

Semi-Supervised Locally Linear Embedding (SSLLE)

Application & Sensitivity Analysis of Critical Hyperparameters



0 AGENDA

- 1 Problem
- 2 Local graph-based manifold learning (LGML)
- 3 Techniques
 - 1 Unsupervised
 - 2 Semi-supervised
 - 3 Challenges
- 4 Sensitivity analysis
 - 1 Setup
 - 2 Results
- 5 Discussion

SSLLE

1 PROBLEM 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

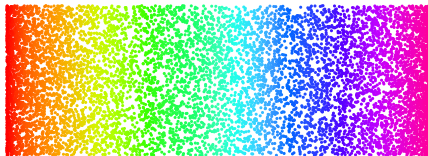


How to find a meaningful, structure-preserving embedding?

1 PROBLEM MANIFOLD LEARNING

Formal goal of manifold learning.

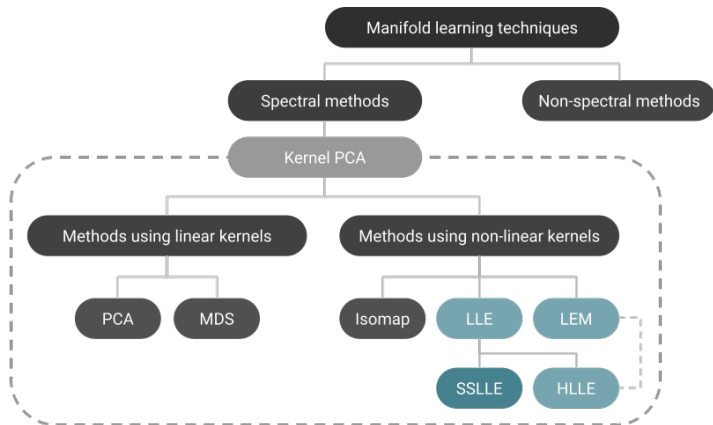
- **Given.** Data $\mathcal{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$, with $\mathbf{x}_i \in \mathbb{R}^D \forall i \in \{1, 2, \dots, N\}$ and $N, D \in \mathbb{N}$, supposedly lying on d -dimensional manifold \mathcal{M}
- ⇒ $\psi : \mathcal{M} \rightarrow \mathbb{R}^d$ with $d \ll D, d \in \mathbb{N}$
- ⇒ $\mathcal{X} \sim \mathcal{M} \subset \mathbb{R}^D$
- **Goal.** Find d -dimensional Euclidean representation
- ⇒ $\mathcal{Y} = (\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_N)$, with $\mathbf{y}_i = \psi(\mathbf{x}_i) \in \mathbb{R}^d \forall i \in \{1, 2, \dots, N\}$.



2 LGML

2 LGML TAXONOMY

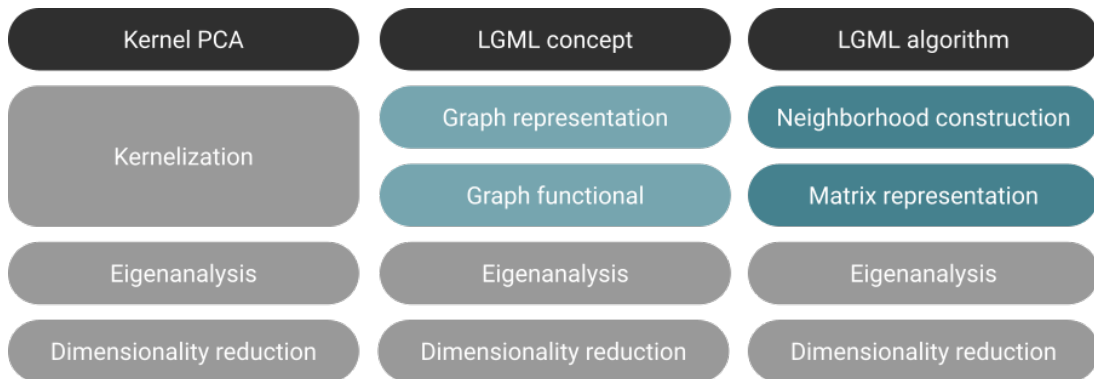
Landscape. Various approaches, many of which may be translated into one another



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

2 LGML CONCEPT

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



2 LGML CONCEPT

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

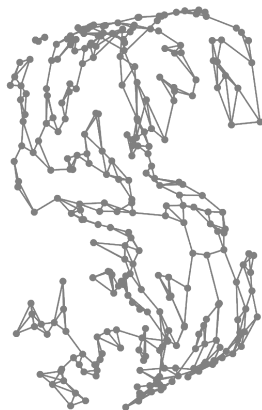
Vertices. Given by observations

Edges. Present between neighboring points

- Typically, k -neighborhoods
- Edge weights determined by nearness

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

- Smoothness **LEM**
- Local linearity **LLE** **SSLLE**
- Curviness **HLLE**
- ...



Achievements: non-linearity & locality

2 LGML CONCEPT

Eigenanalysis. Finding axes of variability in intrinsic manifold structure

- Matrix representation of manifold properties
- Assessment through eigenanalysis
 - Directions of variability \Rightarrow eigenvectors
 - 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

- Notion of smoothness in mapping function
- Second-order penalty on gradient

Graph Laplacian. Discrete approximation of Laplace-Beltrami operator

- Weight matrix. $\mathbf{W} = (w)_{ij} \in \mathbb{R}^{N \times N}$, where $w_{ij} = w_{ij}(\|\mathbf{x}_i - \mathbf{x}_j\|^2)$
- Graph Laplacian. $\mathbf{L} = \mathbf{D} - \mathbf{W} \in \mathbb{R}^{N \times N}$, $\mathbf{D} = \text{diag}(\sum_j w_{ij}) \in \mathbb{R}^{N \times N}$

Generalized eigenvalue problem.

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

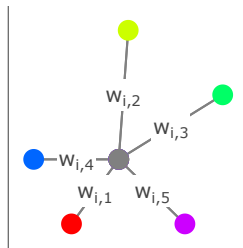
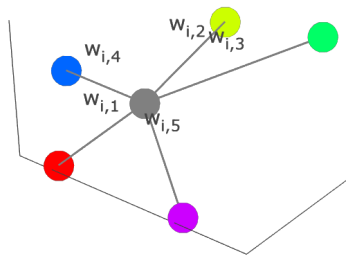
Solution: bottom $d + 1$ eigenvectors

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

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

Embedding loss minimization. Finding optimal embedding coordinates

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

Eigenvalue problem. Define $\mathbf{E} = (\mathbf{I} - \mathbf{W})^T (\mathbf{I} - \mathbf{W})$ and set $\tilde{\mathcal{Y}} = \mathcal{Y}^T$, such that

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

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

- Notion of curviness in mapping function
- Second-order penalty on Hessian
- Strong convergence guarantees but rather complex computations

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

- Continuous functional. $\mathcal{H}(f) = \int_{\mathcal{M}} \|\mathbf{H}_f^{\text{loc}}(\mathbf{p})\|_F^2 d\mathbf{p}$
- Hessian estimators \mathbf{H}_ℓ derived from locally linear neighborhood patches
- Empirical approximator. $\mathcal{H}_{ij} = \sum_{\ell} \sum_m (\mathbf{H}_\ell)_{m,i} (\mathbf{H}_\ell)_{m,j}$
- Finding null space of \mathcal{H}

Solution: bottom $d + 1$ eigenvectors + scaling

3.2 SEMI-SUPERVISED SSLLE

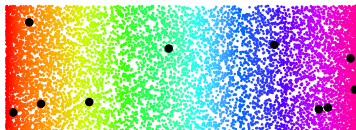
Proposal. Yang et al. (2006)

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 \Rightarrow careful choice of prior points



3.2 SEMI-SUPERVISED SSLLE

Choice of prior points. Basically, three options

- Pre-existing prior information
- Random choice
- Maximum exploration

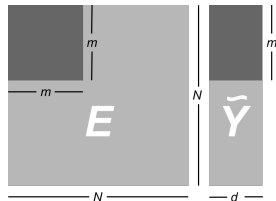
Types of prior information. Exact vs inexact

- Level of confidence encoded in confidence parameter

Algorithmic impact. Recall LLE eigenvalue problem

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

⇒ Partitioning of \mathbf{E} and $\tilde{\mathcal{Y}}$



3.3 CHALLENGES CRITICAL PARAMETERS

Intrinsic dimensionality. True sources of variability

→ Considered known with availability of prior information

Neighborhood size. Global vs local structure

→ Tunable (expensive)

Regularization constant. Singularity for $D < k$

→ Heuristics

Number & location of prior points. Utility of prior knowledge

ANALYSIS

→ Exploration vs labeling cost

Noise level. Quality of prior knowledge

ANALYSIS

→ How exact must prior information be?

Confidence parameter. Belief in prior knowledge

→ Rather robust

4 SENSITIVITY ANALYSIS

4.1 SETUP SCENARIOS

woteva

4.1 SETUP EVALUATION

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4.2 RESULTS **FOO**

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5 DISCUSSION

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.
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