Semi-Supervised Locally Linear Embedding (SSLLE)

Application & Sensitivity Analysis of Critical Parameters

0 AGENDA

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

MANIFOLD LEARNING

Situation: rapidly increasing amount of data thanks to novel applications and data sources

Problem: high data dimensionality detrimental to

1. model functionality
2. interpretability

Manifold assumption: data in high-dimensional observation space truly sampled from low-dimensional manifold

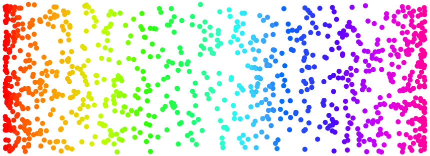
How to find a meaningful, structure-preserving embedding?

1 PROBLEM MANIFOLD LEARNING

Formal goal of manifold learning:

→ **Given:** data $\mathcal{X} = (\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_N)$, 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 $d \ll D, d \in \mathbb{N}$
$\Rightarrow \mathcal{X} \sim \mathcal{M} \subset \mathbb{R}^D$

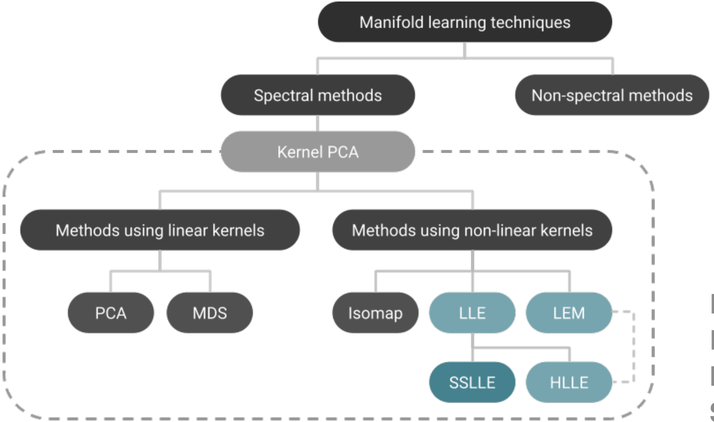
→ **Goal:** find d-dimensional Euclidean representation
$\Rightarrow \mathcal{Y} = (\boldsymbol{y}_1, \boldsymbol{y}_2, ..., \boldsymbol{y}_N)$, with $\boldsymbol{y}_i = \psi(\boldsymbol{x}_i) \in \mathbb{R}^d \; \forall i \in \{1, 2, ..., N\}$.



2 LGML

TAXONOMY

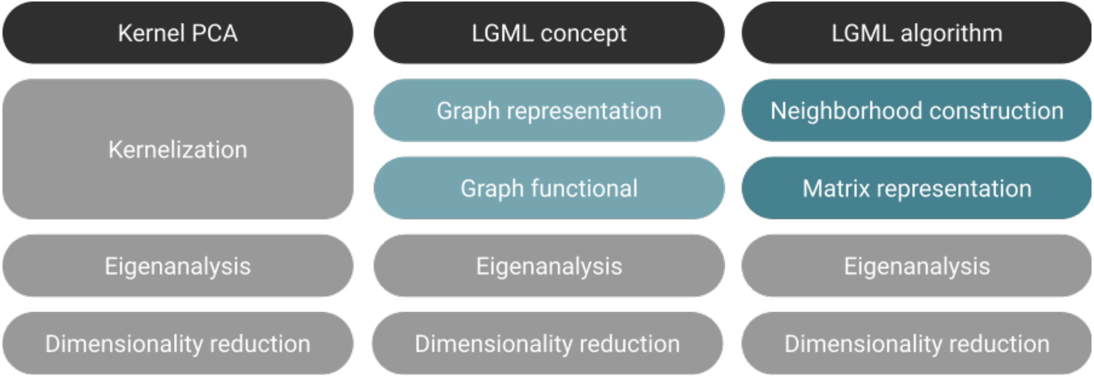
Landscape: various approaches, many of which may be translated into one another



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



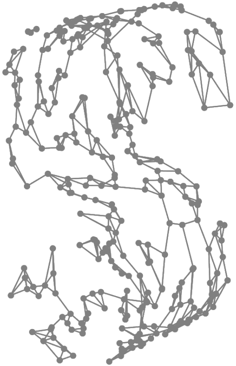
Achievements: non-linearity & locality

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
- $\rightarrow$ Curviness HLLE
- $\rightarrow$ Local linearity LLE SSLLE

3 TECHNIQUES

 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

Solution: eigenanalysis of graph Laplacian $\boldsymbol{L}$

$\rightarrow$ Derived from weight matrix encoding nearness of inputs

$\rightarrow$ Discrete approximation of Laplace-Beltrami operator $\mathcal{L}(f)$

$\rightarrow$ Generalized eigenvalue problem

Solution: bottom $d + 1$ **eigenvectors**

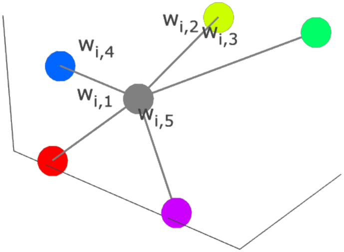
Proposal: Roweis and Saul (2000)

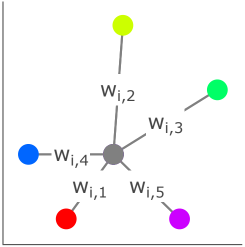
Idea: preserving locally linear reconstructions

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

$\rightarrow$ Reconstruction weights = topological properties

$\rightarrow$ Neighborhood patches invariant to dimensionality reduction





3.1 UNSUPERVISED **LLE**

Reconstruction loss minimization: finding optimal reconstruction weights

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

Embedding loss minimization: finding optimal embedding coordinates

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

Eigenvalue problem: define $\boldsymbol{E} = (\boldsymbol{I} - \boldsymbol{W})^T (\boldsymbol{I} - \boldsymbol{W})$ and set $\tilde{\mathcal{Y}} = \mathcal{Y}^T$, such that

$$\min_{\tilde{\mathcal{Y}}} trace(\tilde{\mathcal{Y}}^T \boldsymbol{E} \tilde{\mathcal{Y}}), \quad \text{s.t. } \frac{1}{N} \tilde{\mathcal{Y}}^T \tilde{\mathcal{Y}} = \boldsymbol{I}, \quad \tilde{\mathcal{Y}}^T \boldsymbol{1} = \boldsymbol{0}. \tag{3}$$

Solution: bottom $d + 1$ eigenvectors

3.1 UNSUPERVISED **HLLE**

Proposal: Donoho and Grimes (2003)

Idea: finding a truly 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

Solution: eigenanalysis of empirical Hessian functional $\mathcal{H}$

$\rightarrow$ Quadratic form of Hessian estimators in linear neighborhood patches

$\rightarrow$ Discrete approximation of continuous Hesssian functional $\mathscr{H}(f)$

$\rightarrow$ Null space problem

Solution: bottom $d + 1$ eigenvectors + scaling

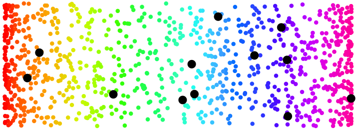
Proposal: Yang et al. (2006)

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

- $\rightarrow$ More active than semi-supervised learning?
- $\rightarrow$ Information available or to be obtained by querying the oracle
- $\rightarrow$ Maximum information at little expense $\Rightarrow$ careful choice of prior points



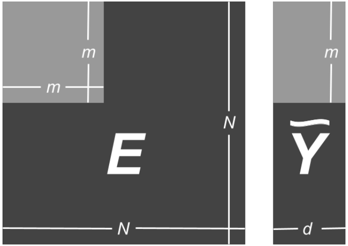
Types of prior information: exact vs inexact

$\rightarrow$ Level of confidence encoded in parameter β

Algorithmic impact: recall LLE eigenvalue problem

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

$\Rightarrow$ partitioning of $\boldsymbol{E}$ and $\tilde{\mathcal{Y}}$



Modified optimization problem: exact information

$$\min_{\tilde{\mathcal{Y}}_2} \begin{bmatrix} \tilde{\mathcal{Y}}_1 & \tilde{\mathcal{Y}}_2 \end{bmatrix} \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \tilde{\mathcal{Y}}_1^T \\ \tilde{\mathcal{Y}}_2^T \end{bmatrix} \tag{4}$$

$$\Leftrightarrow \tilde{\mathcal{Y}}_2^T = M_{22}^{-1} M_{12} \tilde{\mathcal{Y}}_1^T \tag{5}$$

Modified optimization problem: inexact information

$$\min_{\tilde{\mathcal{Y}}_1, \tilde{\mathcal{Y}}_2} \begin{bmatrix} \tilde{\mathcal{Y}}_1 & \tilde{\mathcal{Y}}_2 \end{bmatrix} \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \tilde{\mathcal{Y}}_1^T \\ \tilde{\mathcal{Y}}_2^T \end{bmatrix} + \beta \left\| \tilde{\mathcal{Y}}_1^T - \hat{\tilde{\mathcal{Y}}}_1^T \right\|_F^2 \tag{6}$$

$$\Leftrightarrow \begin{bmatrix} M_{11} + \beta \boldsymbol{I} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \tilde{\mathcal{Y}}_1^T \\ \tilde{\mathcal{Y}}_2^T \end{bmatrix} = \begin{bmatrix} \hat{\tilde{\mathcal{Y}}}_1^T \\ \mathbf{0} \end{bmatrix} \tag{7}$$

CRITICAL PARAMETERS

Choice of landmark points: basically, three options

1. Pre-existing prior information $\Rightarrow$ worst case: poor coverage
2. (Uniform) random sampling
3. Maximum coverage $\Rightarrow$ minimization of condition number $\kappa(M_{22})$

3.3 CHALLENGES CRITICAL PARAMETERS

Number & location of prior points: utility of prior knowledge ANALYSIS

$\rightarrow$ Exploration vs labeling cost

Noise level: quality of prior knowledge ANALYSIS

$\rightarrow$ Support vs harm through prior knowledge

Confidence parameter: strength of belief in prior knowledge

$\rightarrow$ Rather robust

Further hyperparameters: also critical in unsupervised case

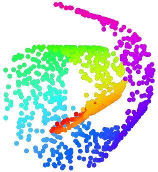
1. Intrinsic dimensionality
2. Neighborhood size
3. Regularization constant

4 SENSITIVITY ANALYSIS

DATA

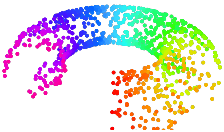
Data: two data sets, $N = 1000$ observations each

Swiss roll: *the* standard synthetic manifold



1. Sample $\boldsymbol{u}_1, \boldsymbol{u}_2 \sim U(0, 1)$ *iid* with $|\boldsymbol{u}_1| = |\boldsymbol{u}_1| = N$
2. Compute $\boldsymbol{t} = 1.5\pi(1 + 2\boldsymbol{u}_1)$ and $\boldsymbol{s} = 21\boldsymbol{u}_2$
3. $\mathcal{X}_{\text{swiss}} = \begin{bmatrix} \boldsymbol{x}_1 & \boldsymbol{x}_2 & \boldsymbol{x}_3 \end{bmatrix} = \begin{bmatrix} \boldsymbol{t}\cos\boldsymbol{t} & \boldsymbol{s} & \boldsymbol{t}\sin\boldsymbol{t} \end{bmatrix}$

Incomplete tire: examined in Yang et al. (2006)



1. Sample $\boldsymbol{u}_1, \boldsymbol{u}_2 \sim U(0, 1)$ *iid* with $|\boldsymbol{u}_1| = |\boldsymbol{u}_1| = N$
2. Compute $\boldsymbol{t} = \frac{5\pi}{3}\boldsymbol{u}_1$ and $\boldsymbol{s} = \frac{5\pi}{3}\boldsymbol{u}_2$
3. $\mathcal{X}_{\text{tire}} = \begin{bmatrix} \boldsymbol{x}_1 & \boldsymbol{x}_2 & \boldsymbol{x}_3 \end{bmatrix}$
   $= \begin{bmatrix} (3 + \cos\boldsymbol{s})\cos\boldsymbol{t} & (3 + \cos\boldsymbol{s})\sin\boldsymbol{t} & \sin\boldsymbol{s} \end{bmatrix}$

4.1 SETUP **SCENARIOS**

Sensitivity analysis I: landmark coverage $\times$ number of landmark points

$\rightarrow$ Landmark coverage $\in \{$poor, random, maximum$\}$

$\rightarrow$ Number of landmark points $\in \{2, 4, 6, 8, 10, 12\}$

Sensitivity analysis II: noise level $\times$ number of landmark points

$\rightarrow$ Landmark coverage kept at optimal configuration

$\rightarrow$ Simulation of inexact prior information through additive Gaussian noise

$\rightarrow$ Corruption of landmark $\boldsymbol{p}$ as $\tilde{\boldsymbol{p}} = \boldsymbol{p} + \boldsymbol{\epsilon} = (p_t, p_s) + (\epsilon_t, \epsilon_s)$
with $\epsilon_i \sim N(0, (\alpha \cdot s_i)^2)$ *iid*, scaled by empirical variance s_i, $i \in \{t, s\}$

$\rightarrow$ Noise level $\alpha \in \{0.1, 0.5, 1.0, 3.0\}$

$\rightarrow$ Number of landmark points $\in \{2, 4, 6, 8, 10, 12\}$

4.1 SETUP **EVALUATION**

Evaluation criterion: AUC(R_{NX}) (Kraemer et al. (2019), Lueks et al. (2011))

$\rightarrow$ Area under the R_{NX} curve

$\rightarrow$ Based on co-ranking matrix

Co-ranking matrix: comparing distance ranks in observation & embedding spaces

$\rightarrow$ Rank distance matrices $(r)_{ij}^{\text{obs}}, (r)_{ij}^{\text{emb}} \in \mathbb{R}^{N \times N}$

$\rightarrow$ Co-ranking matrix $\boldsymbol{Q} = (q)_{\ell m} \in \mathbb{R}^{N \times N}$ with $q_{\ell m} = \left| \{(i,j) : r_{ij}^{\text{emb}} = \ell \wedge r_{ij}^{\text{obs}} = m\} \right|$

$\rightarrow$ Interpretation:

1. All non-zero entries on diagonal $\Rightarrow$ optimal embedding
2. Most non-zero entries on upper triangle $\Rightarrow$ close points torn apart
3. Most non-zero entries on lower triangle $\Rightarrow$ faraway points collapsed

EVALUATION

Co-ranking-based metrics:

→ Number of points remaining in k-neighborhood after projection:

$$Q_{NX}(k) = \frac{1}{kN} \sum_{\ell=1}^{k} \sum_{m=1}^{k} q_{\ell m}$$

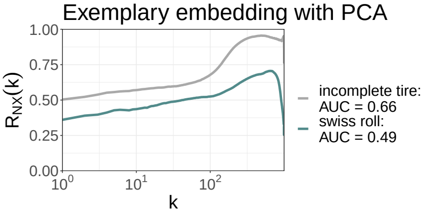
→ $R_{NX}(k) = \dfrac{(N-1)Q_{NX}(k) - k}{N - 1 - k}$

AUC measure:

→ $\text{AUC}(R_{NX}) = \dfrac{\sum_{k=1}^{N-2} R_{NX}(k)}{\sum_{k=1}^{N-2} 1/k} \in [0, 1]$

→ Interpretation:

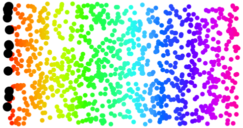
1. $\text{AUC}(R_{NX}) = 0 \Rightarrow$ random embedding
2. $\text{AUC}(R_{NX}) = 1 \Rightarrow$ optimal embedding

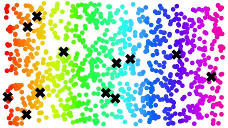


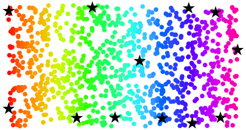
SENSITIVITY ANALYSIS I

Key variation: poor, random, maximum coverage

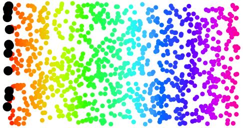
Swiss roll

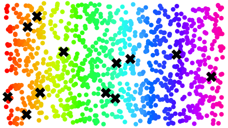


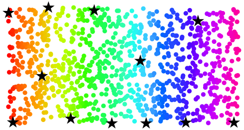




Incomplete tire



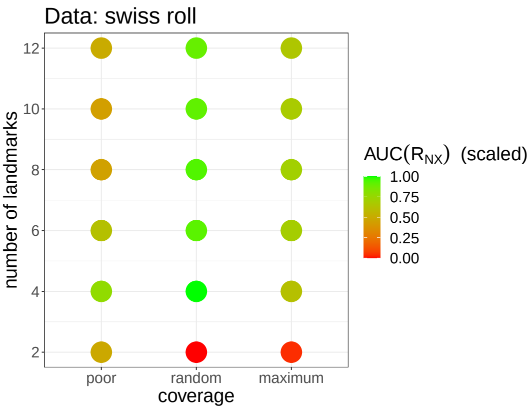


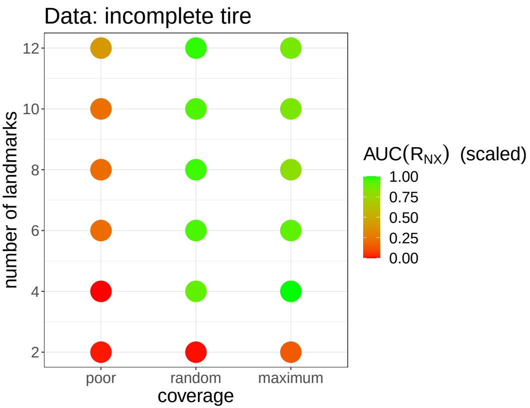


● poor coverage × random coverage ⋆ maximum coverage

SENSITIVITY ANALYSIS I

Quantitative results: seemingly better performance of random coverage

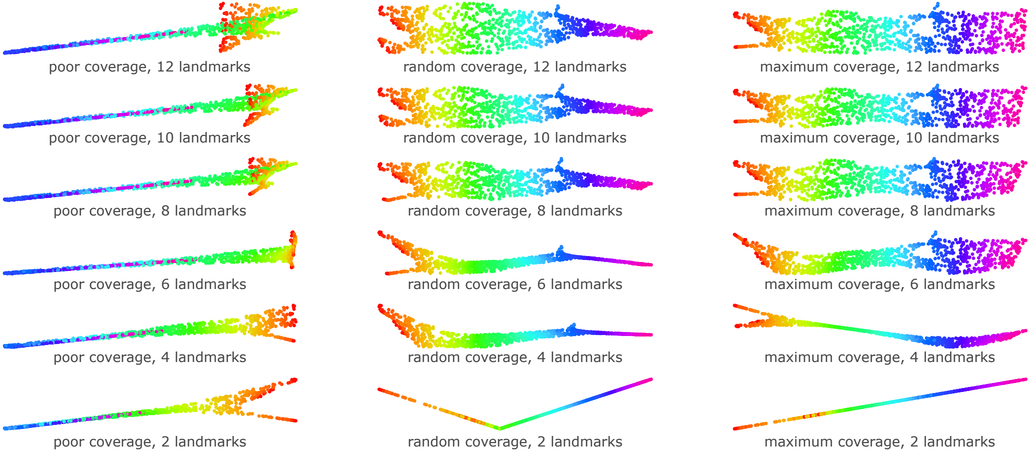




AUC(R_{NX}) has been scaled to take on a minimum of 0 and maximum of 1 in both figures for better visibility of differences.
Original scales: swiss roll – AUC$(R_{NX}) \in [0.2655, 0.4086]$, incomplete tire – AUC$(R_{NX}) \in [0.2772, 0.6231]$

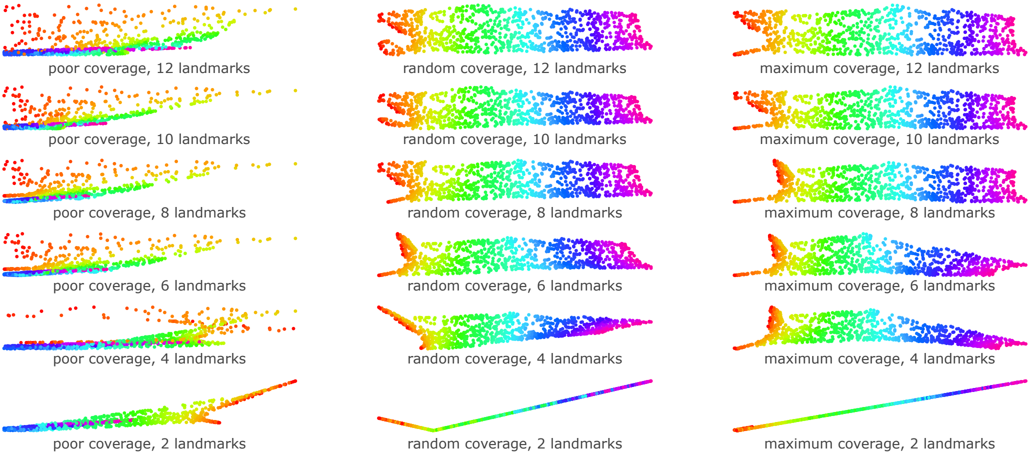
4.2 RESULTS SENSITIVITY ANALYSIS I

Qualitative results: swiss roll



4.2 RESULTS SENSITIVITY ANALYSIS I

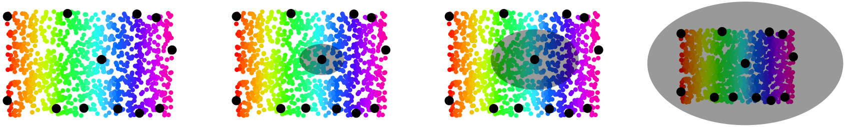
Qualitative results: incomplete tire



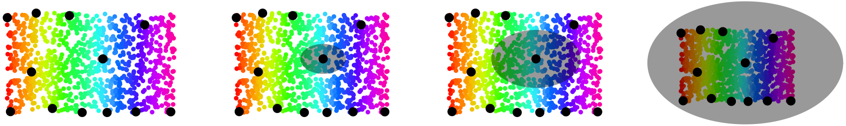
SENSITIVITY ANALYSIS II

Key variation: noise level $\alpha \in \{0.1, 0.5, 1.0, 3.0\}$

Swiss roll



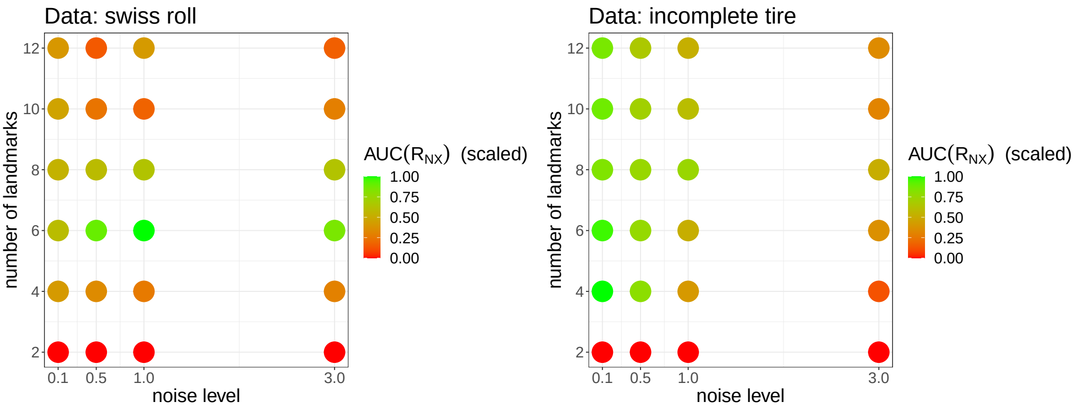
Incomplete tire



Potential displacement by random noise, exemplified at one prior point location.
Ellipses have semi-axes of length = one standard deviation of the Gaussian noise variable, i.e., noise level scaled by standard deviation s_i in t and s direction, respectively: $\alpha \cdot s_i$ with $i \in \{t, s\}$.
Landmarks have been found via maximum coverage.

SENSITIVITY ANALYSIS II

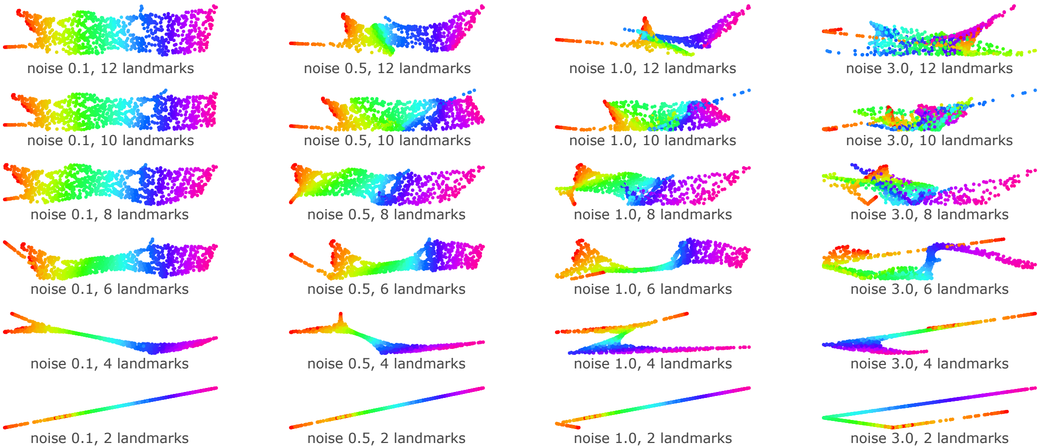
Quantitative results: some compensation of noise by larger number of landmarks



$\mathrm{AUC}(R_{NX})$ has been scaled to take on a minimum of 0 and maximum of 1 in both figures for better visibility of differences.
Original scales: swiss roll – $\mathrm{AUC}(R_{NX}) \in [0.2720, 0.4167]$, incomplete tire – $\mathrm{AUC}(R_{NX}) \in [0.3171, 0.6172]$

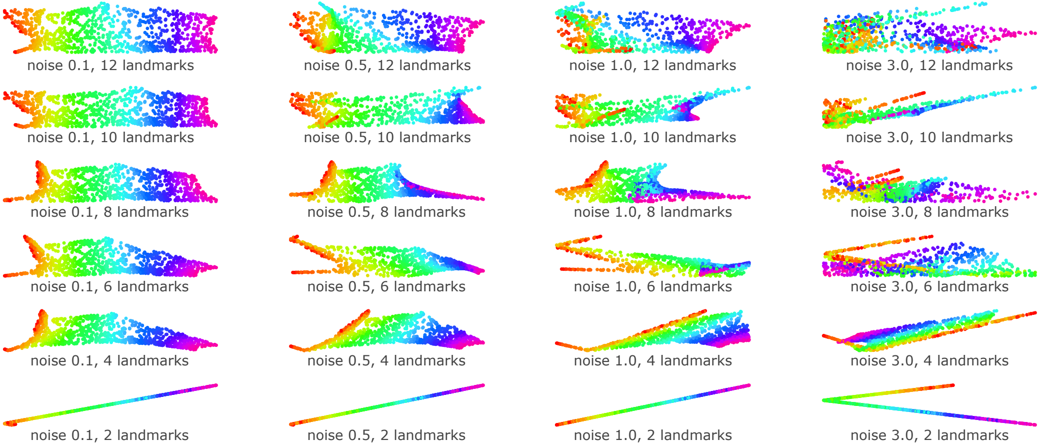
SENSITIVITY ANALYSIS II

Qualitative results: swiss roll



SENSITIVITY ANALYSIS II

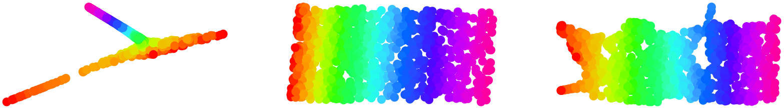
Qualitative results: incomplete tire



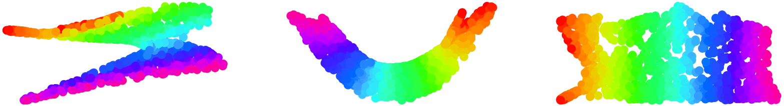
CONCLUDING COMPARISON

Comparison: LLE vs HLLE vs SSLLE

Swiss roll



Incomplete tire



SSLLE: own implementation (see Github), LLE & HLLE: implementation in R's `dimRed` package (Kraemer, 2019).
SSLLE with maximum coverage, 12 landmarks and exact prior information, LLE and HLLE with number of neighbors as deemed optimal by SSLLE implementation (no other hyperparameters to set).

5 DISCUSSION

5 DISCUSSION

	Strengths	Drawbacks
General	Reasonably simple Few parameters Tractable computations	Vital dependency on graph approximation No indication of intrinsic dimensionality Fundamental weakness in optimization problem Possibly very tight eigenvalue spectrum Meaningfulness of embedding not guaranteed Weak preservation of geometric properties
Semi-supervised extension	Simple but impactful improvement Better handling of more complex manifolds Small number of landmarks sufficient	Potentially high labeling cost Label noise problematic Prior point location crucial

SSLLE: imperfect but potentially powerful approach to LGML

MAIN 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.

Bengio, Y., Delalleau, O., Roux, N. L., Paiement, J.-F., Vincent, P. and Ouimet, M. (2004). Learning eigenfunction links spectral embedding and kernel pca, *Neural Computation* **16**: 2197–2219.

Cayton, L. (2005). Algorithms for manifold learning, *Technical Report CS2008-0923*, University of California, San Diego (UCSD).

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.

Ghojogh, B., Ghodsi, A., Karray, F. and Crowley, M. (2020). Locally linear embedding and its variants: Tutorial and survey.

Kraemer, G. (2019). *dimRed: A Framework for Dimensionality Reduction*. R package version 0.2.3.
URL: *https://CRAN.R-project.org/package=dimRed*

Kraemer, G., Reichstein, M. and Mahecha, M. D. (2019). dimred and coranking -— unifying dimensionality reduction in r, *Technical report*.

Lueks, W., Mokbel, B., Biehl, M. and Hammer, B. (2011). How to evaluate dimensionality reduction? improving the co-ranking matrix, *arXiv: Machine Learning* .

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

Saul, L. K., Weinberger, K. Q., Sha, F., Ham, J. and Lee, D. D. (2006). Spectral methods for dimensionality reduction, *in* O. Chapelle, B. Scholkopf and A. Zien (eds), *Semi-Supervised Learning*, MIT Press Scholarship Online, chapter 1.

van der Maaten, L., Postma, E. and van den Herik, J. (2009). Dimensionality reduction: A comparative review, *Technical Report TiCC TR 2009-005*, Tilburg University.

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