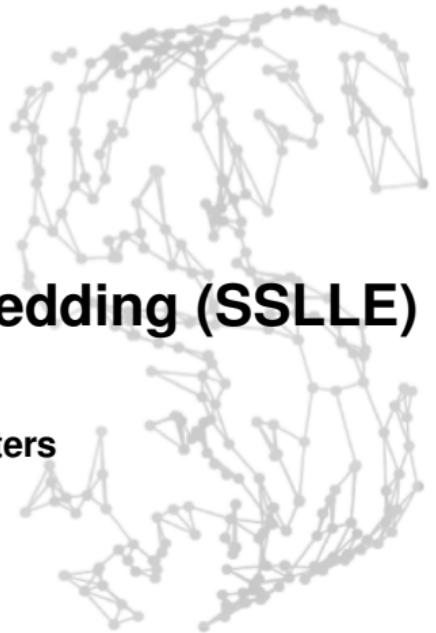


Semi-Supervised Locally Linear Embedding (SSLLE)

Application & Sensitivity Analysis of Critical Hyperparameters



0 AGENDA

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

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

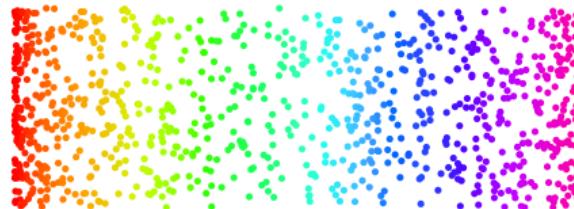


How to find a meaningful, structure-preserving embedding?

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}
 - $\Rightarrow \psi : \mathcal{M} \rightarrow \mathbb{R}^d$ with $d \ll D, d \in \mathbb{N}$
 - $\Rightarrow \mathcal{X} \sim \mathcal{M} \subset \mathbb{R}^D$
- **Goal.** Find d -dimensional Euclidean representation
 - $\Rightarrow \mathcal{Y} = (\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_N)$, 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
HLLE Hessian LLE
SSLLE Semi-supervised LLE

2 LGML CONCEPT

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

Kernel PCA

LGML concept

LGML algorithm

Kernelization

Graph representation

Neighborhood construction

Graph functional

Matrix representation

Eigenanalysis

Eigenanalysis

Eigenanalysis

Dimensionality reduction

Dimensionality reduction

Dimensionality reduction

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 ⇒ eigenvectors
 - Respective degrees of variability ⇒ 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

Solution. Eigenanalysis of graph Laplacian L

- Derived from weight matrix encoding nearness of inputs
- Discrete approximation of Laplace-Beltrami operator $\mathcal{L}(f)$
- Generalized eigenvalue problem

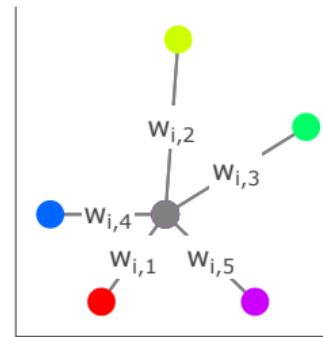
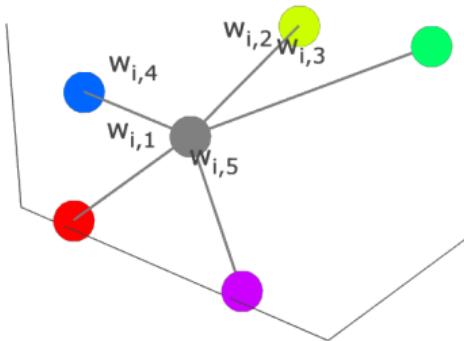
Solution: bottom $d + 1$ eigenvectors

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

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

Embedding loss minimization. Finding optimal embedding coordinates

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

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

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

Solution: bottom $d + 1$ eigenvectors

3.1 UNSUPERVISED HLLE

Proposal. Donoho and Grimes (2003)

Idea. Finding a truly linear mapping while preserving local isometry

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

Solution. Eigenanalysis of empirical Hessian functional \mathcal{H}

- Derived as a quadratic form of Hessian estimators in linear neighborhood patches
- Discrete approximation of continuous Hesssian functional $\mathcal{H}(f)$
- Null space problem

Solution: bottom $d + 1$ eigenvectors + scaling

3.2 SEMI-SUPERVISED SSLLE

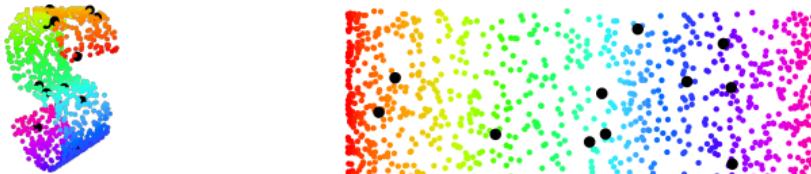
Proposal. Yang et al. (2006)

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

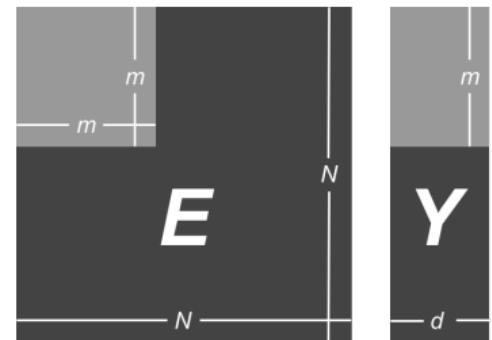
Types of prior information. Exact vs inexact

→ Level of confidence encoded in parameter β

Algorithmic impact. Recall LLE eigenvalue problem

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

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



3.2 SEMI-SUPERVISED SSLLE

Modified optimization problem. Exact information

$$\min_{\mathcal{Y}_2} [\mathcal{Y}_1 \quad \mathcal{Y}_2] \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \mathcal{Y}_1^T \\ \mathcal{Y}_2^T \end{bmatrix} \quad (4)$$

$$\Leftrightarrow \mathcal{Y}_2^T = M_{22}^{-1} M_{12} \mathcal{Y}_1^T \quad (5)$$

Modified optimization problem. Inexact information

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

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

3.3 CHALLENGES CRITICAL PARAMETERS

Choice of landmark points. Basically, three options

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



3.3 CHALLENGES CRITICAL PARAMETERS

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. Strength of belief in prior knowledge

- Rather robust

Further hyperparameters. Also critical in unsupervised case

- Intrinsic dimensionality
- Neighborhood size
- Regularization constant

4 SENSITIVITY ANALYSIS

4.1 SETUP DATA

Data. Two data sets, $N = 1000$ observations each

Swiss roll. The standard synthetic manifold

- 1 Sample $\mathbf{u}_1, \mathbf{u}_2 \sim U(0, 1)$ iid with $|\mathbf{u}_1| = |\mathbf{u}_2| = N$
- 2 Compute $\mathbf{t} = 1.5\pi(1 + 2\mathbf{u}_1)$ and $\mathbf{s} = 21\mathbf{u}_2$
- 3 $\mathcal{X}_{\text{swiss}} = [\mathbf{x}_1 \quad \mathbf{x}_2 \quad \mathbf{x}_3] = [\mathbf{t} \cos \mathbf{t} \quad \mathbf{s} \quad \mathbf{t} \sin \mathbf{t}]$



Incomplete tire. Examined in Yang et al. (2006)

- 1 Sample $\mathbf{u}_1, \mathbf{u}_2 \sim U(0, 1)$ iid with $|\mathbf{u}_1| = |\mathbf{u}_2| = N$
- 2 Compute $\mathbf{t} = \frac{5\pi}{3}\mathbf{u}_1$ and $\mathbf{s} = \frac{5\pi}{3}\mathbf{u}_2$
- 3 $\mathcal{X}_{\text{tire}} = [\mathbf{x}_1 \quad \mathbf{x}_2 \quad \mathbf{x}_3]$
 $= [(3 + \cos \mathbf{s}) \cos \mathbf{t} \quad (3 + \cos \mathbf{s}) \sin \mathbf{t} \quad \sin \mathbf{s}]$



4.1 SETUP SCENARIOS

Sensitivity analysis I. Landmark coverage \times number of landmark points

- Landmark coverage $\in \{\text{poor, random, maximum}\}$
- Number of landmark points $\in \{2, 4, 6, 8, 10, 12\}$

Sensitivity analysis II. Noise level \times number of landmark points

- Landmark coverage kept at optimal configuration
- Simulation of inexact prior information through additive Gaussian noise
- Corruption of landmark \mathbf{p} as $\tilde{\mathbf{p}} = \mathbf{p} + \boldsymbol{\epsilon} = (p_t, p_s) + (\epsilon_t, \epsilon_s)$
with $\epsilon_i \sim N(0, (\alpha \cdot s_i)^2)$ scaled by empirical variance s_i , $i \in \{t, s\}$
- Noise level $\alpha \in \{0.1, 0.5, 1.0, 3.0\}$
- Number of landmark points $\in \{2, 4, 6, 8, 10, 12\}$

4.1 SETUP EVALUATION

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

- Area under the R_{NX} curve
- Based on co-ranking matrix

Co-ranking matrix. Comparing distance ranks in observation & embedding spaces

- Rank distance matrices. $(r)_{ij}^{\text{obs}}$ and $(r)_{ij}^{\text{emb}}$
- Co-ranking matrix. $\mathbf{Q} = (q)_{\ell m}$ with $q_{\ell m} = |\{(i, j) : r_{ij}^{\text{emb}} = \ell \wedge r_{ij}^{\text{obs}} = m\}|$
- 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

4.1 SETUP EVALUATION

Co-ranking-based metrics. Comparing distance ranks in observation & embedding spaces

- Number of points remaining in k -neighborhood after projection.

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

$$\rightarrow R_{NX}(k) = \frac{(N-1)Q_{NX}(k) - k}{N-1-k}$$

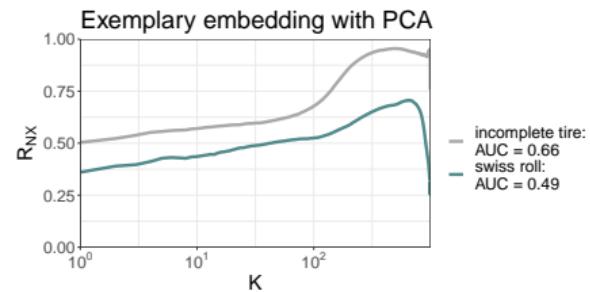
AUC measure.

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

- Interpretation.

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

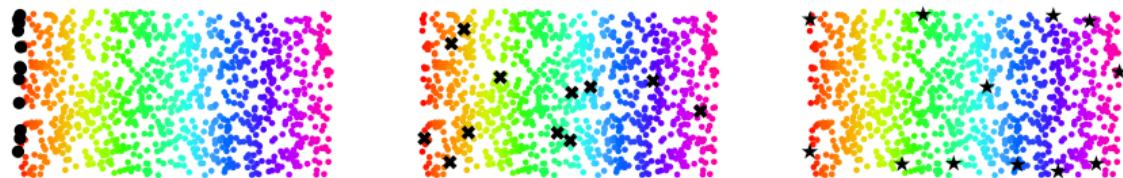
2 $\text{AUC}(R_{NX}) = 1 \Rightarrow$ optimal embedding



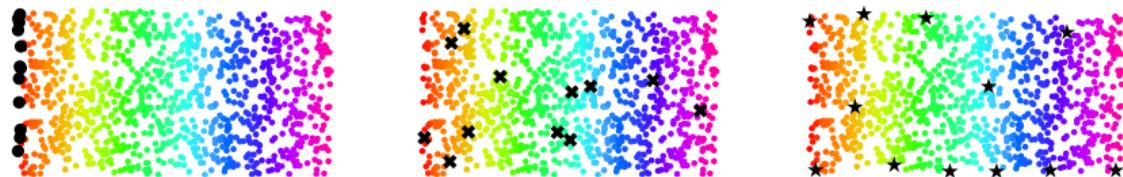
4.2 RESULTS SENSITIVITY ANALYSIS I

Key variation. Poor, random, maximum coverage

Swiss roll



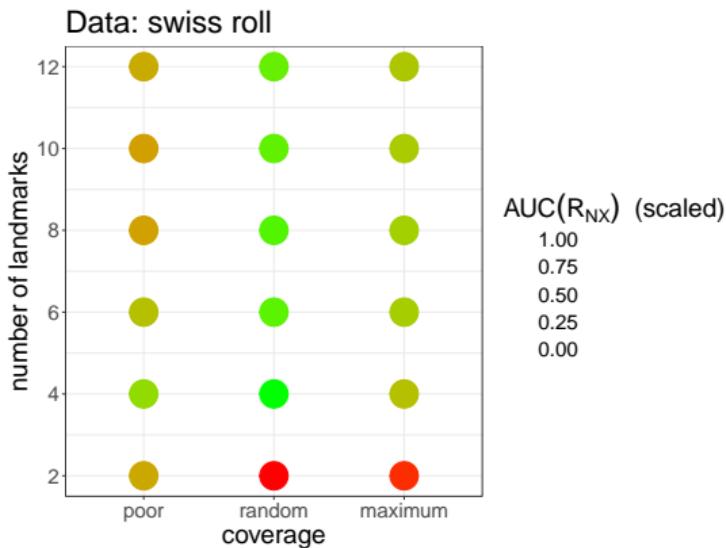
Incomplete tire



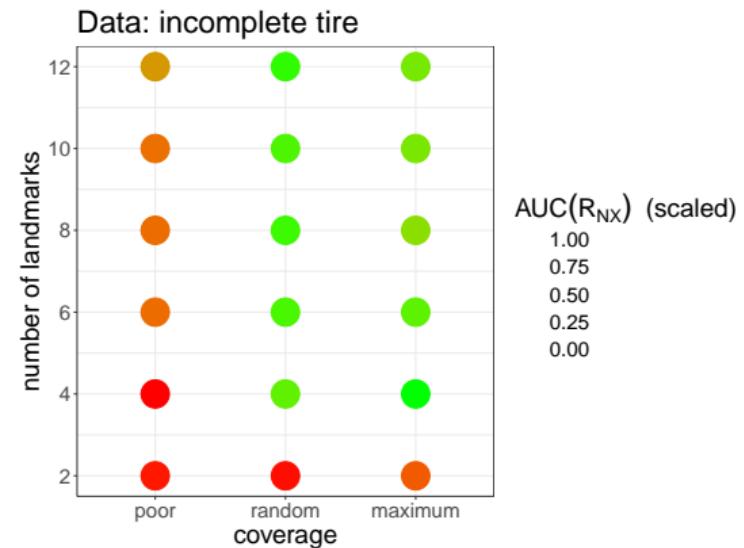
- poor coverage × random coverage ★ maximum coverage

4.2 RESULTS SENSITIVITY ANALYSIS I

Quantitative results. Seemingly better performance of random coverage

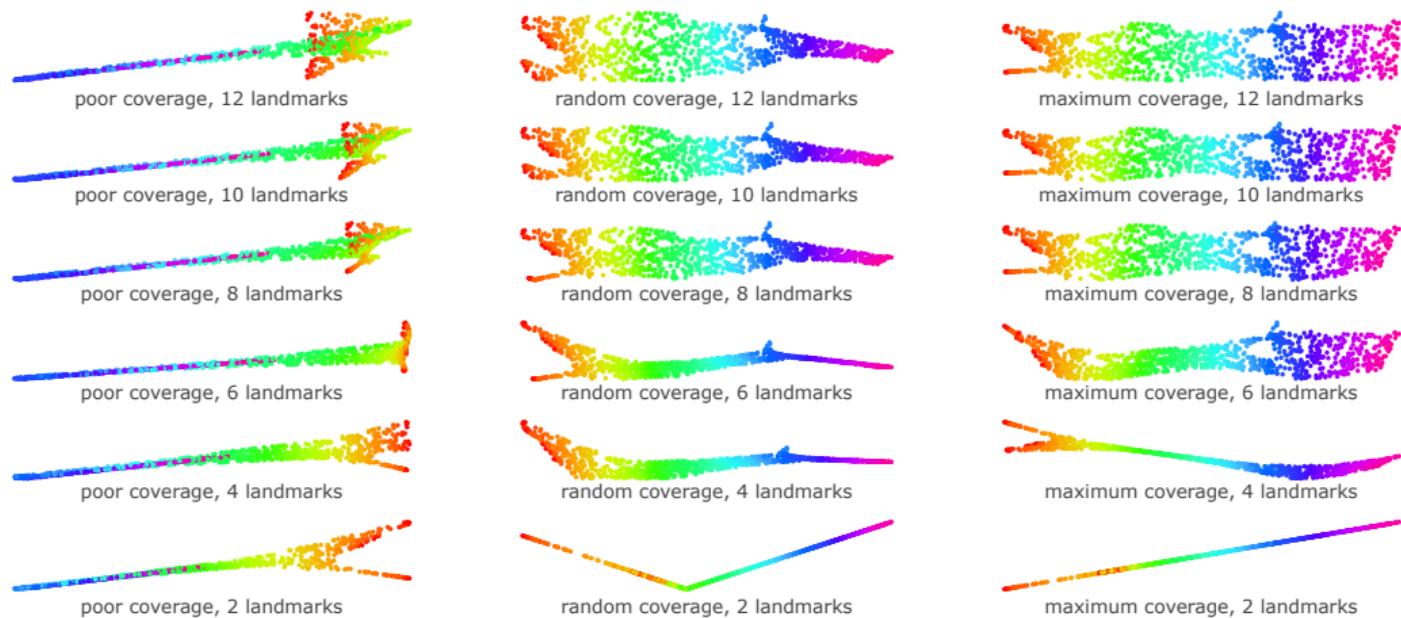


AUC(R_{NX}) has been scaled to take on a minimum of 0 and maximum of 1 in both figures for better visibility of differences.
Original scales. Swiss roll: AUC(R_{NX}) $\in [0.2655, 0.4086]$, incomplete tire: AUC(R_{NX}) $\in [0.2772, 0.6231]$



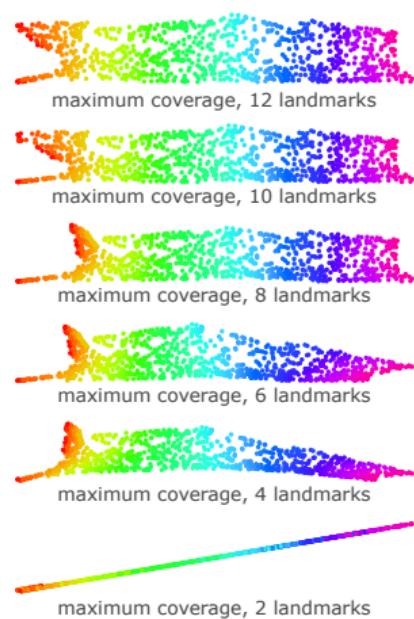
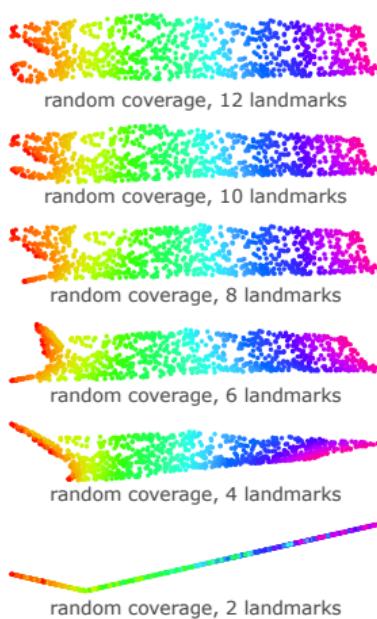
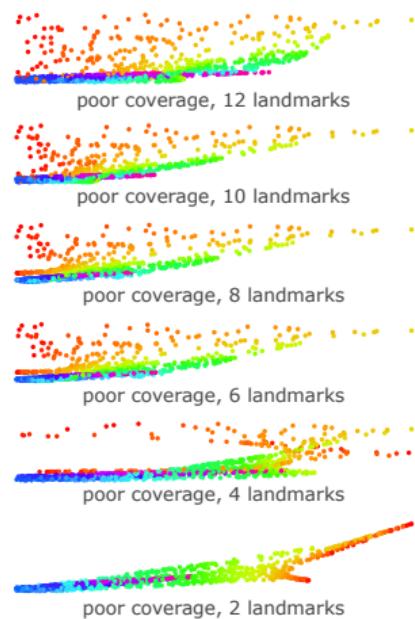
4.2 RESULTS SENSITIVITY ANALYSIS I

Qualitative results. Swiss roll



4.2 RESULTS SENSITIVITY ANALYSIS I

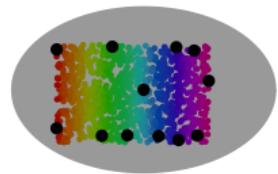
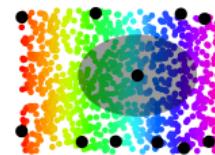
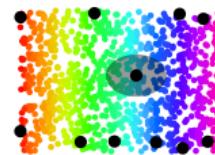
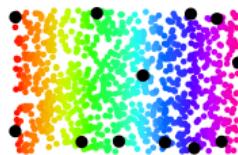
Qualitative results. Incomplete tire



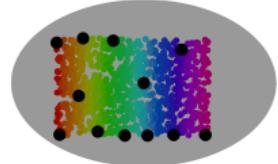
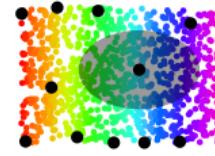
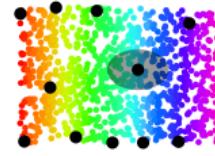
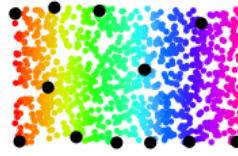
4.2 RESULTS SENSITIVITY ANALYSIS II

Key variation. Noise level $\alpha \in \{0.1, 0.5, 1.0, 3.0\}$

Swiss roll



Incomplete tire

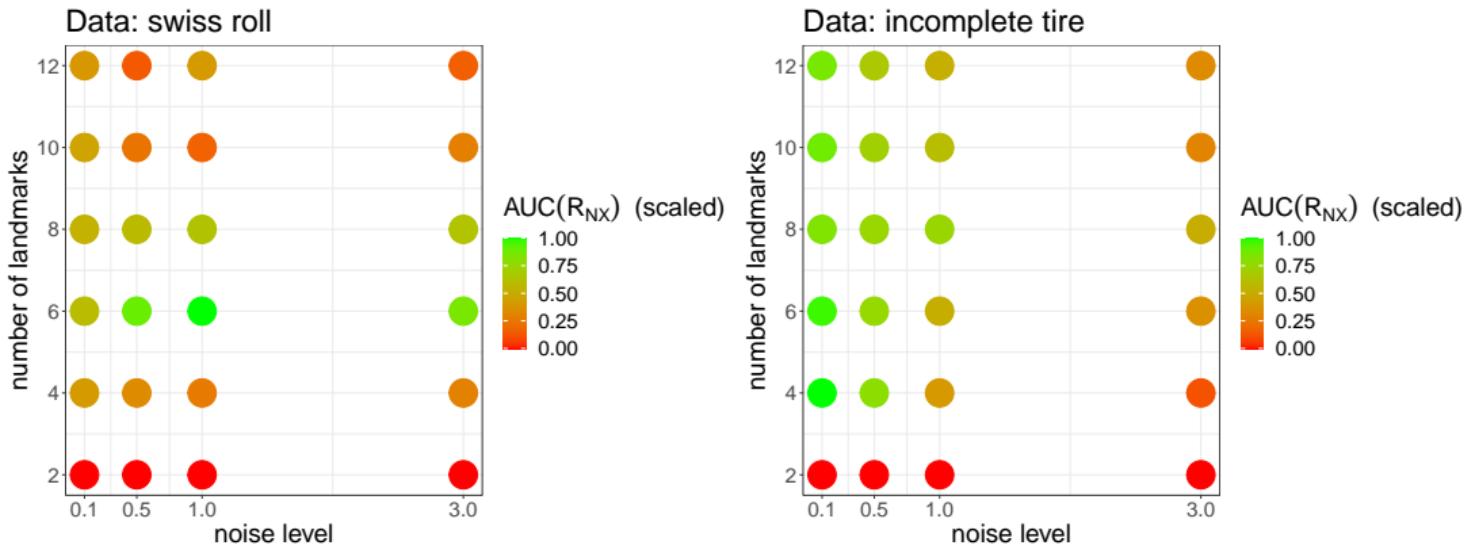


Expected displacement by random noise, exemplified at one prior point location.

Ellipses have semi-axes of length $\alpha \cdot s_i$, i.e., noise level scaled by standard deviation s_i in t and s direction, respectively, so $i \in \{t, s\}$.

4.2 RESULTS SENSITIVITY ANALYSIS II

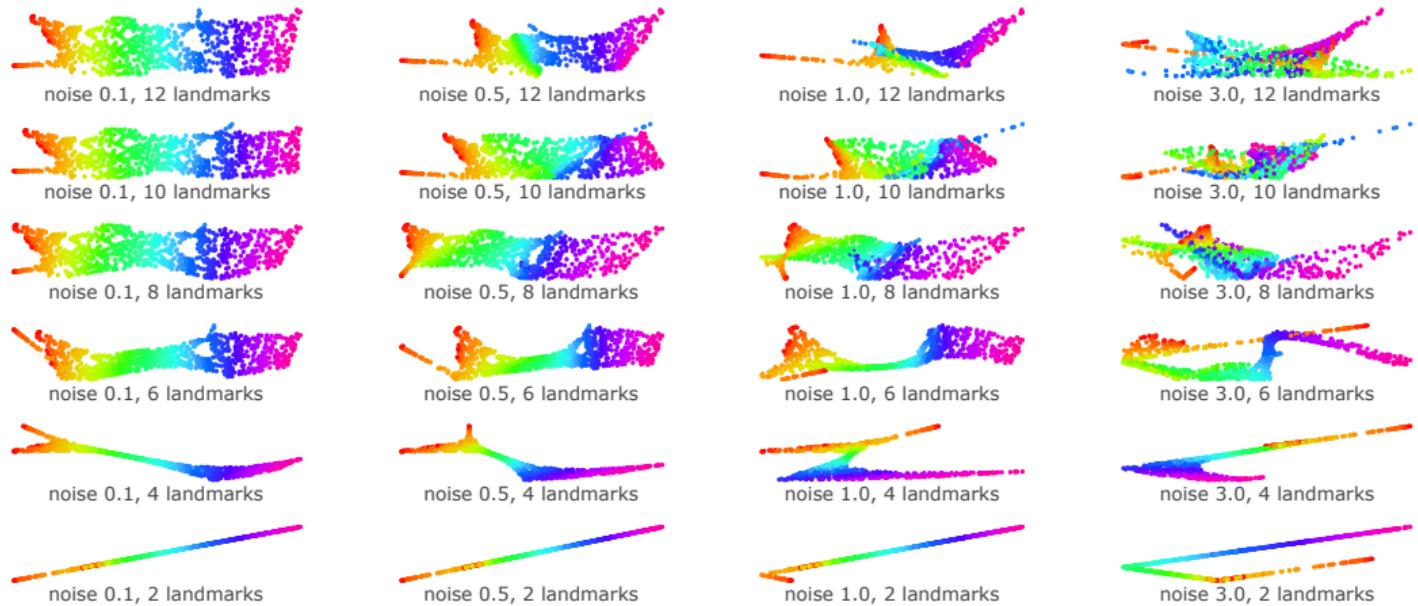
Quantitative results. Some compensation of noise by larger number of landmarks



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}) $\in [0.2720, 0.4167]$, incomplete tire: AUC(R_{NX}) $\in [0.3171, 0.6172]$

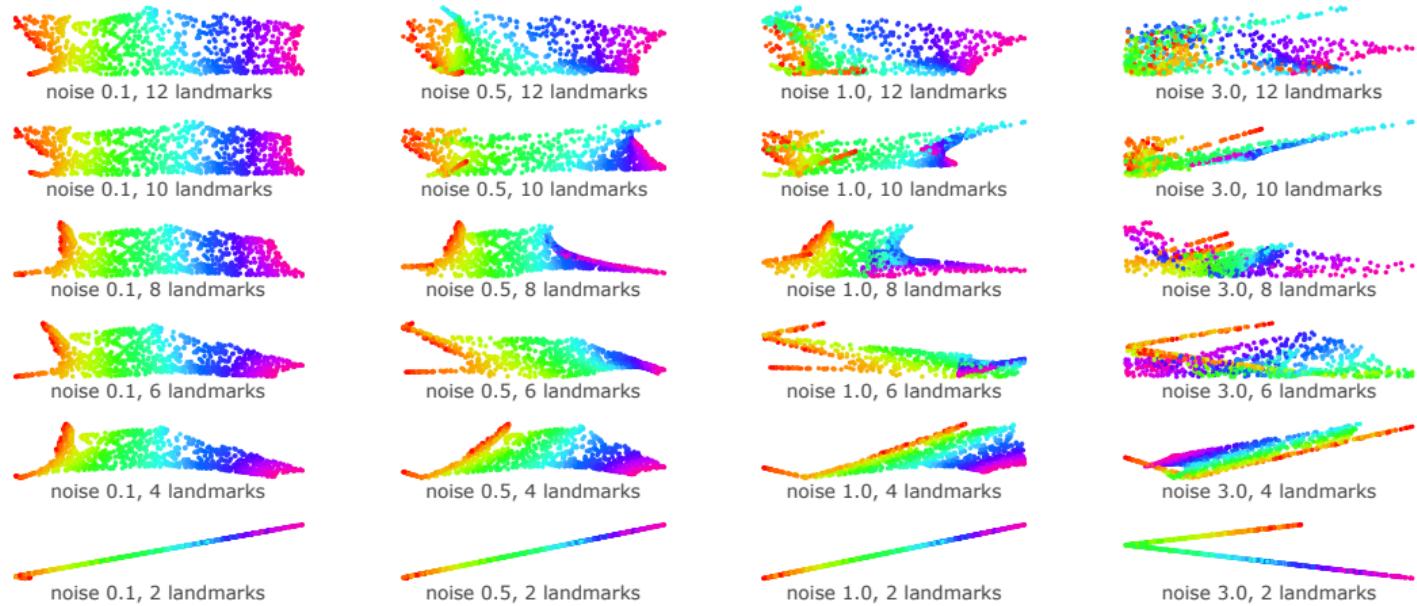
4.2 RESULTS SENSITIVITY ANALYSIS II

Qualitative results. Swiss roll



4.2 RESULTS SENSITIVITY ANALYSIS II

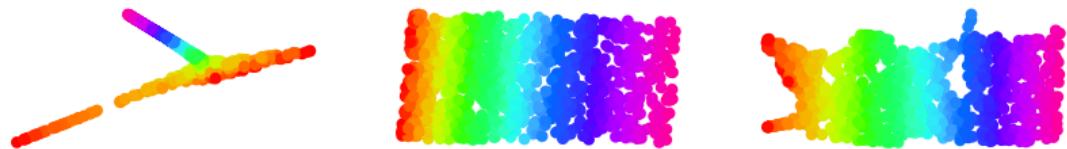
Qualitative results. Incomplete tire



4.2 RESULTS CONCLUDING COMPARISON

Comparison. LLE vs HLLE vs SSLLE

Swiss roll



Incomplete tire



SSLLE with maximum coverage, 12 landmarks and exact prior information.

LLE and HLLE computed using implementation in R's `dimRed` package (Kraemer, 2019); 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 very powerful approach to LGML

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