Non-Isometric Manifold Learning

Analysis and an Algorithm

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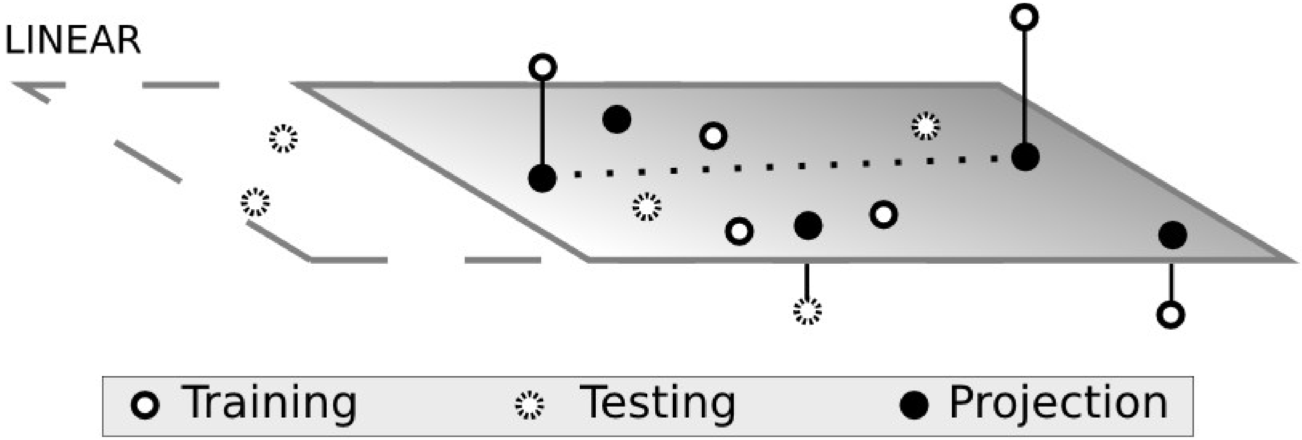
I. Motivation

1. Extend manifold learning to applications other than embedding

2. Establish notion of test error and generalization for manifold learning

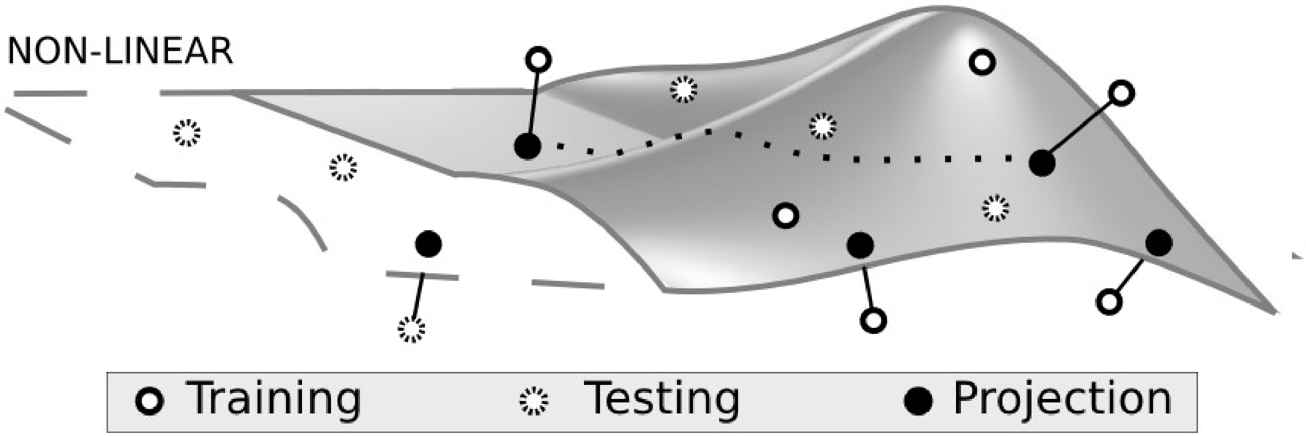
Linear Manifolds (subspaces)



Typical operations:

- project onto subspace
- distance to subspace
- distance between points
- generalize to unseen regions

Non-Linear Manifolds

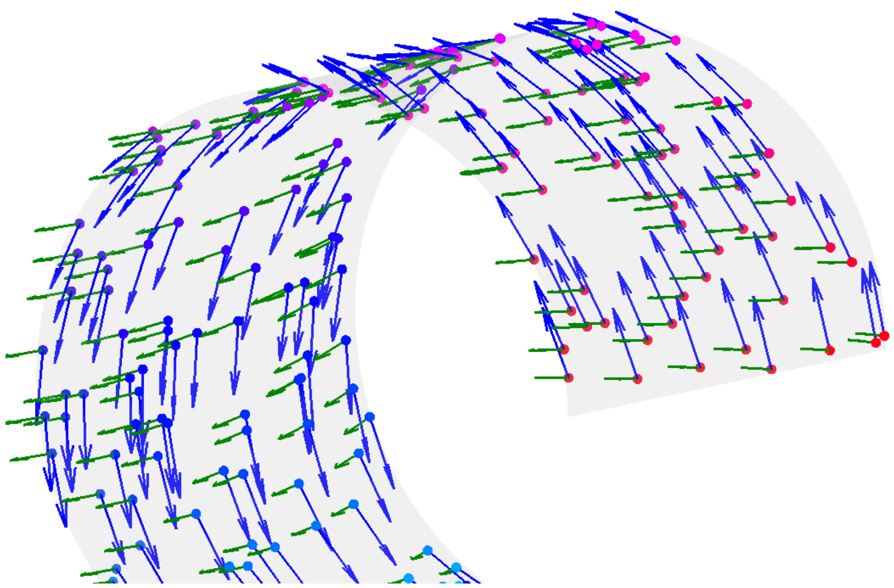


Desired operations:

- project onto manifold
- distance to manifold
- geodesic distance
- generalize to unseen regions

II. Locally Smooth Manifold Learning (LSML)

Represent manifold by its tangent space



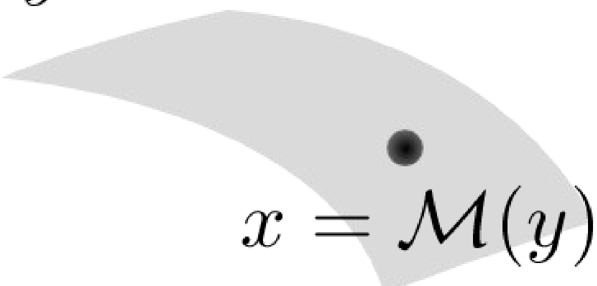
Non-local Manifold Tangent Learning [Bengio et al. NIPS05]

Learning to Traverse Image Manifolds [Dollar et al. NIPS06]

Learning the tangent space

Data on *d* dim. manifold in *D* dim. space

$y \in \mathbb{R}^d \quad x \in \mathbb{R}^D$

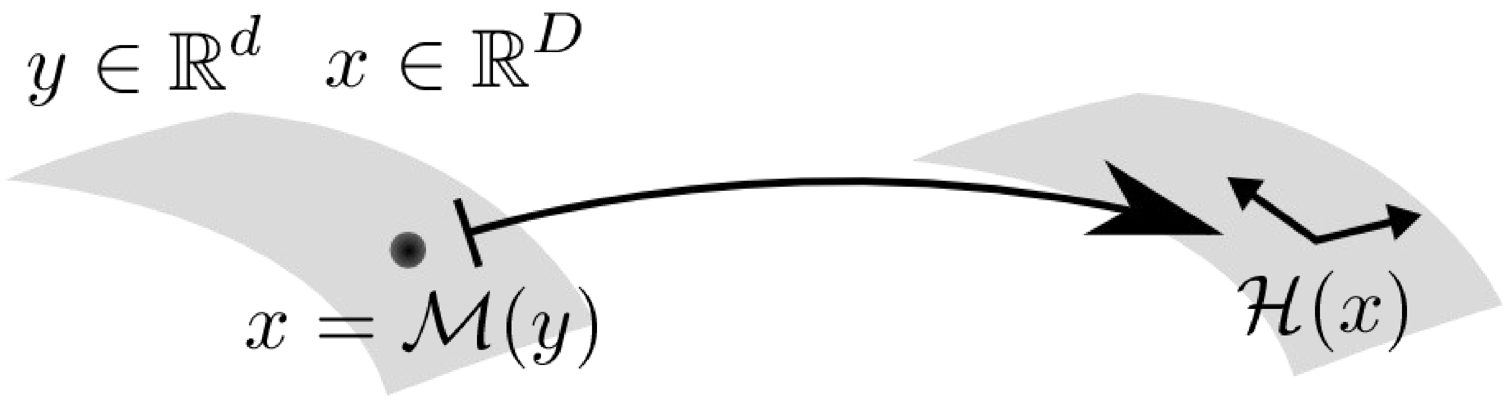


$x = \mathcal{M}(y)$

$$\mathcal{M} : \begin{cases} \mathbb{R}^d & \longrightarrow & \mathbb{R}^D \\ \mathrm{y} & \longmapsto & \mathrm{x} \end{cases}$$

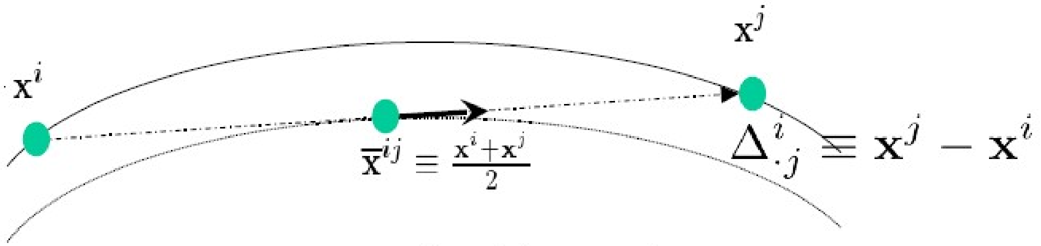
Learning the tangent space

Learn function from point to tangent basis

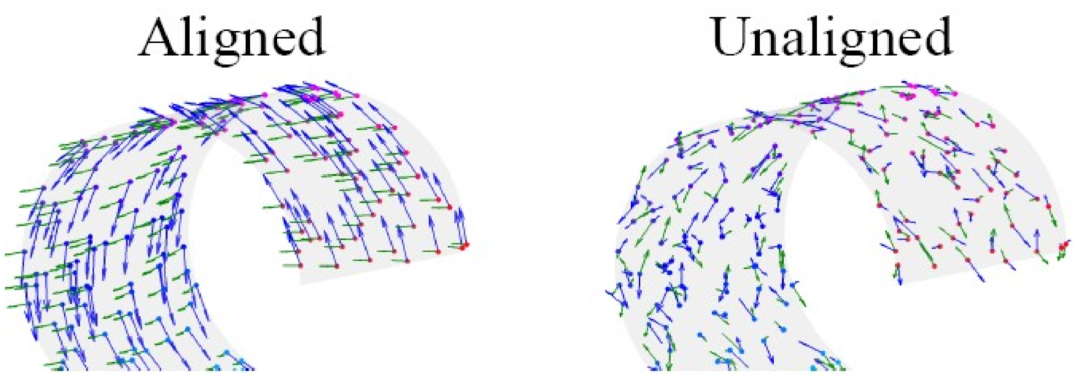


$$\mathcal{H} : \begin{cases} \mathbb{R}^D & \longrightarrow \quad \mathbb{R}^{D \times d} \\ \mathbf{x} & \longmapsto \quad \left[\frac{\partial}{\partial \mathbf{y}_1} \mathcal{M}(\mathbf{y}) \quad \cdots \quad \frac{\partial}{\partial \mathbf{y}_d} \mathcal{M}(\mathbf{y}) \right] \end{cases}$$

Loss function



$$\mathcal{H}_\theta(\overline{\mathbf{x}}^{ij})\boldsymbol{\epsilon}^{ij} \approx \Delta^i_{\cdot j}$$



$$\mathrm{err}(\theta) = \min_{\{\boldsymbol{\epsilon}^{ij}\}} \sum_{i,j \in \mathcal{N}^i} \left\| \mathcal{H}_\theta(\overline{\mathbf{x}}^{ij})\boldsymbol{\epsilon}^{ij} - \Delta^i_{\cdot j} \right\|_2^2$$

Optimization procedure

Linear form: $\mathcal{H}_\theta(\overline{\mathbf{x}}^{ij}) = \left[\Theta^1 \mathbf{f}^{ij} \cdots \Theta^D \mathbf{f}^{ij}\right]^\top$

$$\mathrm{err}(\theta) = \min_{\{\epsilon^{ij}\}} \sum_{i,j \in \mathcal{N}^i} \sum_{k=1}^{D} \left(\mathbf{f}^{ij\top} \Theta^{k\top} \boldsymbol{\epsilon}^{ij} - \Delta^i_{kj} \right)^2$$

Initialize Θ randomly.

while $\mathrm{err}(\Theta)$ decreases **do**

$\forall i, j$, solve for the best $\boldsymbol{\epsilon}^{ij}$ given the Θ^ks:

$$\boldsymbol{\epsilon}^{ij} = (H^{ij\top} H^{ij} + \lambda_\epsilon I)^+ H^{ij\top} \Delta^i_{\cdot j}$$

$\forall k$, solve for the best Θ^k given the $\boldsymbol{\epsilon}^{ij}$'s:

$$\text{Let: } A = \begin{bmatrix} \vdots \\ \boldsymbol{\epsilon}^{ij\top} \otimes \mathbf{f}^{ij\top} \\ \vdots \end{bmatrix}, \mathbf{b}^k = \begin{bmatrix} \vdots \\ \Delta^i_{kj} \\ \vdots \end{bmatrix}$$

$$\mathrm{vec}\left(\Theta^{k\top}\right) = (A^\top A + \lambda_\Theta (I \otimes (\Delta_F{}^\top \Delta_F))^{-1} A^\top \mathbf{b}^k$$

end while

III. Analyzing Manifold Learning Methods

- Need evaluation methodology to:
  - objectively compare methods
  - control model complexity
  - extend to non-isometric manifolds

Evaluation metric

By definition, for isometric manifolds embedding should preserve distance

$$\text{err}_{\text{GD}} \equiv \frac{1}{n^2} \sum_{ij} \frac{|d_{ij} - d'_{ij}|}{d_{ij}}$$

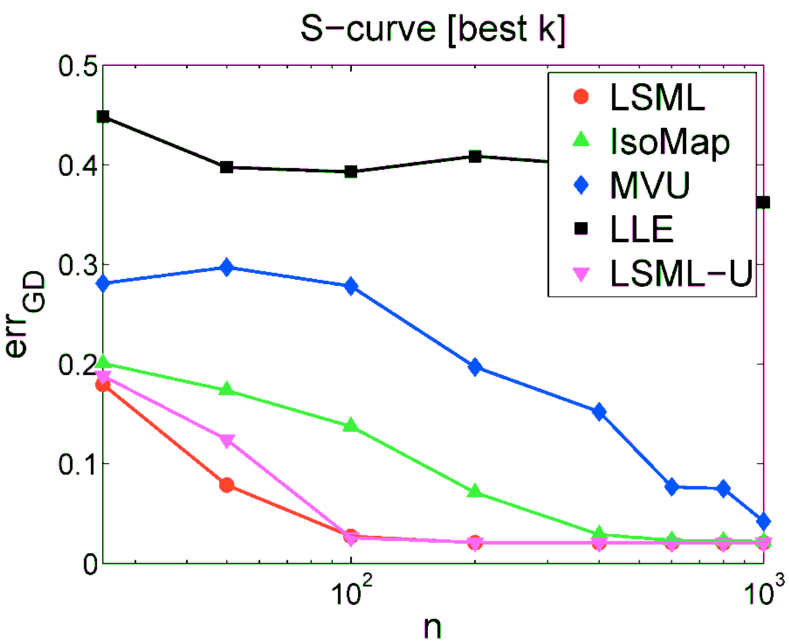
(d'_{ij} ← Estimated dist; d_{ij} ← True distance)

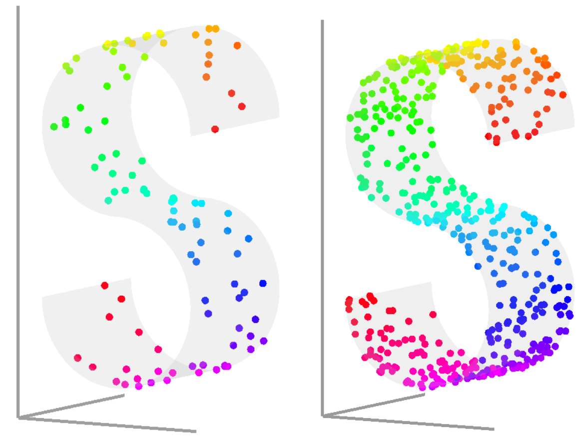
Requires two sets of samples from manifold:

1. S_n – for training
2. S_∞ – for computing "true" geodesics (Isomap)

Applicable for manifolds that can be densely sampled

Finite Sample Performance

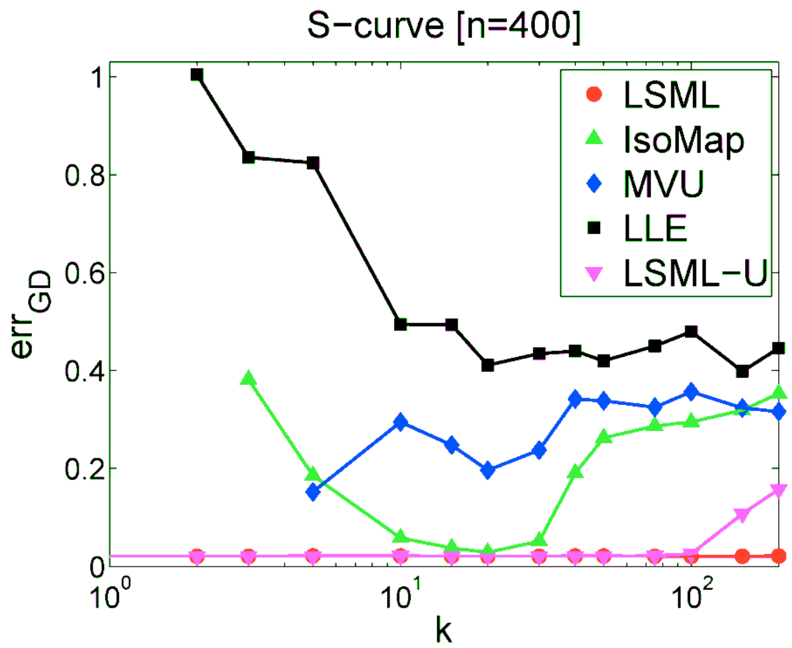


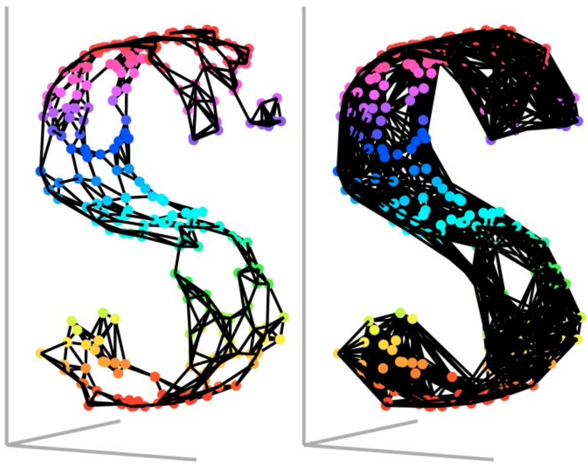


Performance: LSML > ISOMAP > MVU >> LLE

Applicability: LSML >> LLE > MVU > ISOMAP

Model Complexity





All methods have at least one parameter: k

Bias-Variance tradeoff

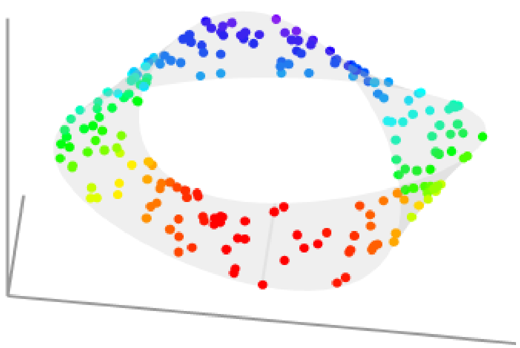
LSML test error

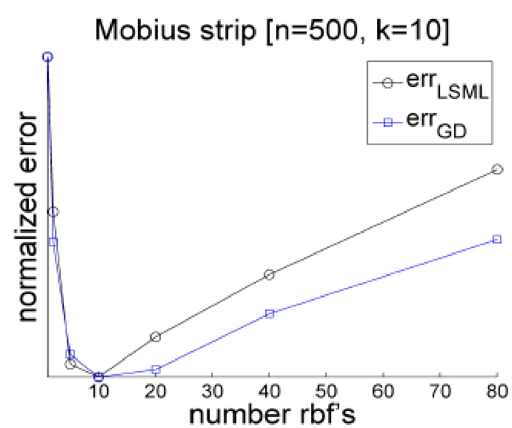
Typically, S_∞ not available

- Need notion of generalization: **testable prediction**
- Model assessment / Model selection

Define: $$\mathrm{err}_{\mathrm{LSML}} \equiv \sum_i \min_{\boldsymbol{\epsilon}^{ii'}} \left\| \mathcal{H}_\theta(\overline{\mathbf{x}}^{ii'})\boldsymbol{\epsilon}^{ii'} - (\mathbf{x}^i - \mathbf{x}^{i'}) \right\|_2^2$$

Claim: $\mathrm{err}_{\mathrm{LSML}}$ / $\mathrm{err}_{\mathrm{GD}}$ strongly correlated:





LSML test error

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- Use much as test error in supervised learning
- Cannot be used to select *d*
- Can also measure error for manifold transfer

IV. Using the Tangent Space

- projection
- manifold de-noising
- geodesic distance
- generalization

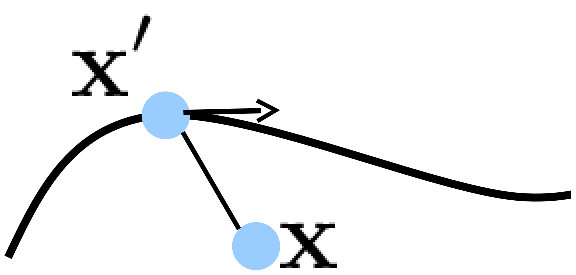
Projection

x' is the projection of *x* onto a manifold if it satisfies:

$$\min_{\mathbf{x}'} \|\mathbf{x} - \mathbf{x}'\|_2^2$$

gradient descent is performed after initializing the projection *x*' to some point on the manifold:

$$\mathbf{x}' \leftarrow \mathbf{x}' + \alpha H' H'^{\top} (\mathbf{x} - \mathbf{x}')$$



$H' \longleftarrow$ tangents at $\mathbf{x}'$

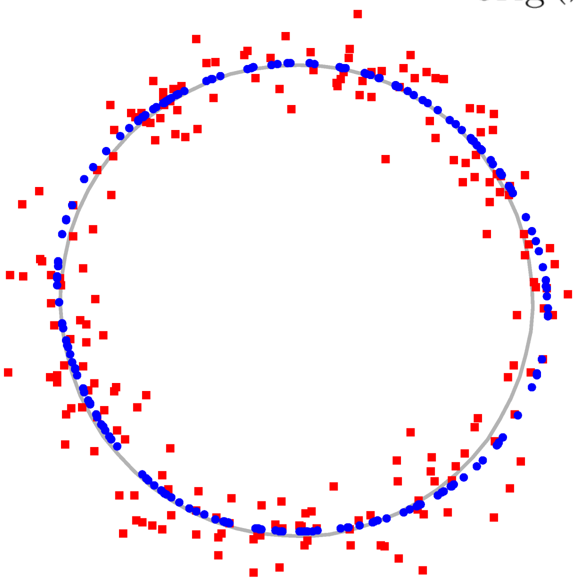
$H' H'^{\top} \longleftarrow$ projection matrix

Manifold de-noising

Goal: recover points on manifold (χ) from points corrupted by noise ($\mathbf{X}$)

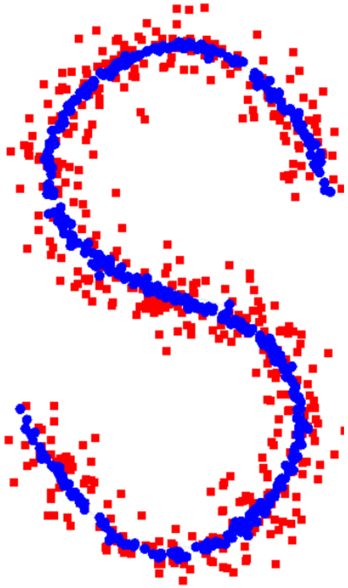
$$\mathrm{err}_{\mathcal{M}}(\chi) = \min_{\{\boldsymbol{\epsilon}^{ij}\}} \sum_{i,j \in \mathcal{N}^i} \left\| \mathcal{H}_\theta(\overline{\chi}^{ij})\boldsymbol{\epsilon}^{ij} - (\chi^i - \chi^j) \right\|_2^2$$

$$\mathrm{err}_{\mathrm{orig}}(\chi) = \sum_{i=1}^{n} \left\| \chi^i - \mathbf{x}^i \right\|_2^2$$



$\mathbf{X}$ - original

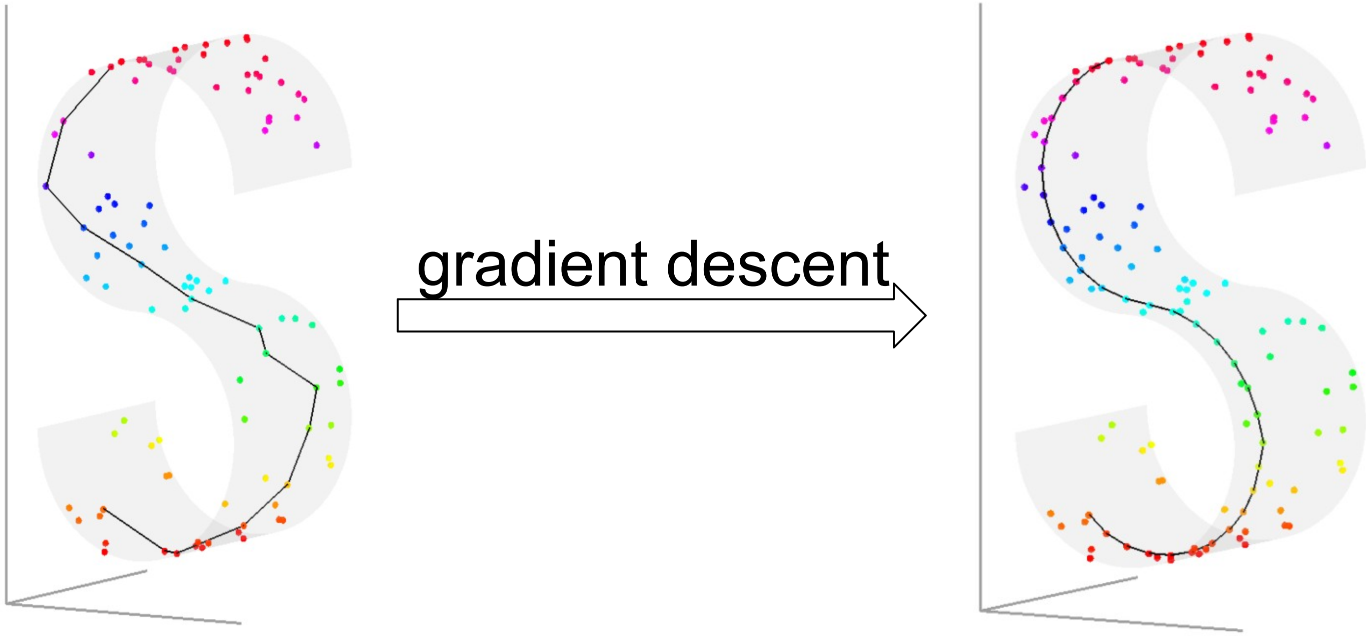
χ - de-noised



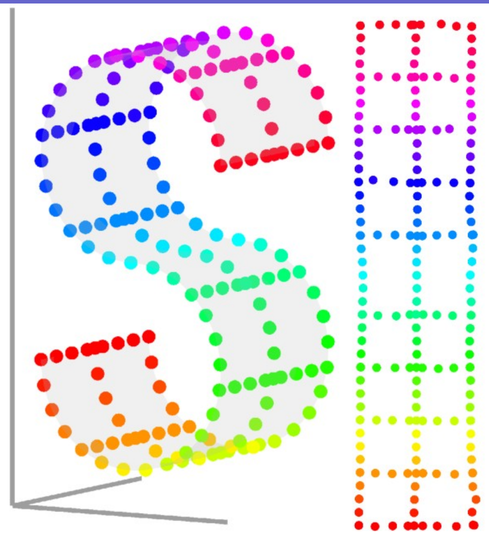
Geodesic distance

Shortest path: $$\mathrm{err}_{\mathrm{length}}(\chi) = \sum_{i=2}^{m} \left\| \chi^i - \chi^{i-1} \right\|_2^2$$

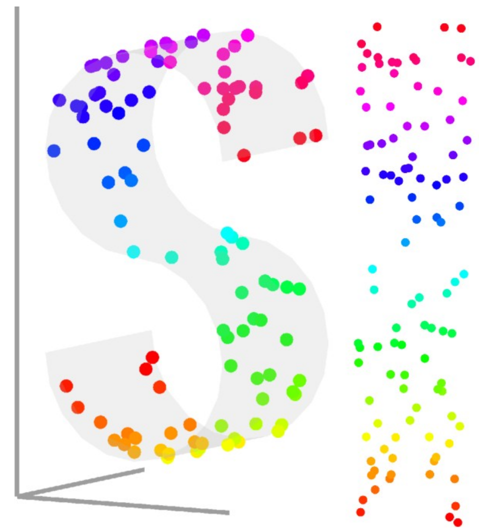
On manifold: $$\mathrm{err}_{\mathcal{M}}(\chi) = \min_{\{\boldsymbol{\epsilon}^{ij}\}} \sum_{i,j \in \mathcal{N}^i} \left\| \mathcal{H}_\theta(\overline{\chi}^{ij})\boldsymbol{\epsilon}^{ij} - (\chi^i - \chi^j) \right\|_2^2$$

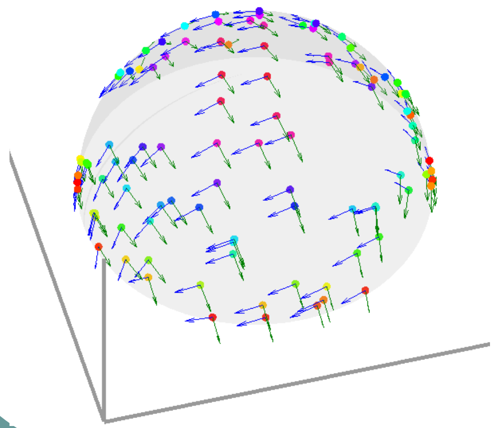


Geodesic distance

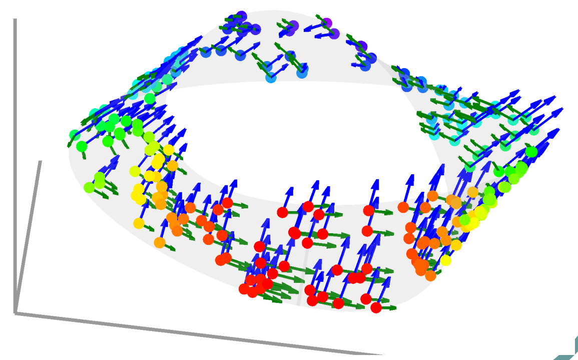


← embedding of sparse and structured data →

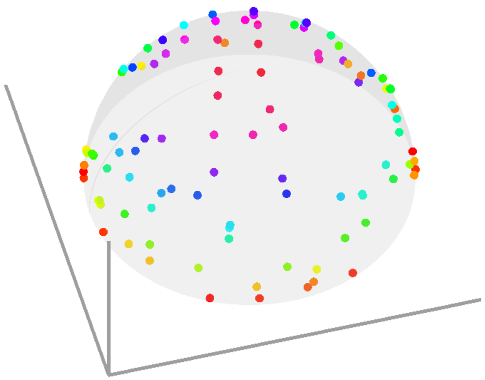


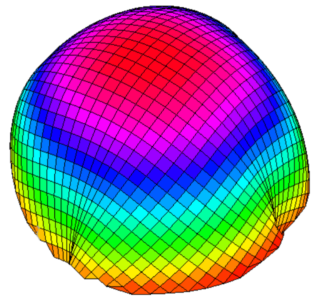


←can apply to non-isometric manifolds →

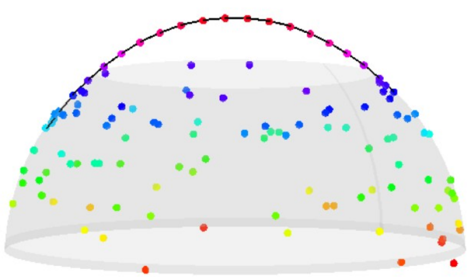


Generalization





← Reconstruction within the support of training data



← Generalization beyond support of training data →

Thank you!