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

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

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

$\mathcal{M} : \{ \begin{array}{c} \mathbb{R}^d \\ y \end{array} \rightarrow \mathbb{R}^D \\ \begin{array}{c} \mathbb{R}^D \\ x \end{array}$
Learning the tangent space

Learn function from point to tangent basis

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

\[ x = \mathcal{M}(y) \]

\[ \mathcal{H} : \{ \mathbb{R}^D \rightarrow \mathbb{R}^{D \times d} \}

\[ x \mapsto \left[ \frac{\partial}{\partial y_1} \mathcal{M}(y) \quad \ldots \quad \frac{\partial}{\partial y_d} \mathcal{M}(y) \right] \]
Loss function

\[ H_\theta(\overline{x}^{i,j}) \epsilon^{i,j} \approx \Delta^{i,j} \]

\[ \text{err}(\theta) = \min_{\{\epsilon^{i,j}\}} \sum_{i,j \in N^i} \left\| H_\theta(\overline{x}^{i,j}) \epsilon^{i,j} - \Delta^{i,j} \right\|^2 \]
Optimization procedure

Linear form: \( \mathcal{H}_\theta(\bar{x}^{ij}) = [\Theta^1 f^{ij} \cdots \Theta^D f^{ij}]^T \)

\[
\text{err}(\theta) = \min_{\{\epsilon_{ij}\}} \sum_{i,j \in N} \sum_{k=1}^{D} \left( f^{ij}^T \Theta_k^T \epsilon_{ij} - \Delta_{kij} \right)^2
\]

Initialize \( \Theta \) randomly.

\textbf{while} \( \text{err}(\theta) \) decreases \textbf{do}

\( \forall i,j, \) solve for the best \( \epsilon_{ij} \) given the \( \Theta^k \) 's:

\[
\epsilon_{ij} = (H^{ij^T} H^{ij} + \lambda_c I)^+ H^{ij^T} \Delta_{ij}
\]

\( \forall k, \) solve for the best \( \Theta^k \) given the \( \epsilon_{ij} \) 's:

Let: \( A = \begin{bmatrix} \epsilon_{ij}^T \otimes f^{ij^T} \\ \vdots \end{bmatrix}, b^k = \begin{bmatrix} \Delta_{kij}^i \\ \vdots \end{bmatrix} \)

\[
\text{vec} \left( \Theta^k^T \right) = (A^T A + \lambda_c (I \otimes (\Delta_F^T \Delta_F))^{-1} A^T b^k
\]

\textbf{end while}
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

\[
\text{err}_{GD} \equiv \frac{1}{n^2} \sum_{ij} \left| d_{ij} - d'_{ij} \right| \quad \text{Estimated dist}
\]

\[
d_{ij} \quad \text{True distance}
\]

Requires two sets of samples from manifold:
1. \( S_n \) – for training
2. \( S_\infty \) – 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
Typically, $S'_\infty$ not available

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

Define:  \[ \text{err}_{\text{LSML}} \equiv \sum \min_{\epsilon_i} \left\| \mathcal{H}_\theta(x_i \epsilon_i') \epsilon_{ii'} - (x_i - x_i') \right\|_2^2 \]

Claim:  \[ \text{err}_{\text{LSML}} / \text{err}_{\text{GD}} \text{ strongly correlated:} \]
Typically, $S_\infty$ not available

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

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

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

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

Gradient descent is performed after initializing the projection $x'$ to some point on the manifold:

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

$tangents at \ x'$

$H' H'^\top \leftarrow projection matrix$
Manifold de-noising

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

$$
\text{err}_M(\mathcal{X}) = \min_{\{\epsilon_i\}} \sum_{i,j \in \mathcal{N}_i} \left\| \mathcal{H}_\theta(\overline{x}^{ij})\epsilon^{ij} - (x^i - x^j) \right\|^2_2
$$

$$
\text{err}_{\text{orig}}(\mathcal{X}) = \sum_{i=1} \left\| x^i - \mathcal{X}^i \right\|^2_2
$$

- $\mathbf{X}$ - original
- $\mathcal{X}$ - de-noised
**Geodesic distance**

**Shortest path:**

\[
\text{err}_{\text{length}}(\chi) = \sum_{i=2}^{m} \left\| \chi^i - \chi^{i-1} \right\|_2^2
\]

**On manifold:**

\[
\text{err}_M(\chi) = \min_{\{\epsilon^{ij}\}} \sum_{i,j \in \mathcal{N}^i} \left\| \mathcal{H}_\theta(\overline{x}^{ij}) \epsilon^{ij} - (\chi^i - \chi^j) \right\|_2^2
\]

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**Diagram:**

Gradent descent.
Geodesic distance

← embedding of sparse and structured data →

← can apply to non-isometric manifolds →
Generalization beyond support of training data

← Reconstruction within the support of training data

← Generalization beyond support of training data →
Thank you!