

Introduction to Manifold Learning

A Geometry View on Machine Learning

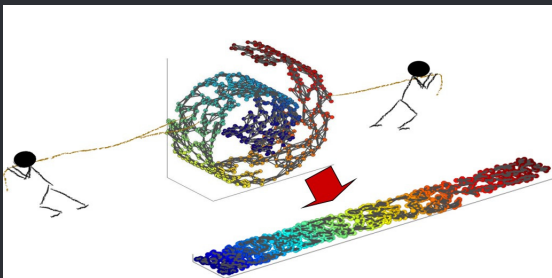
Xiaoyu Xue

Manifold Learning

1. Manifold
2. Manifold based Dimensionality Reduction
 - 2.1 Principal Component Analysis
 - 2.2 Multidimensional scaling
 - 2.3 ISOMAP
 - 2.4 Local Linear Embedding
 - 2.5 Laplacian Eigenmaps
 - 2.6 Vector Field based Dimensionality Reduction
3. Manifold Regularization : Semi-Supervised Setting

Manifold Learning

- The data space may not be a Euclidean space, but a nonlinear manifold
- Unfold a manifold, and preserve the geometry structure.
- Euclidean distance \Rightarrow geodesic distance



Manifold Learning

Find a Euclidean embedding, and then perform traditional learning algorithms in the Euclidean space.

Definition of Manifold Learning

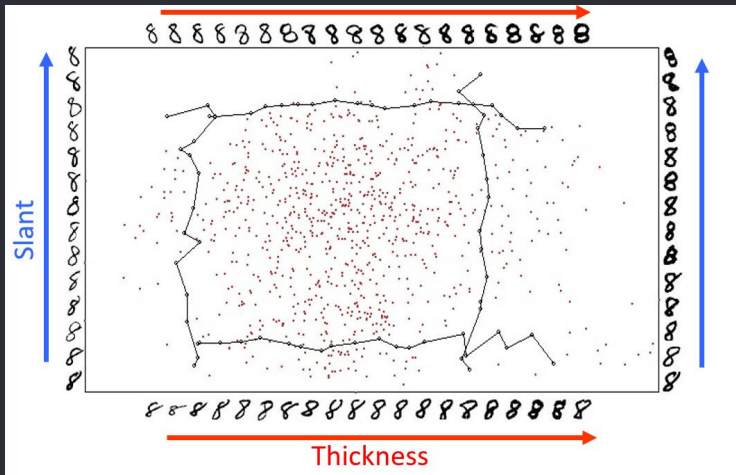
Given data points $\mathbf{x}_1, \dots, \mathbf{x}_m \in \mathcal{M} \subset \mathbb{R}^n$, try to find a map $f : \mathcal{M} \rightarrow \mathbb{R}^d, d \ll n$, where $f = (f_1, \dots, f_d), f_i : \mathcal{M} \rightarrow \mathbb{R}$

- The manifold is unknown! We have only samples!
- How to compute the distance on \mathcal{M} ?
- How to find the mapping function f

Manifold of Face Images



Manifold of Handwritten Digits



Manifold Learning

1. Manifold
2. Manifold based Dimensionality Reduction
 - 2.1 Principal Component Analysis
 - 2.2 Multidimensional scaling
 - 2.3 ISOMAP
 - 2.4 Local Linear Embedding
 - 2.5 Laplacian Eigenmaps
 - 2.6 Vector Field based Dimensionality Reduction
3. Manifold Regularization : Semi-Supervised Setting

PCA: Traditional Dimensionality Reduction Method

Principal Component Analysis using linear projection to project data to some directions which have maximum variances

$$\begin{aligned}\mathbf{p}_{opt} &= \arg \max_{\mathbf{p}} \sum_{i=1}^m (y_i - \bar{y})^2 \\ &= \arg \max_{\mathbf{p}} \mathbf{p}^T \mathbf{C} \mathbf{p} \\ &\text{s.t. } \mathbf{p}^T \mathbf{p} = 1\end{aligned}$$

- If the manifold is linear, PCA can find the optimal result
- PCA can not process nonlinear manifold

MDS and ISOMAP

Multidimensional scaling tries to preserve the Euclidean distances

$$\Delta := \begin{pmatrix} \delta_{1,1} & \delta_{1,2} & \dots & \delta_{1,m} \\ \delta_{2,1} & \delta_{2,2} & \dots & \delta_{2,m} \\ \vdots & \vdots & & \vdots \\ \delta_{m,1} & \delta_{m,2} & \dots & \delta_{m,m} \end{pmatrix}$$

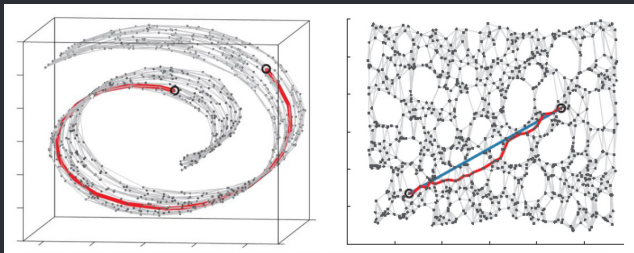
The δ is the Euclidean distance of every two points $\delta_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|$

$$\min_{\mathbf{y}_1, \dots, \mathbf{y}_m} \sum_{i < j} (\|\mathbf{y}_i - \mathbf{y}_j\| - \delta_{i,j})^2, \quad \dim(\mathbf{y}_i) \ll \dim(\mathbf{x}_i)$$

MDS and ISOMAP

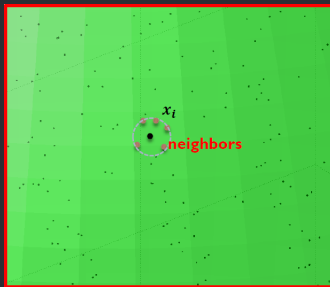
ISOMAP tries to keep the geodesic distances instead of the Euclidean distances.

- How to evaluate the geodesic distances with limited samples?
- Construct the adjacency Graph, and calculate the shortest distances (Dijkstra or Floyd algorithm)



Local Linear Embedding

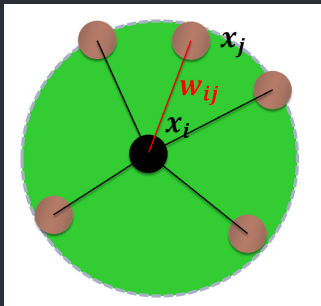
Local Linear Embedding(2000 Science) is another famous manifold learning method. It tries to preserve the local linear relationship.



$$\begin{aligned} \min \epsilon(W) &= \min \sum_i \|x_i - \sum_j W_{ij} x_j\| \\ \text{s.t. } &\sum_j W_{ij} = 1 \end{aligned}$$

Local Linear Embedding

Local Linear Embedding(2000 Science) is another famous manifold learning method. It tries to preserve the local linear relationship.



$$\min \Phi(\mathbf{y}) = \min \sum_i \|\mathbf{y}_i - \sum_j w_{ij} \mathbf{y}_j\|^2$$

Laplacian Eigenmaps

In Laplacian Eigenmaps, a conclusion has been proofed:

$$|f(\mathbf{z}) - f(\mathbf{x})| < \|\nabla f(\mathbf{x})\| \cdot \|\mathbf{z} - \mathbf{x}\| + o(\|\mathbf{z} - \mathbf{x}\|)$$

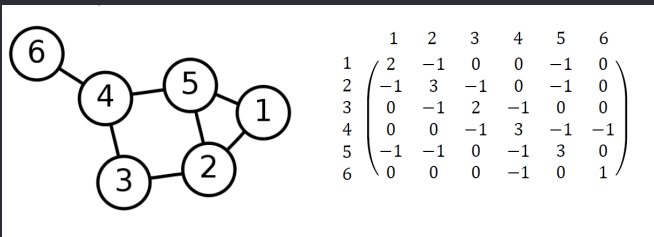
- If \mathbf{x}_i and \mathbf{x}_j are close to each other and the gradient of map f is small, we can sure that $f(\mathbf{x}_i)$ and $f(\mathbf{x}_j)$ preserve local structure.

Construct Laplace matrix and get object function

$$\min \sum_{i,j} (y_i - y_j)^2 W_{ij} \Rightarrow L\mathbf{y} = \lambda D\mathbf{y}$$

Laplace Operator on Graph

- L is the Laplace operator, which measures the smooth of the function on manifold
- On Graph, L is Laplace matrix



Global vs Local

- Global method : ISOMAP
- Local method : LLE, LE
- Global method can keep more informations of data
- But the amount of computation of Global methods is huge

Out of sample problem

- LE and LLE can not applied new samples.
- Use linear projection: $y = \mathbf{p}^T \mathbf{x}$
- LE \rightarrow LPP : $XLX^T \mathbf{p} = \lambda D \mathbf{p}$
- LLE \rightarrow NPE : $XM X^T \mathbf{p} = \lambda XX^T \mathbf{p}$

Vector Field based Dimensionality Reduction

Parallel Vector Field Embedding

The goal to find a map $F = (f_1, \dots, f_d) : \mathcal{M} \subset \mathbb{R}^n \rightarrow \mathbb{R}^d$

- F is a local isometry
- dF is orthonormal
- df_i is parallel vector fields $\Rightarrow \nabla df_i = 0$

Steps:

1. $E(V) = \int_{\mathcal{M}} \|\nabla V\|^2 dx, \quad \text{s.t.} \int_{\mathcal{M}} \|V\|^2 = 1$
2. $\min \Phi(f) = \int_{\mathcal{M}} \|\nabla f - V\|^2 dx$

A new perspective for manifold learning

Swiss Roll

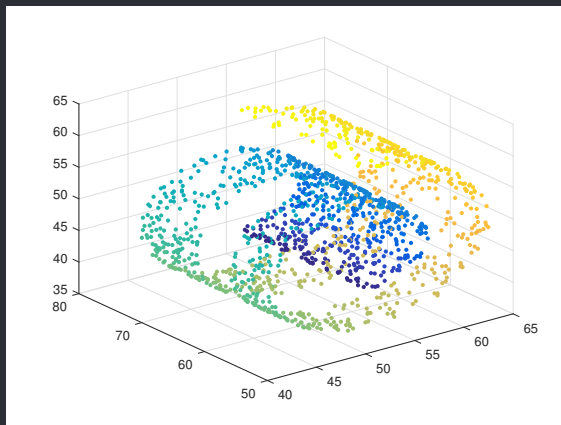


Figure: Swiss Roll

PFE

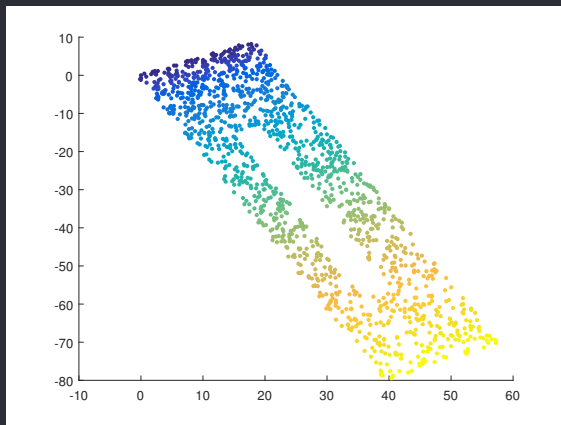


Figure: PFE

PCA

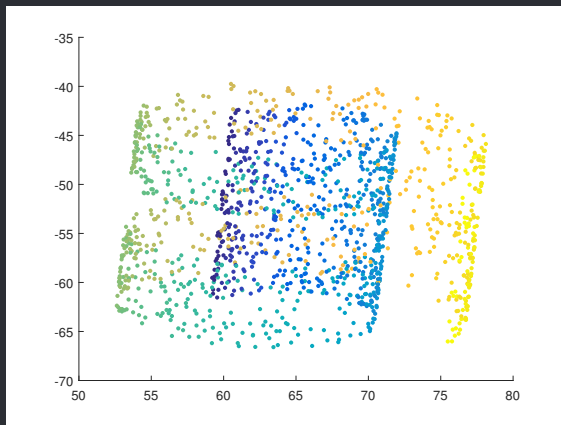


Figure: PCA

ISOMAP

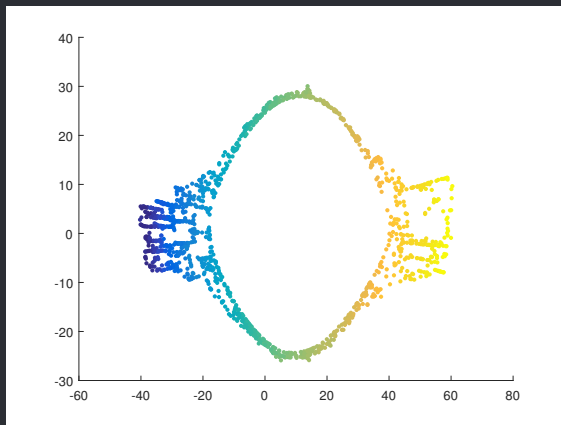


Figure: ISOMAP

LLE

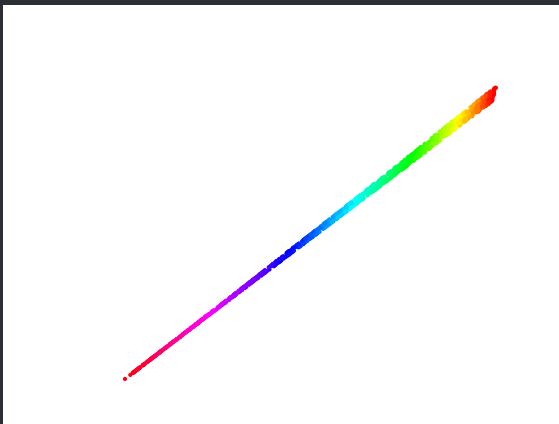


Figure: LLE

LE

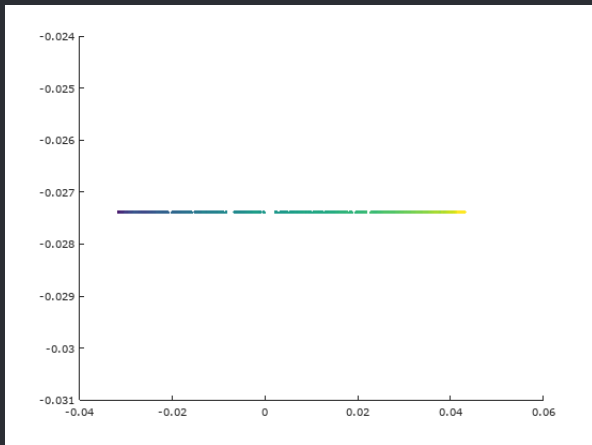


Figure: LE

NPE

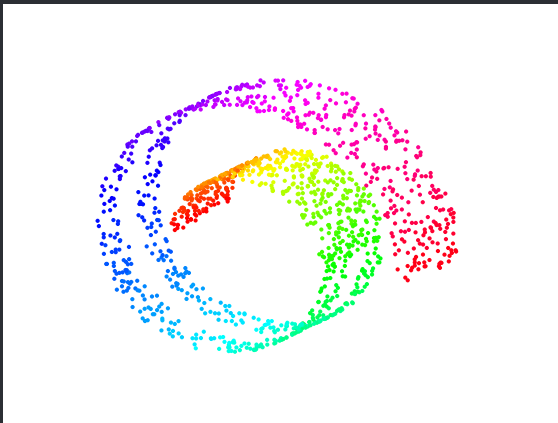


Figure: NPE

LPP



Figure: LPP

Manifold Learning

1. Manifold
2. Manifold based Dimensionality Reduction
 - 2.1 Principal Component Analysis
 - 2.2 Multidimensional scaling
 - 2.3 ISOMAP
 - 2.4 Local Linear Embedding
 - 2.5 Laplacian Eigenmaps
 - 2.6 Vector Field based Dimensionality Reduction
3. Manifold Regularization : Semi-Supervised Setting

Manifold Regularization

- Measured (labeled) points: discriminant structure

$$\min \sum_{i=1}^k (y_i - f(\mathbf{z}_i))^2$$

- Unmeasured (unlabeled) points: geometrical structure

$$\min \sum_{i,j} (f(\mathbf{x}_i) - f(\mathbf{x}_j))^2 S_{ij}$$

$$\min_f \sum_{i=1}^k (y_i - f(\mathbf{z}_i))^2 + \frac{\lambda}{2} \sum_{i,j} (f(\mathbf{x}_i) - f(\mathbf{x}_j))^2 S_{ij}$$

Laplacian Regularized Least Square

- Linear objective function

$$\min_{\mathbf{w}} \sum_{i=1}^k (y_i - \mathbf{w}^T \mathbf{z}_i)^2 + \frac{\lambda_1}{2} \sum_{i,j=1}^m (\mathbf{w}^T \mathbf{x}_i - \mathbf{w}^T \mathbf{x}_j)^2 S_{ij} + \lambda_2 \|\mathbf{w}\|^2$$

- Solution

$$\mathbf{w} = (\mathbf{Z}\mathbf{Z}^T + \lambda_1 \mathbf{X}\mathbf{L}\mathbf{X}^T + \lambda_2 \mathbf{I})^{-1} \mathbf{Z}\mathbf{y}$$

- $\mathbf{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_k)$: labeled points
- $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_m)$: all points

Thanks !