

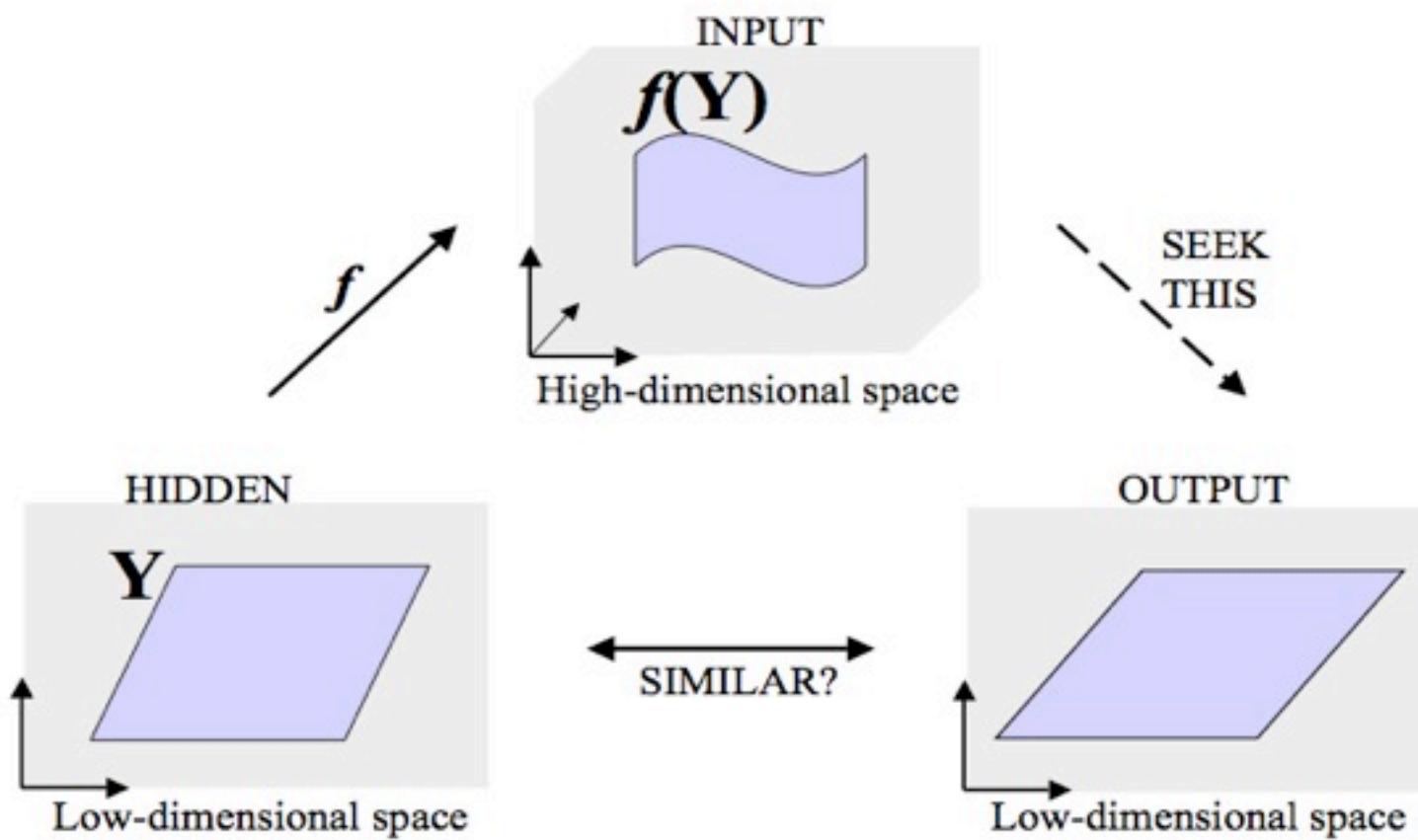
# Extended Locally Linear Embedding



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# Generative Models in Manifold Learning



# Spectral Geometric Embedding

Given  $x_1, \dots, x_n \in \mathcal{M} \subset \mathbb{R}^N$ ,

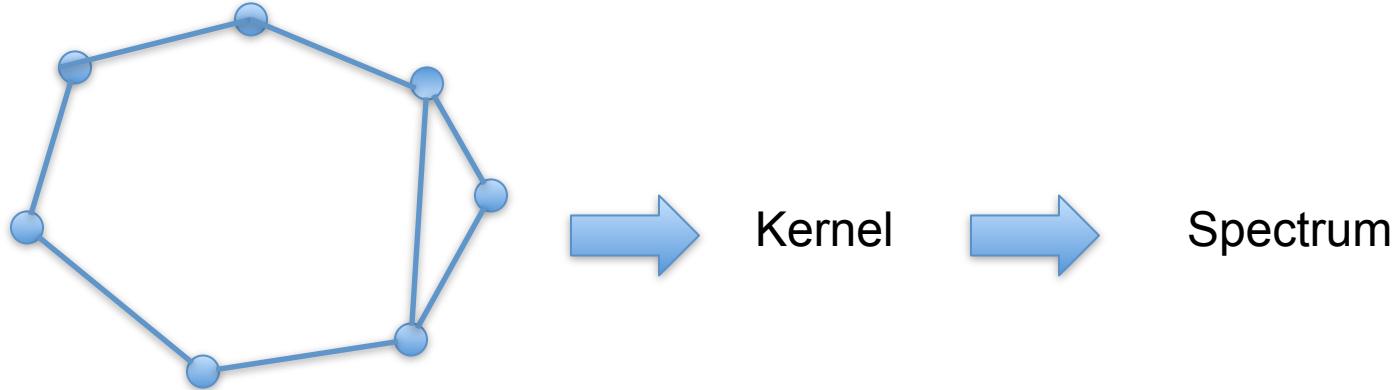
Find  $y_1, \dots, y_n \in \mathbb{R}^d$  where  $d \ll N$

- ISOMAP (Tenenbaum, et al, 00)
- LLE (Roweis, Saul, 00)
- Laplacian Eigenmaps (Belkin, Niyogi, 01)
- Local Tangent Space Alignment (Zhang, Zha, 02)
- Hessian Eigenmaps (Donoho, Grimes, 02)
- Diffusion Maps (Coifman, Lafon, et al, 04)

Related: Kernel PCA (Schoelkopf, et al, 98)

# Meta-Algorithm

- Construct a neighborhood graph
- Construct a positive semi-definite kernel
- Find the spectrum decomposition



# Recall: ISOMAP

1. Construct Neighborhood Graph.
2. Find **shortest path (geodesic)** distances.

$D_{ij}$  is  $n \times n$

3. Embed using Multidimensional Scaling.

# Recall: LLE

- Construct a neighborhood Graph  $G=(V,E)$
- Solve weights

$$\min_{\sum_j w_{ij}=1} \|X_i - \sum_{j \in \mathcal{N}(i)} w_{ij} \bar{X}_j\|^2, \quad \bar{X}_j = X_j - X_i.$$

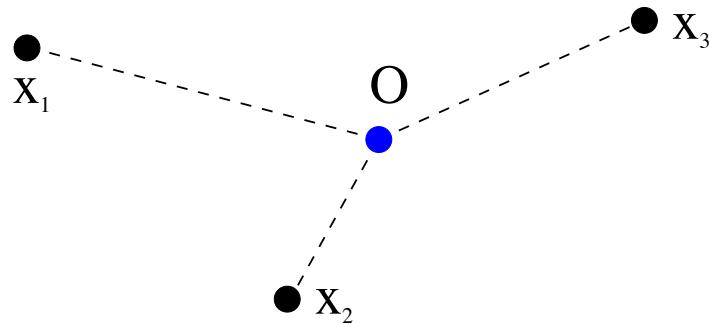
- Compute Embedding

$$\min_Y \sum_{i=1}^n \|Y_i - \sum_{j=1}^n W_{ij} Y_j\|^2 = \text{trace}((I - W)Y^T Y(I - W)^T).$$

$$W_{ij}^{n \times n} = \begin{cases} w_{ij} & j \in \mathcal{N}(i), \\ 0 & \text{other's.} \end{cases}$$

This is equivalent to find smallest eigenvectors of  $K = (I - W)^T(I - W)$ .

# Laplacian and LLE



$$\sum w_i x_i = 0$$

$$\sum w_i = 1$$

Hessian  $H$ . Taylor expansion :

$$f(x_i) = f(0) + x_i^t \nabla f + \frac{1}{2} x_i^t H x_i + o(\|x_i\|^2)$$

$$(I - W)f(0) = f(0) - \sum w_i f(x_i) \approx f(0) - \sum w_i f(0) - \sum_i w_i x_i^t \nabla f - \frac{1}{2} \sum_i w_i x_i^t H x_i =$$

$$= -\frac{1}{2} \sum_i x_i^t H x_i \approx -\text{tr} H = \Delta f$$

# Discrete Laplacian

Find  $y_1, \dots, y_n \in R$

$$\min \sum_{i,j} (y_i - y_j)^2 W_{ij}$$

Tries to preserve **locality**

# A Fundamental Identity

But

$$\frac{1}{2} \sum_{i,j} (y_i - y_j)^2 W_{ij} = \mathbf{y}^T L \mathbf{y}$$

$$\begin{aligned} \sum_{i,j} (y_i - y_j)^2 W_{ij} &= \sum_{i,j} (y_i^2 + y_j^2 - 2y_i y_j) W_{ij} \\ &= \sum_i y_i^2 D_{ii} + \sum_j y_j^2 D_{jj} - 2 \sum_{i,j} y_i y_j W_{ij} \\ &= 2\mathbf{y}^T L \mathbf{y} \end{aligned}$$

# Embedding of Unnormalized Laplacian Eigenmap

$$\lambda = 0 \rightarrow \mathbf{y} = \mathbf{1}$$

$$\min_{\mathbf{y}^T \mathbf{1}=0} \mathbf{y}^T L \mathbf{y}$$

Let  $Y = [\mathbf{y}_1 \mathbf{y}_2 \dots \mathbf{y}_m]$

$$\sum_{i,j} ||Y_i - Y_j||^2 W_{ij} = \text{trace}(Y^T L Y)$$

subject to  $Y^T Y = I$ .

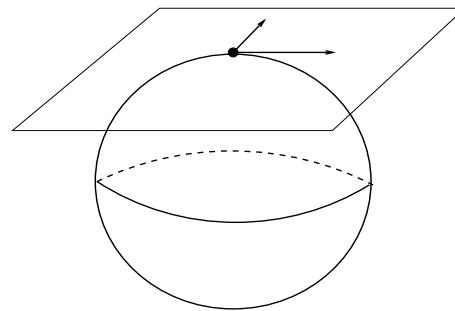
Use eigenvectors of  $L$  to embed.

# Manifold Laplacian

Recall ordinary Laplacian in  $\mathbb{R}^k$   
This maps

$$f(x_1, \dots, x_k) \rightarrow \left( - \sum_{i=1}^k \frac{\partial^2 f}{\partial x_i^2} \right)$$

Manifold Laplacian is the same on the tangent space.



# On the Manifold

smooth map  $f : \mathcal{M} \rightarrow R$

$$\int_{\mathcal{M}} \|\nabla_{\mathcal{M}} f\|^2 \approx \sum_{i \sim j} W_{ij} (f_i - f_j)^2$$

Recall standard gradient in  $\mathbb{R}^k$  of  $f(z_1, \dots, z_k)$

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial z_1} \\ \frac{\partial f}{\partial z_2} \\ \vdots \\ \vdots \\ \frac{\partial f}{\partial z_k} \end{bmatrix}$$

# Stokes Theorem

A Basic Fact

$$\int_{\mathcal{M}} \|\nabla_{\mathcal{M}} f\|^2 = \int f \cdot \Delta_{\mathcal{M}} f$$

This is like

$$\sum_{i,j} W_{ij} (f_i - f_j)^2 = \mathbf{f}^T \mathbf{L} \mathbf{f}$$

where

$\Delta_{\mathcal{M}} f$  is the manifold Laplacian

# Manifold Laplacian Eigenvectors

Eigensystem

$$\Delta_{\mathcal{M}} f = \lambda_i \phi_i$$

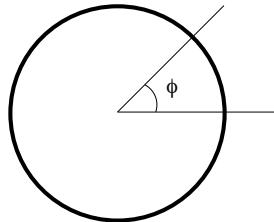
$\lambda_i \geq 0$  and  $\lambda_i \rightarrow \infty$

$\{\phi_i\}$  form an orthonormal basis for  $L^2(\mathcal{M})$

$$\int \|\nabla_{\mathcal{M}} \phi_i\|^2 = \lambda_i$$

Manifold Laplacian is non-compact!

# Example: Circle



$$-\frac{d^2u}{dt^2} = \lambda u \text{ where } u(0) = u(2\pi)$$

Eigenvalues are

$$\lambda_n = n^2$$

Eigenfunctions are

$$\sin(nt), \cos(nt)$$

Spherical Harmonics in high-D sphere!

# Spectral Growth

$$\lambda_1 \leq \lambda_2 \dots \leq \lambda_j \leq \dots$$

Then

$$A + \frac{2}{d} \log(j) \leq \log(\lambda_j) \leq B + \frac{2}{d} \log(j + 1)$$

Example: on  $S^1$

$$\lambda_j = j^2 \implies \log(\lambda_j) = \frac{2}{1} \log(j)$$

(Li and Yau; Weyl's asymptotics)

# Solution of Heat Equations

Heat equation in  $\mathbb{R}^n$ :

$u(x, t)$  – heat distribution at time  $t$ .

$u(x, 0) = f(x)$  – initial distribution.  $x \in \mathbb{R}^n, t \in \mathbb{R}$ .

$$\Delta_{\mathbb{R}^n} u(x, t) = \frac{du}{dt}(x, t)$$

Solution – convolution with the heat kernel:

$$u(x, t) = (4\pi t)^{-\frac{n}{2}} \int_{\mathbb{R}^n} f(y) e^{-\frac{\|x-y\|^2}{4t}} dy$$

# Discretization of Heat Eq.

Functional approximation:

Taking limit as  $t \rightarrow 0$  and writing the derivative:

$$\Delta_{\mathbb{R}^n} f(x) = \frac{d}{dt} \left[ (4\pi t)^{-\frac{n}{2}} \int_{\mathbb{R}^n} f(y) e^{-\frac{\|x-y\|^2}{4t}} dy \right]_0$$

$$\Delta_{\mathbb{R}^n} f(x) \approx -\frac{1}{t} (4\pi t)^{-\frac{n}{2}} \left( f(x) - \int_{\mathbb{R}^n} f(y) e^{-\frac{\|x-y\|^2}{4t}} dy \right)$$

Empirical approximation:

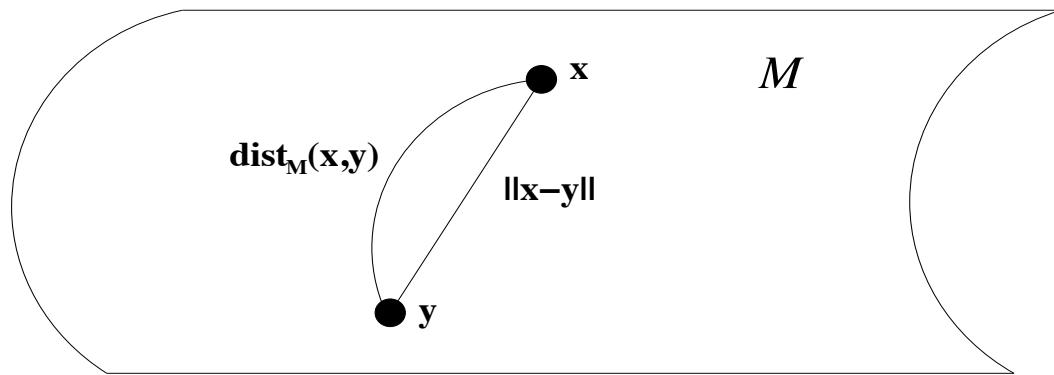
Integral can be estimated from empirical data.

$$\Delta_{\mathbb{R}^n} f(x) \approx -\frac{1}{t} (4\pi t)^{-\frac{n}{2}} \left( f(x) - \sum_{x_i} f(x_i) e^{-\frac{\|x-x_i\|^2}{4t}} \right)$$

# Some Difficulties for Manifolds

Some difficulties arise for manifolds:

- Do not know distances.
- Do not know the heat kernel.



Careful analysis needed.

# The Heat Kernel Approximation

- $H_t(x, y) = \sum_i e^{-\lambda_i t} \phi_i(x) \phi_i(y)$
- in  $\mathbb{R}^d$ , closed form expression

$$H_t(x, y) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{\|x-y\|^2}{4t}}$$

- Goodness of approximation depends on the gap
$$\left| H_t(x, y) - \frac{1}{(4\pi t)^{d/2}} e^{-\frac{\|x-y\|^2}{4t}} \right|$$
- $H_t$  is a Mercer kernel intrinsically defined on manifold.  
Leads to SVMs on manifolds.

# Pointwise Convergence

$$f : \mathcal{M} \rightarrow \mathbb{R} \quad x \in \mathcal{M} \quad x_1, \dots, x_n \in \mathcal{M}$$

Graph Laplacian:

$$L_n^t(f)(x) = f(x) \sum_j e^{-\frac{\|x-x_j\|^2}{t}} - \sum_j f(x_j) e^{-\frac{\|x-x_j\|^2}{t}}$$

**Theorem** [pointwise convergence]  $t_n = n^{-\frac{1}{k+2+\alpha}}$

$$\lim_{n \rightarrow \infty} \frac{(4\pi t_n)^{-\frac{k+2}{2}}}{n} L_n^{t_n} f(x) = \Delta_{\mathcal{M}} f(x)$$

Belkin 03, Lafon Coifman 04, Belkin Niyogi 05, Hein et al 05

# Convergence of Eigenfunctions

**Theorem** [convergence of eigenfunctions]

$$\lim_{t \rightarrow 0, n \rightarrow \infty} \text{Eig}[L_n^{t_n}] \rightarrow \text{Eig}[\Delta_{\mathcal{M}}]$$

Belkin Niyogi 06

# Laplacian Eigenmaps (I)

## [Belkin-Niyogi]

**Step 1** [Constructing the Graph]

$$e_{ij} = 1 \Leftrightarrow \mathbf{x}_i \text{ "close to" } \mathbf{x}_j$$

1.  $\epsilon$ -neighborhoods. [parameter  $\epsilon \in \mathbb{R}$ ] Nodes  $i$  and  $j$  are connected by an edge if

$$\|\mathbf{x}_i - \mathbf{x}_j\|^2 < \epsilon$$

2.  $n$  nearest neighbors. [parameter  $n \in \mathbb{N}$ ] Nodes  $i$  and  $j$  are connected by an edge if  $i$  is among  $n$  nearest neighbors of  $j$  or  $j$  is among  $n$  nearest neighbors of  $i$ .

# Laplacian Eigenmaps (II)

**Step 2.** [*Choosing the weights*].

1. **Heat kernel.** [parameter  $t \in \mathbb{R}$ ]. If nodes  $i$  and  $j$  are connected, put

$$W_{ij} = e^{-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{t}}$$

2. **Simple-minded.** [No parameters].  $W_{ij} = 1$  if and only if vertices  $i$  and  $j$  are connected by an edge.

# Laplacian Eigenmaps (III)

**Step 3.** [Eigenmaps] Compute eigenvalues and eigenvectors for the generalized eigenvector problem:

$$Lf = \lambda Df$$

$D$  is diagonal matrix where

$$D_{ii} = \sum_j W_{ij}$$

$$L = D - W$$

Let  $\mathbf{f}_0, \dots, \mathbf{f}_{k-1}$  be eigenvectors.

Leave out the eigenvector  $\mathbf{f}_0$  and use the next  $m$  lowest eigenvectors for embedding in an  $m$ -dimensional Euclidean space.

# Connection to Markov Chain

- $L = D - W$
- $P = I - D^{-1}L = D^{-1}W$  is a markov matrix
- $v$  is generalized eigenvector of  $L$ :  $L v = \lambda D v$
- $v$  is also a right eigenvector of  $P$  with eigenvalue  $1 - \lambda$
- $P$  is **lumpable** iff  $v$  is piece-wise constant
- So Laplacian eigenmaps have Markov Chain interpretations (Diffusion Map)

# Another choice of eigenmaps

- Normalized positive semi-definite Laplacian

$$L_n = D^{-1/2}(D - W)D^{-1/2} = I - D^{-1/2}WD^{-1/2}$$

- $\phi_i$  is an eigenvector of  $L_n$  with eigenvalue  $\lambda_i$
- Laplacian eigenmap/Diffusion map:

$$Y = \begin{pmatrix} \lambda_1^{1/2} \phi_1 & \lambda_2^{1/2} \phi_2 & \dots & \lambda_d^{1/2} \phi_d \end{pmatrix}$$

- $D^{1/2} v_i = \phi_i$
- Why not this eigenmap? Which eigenvector shall we use?

# Generalized Heat Kernels

- Find Gaussian kernel
- Normalize kernel

$$K_\varepsilon(x,y) = \exp\left(-\frac{\|x-y\|^2}{\varepsilon^2}\right)$$

$$K^{(\alpha)}(x,y) = \frac{K_\varepsilon(x,y)}{p^\alpha(x)p^\alpha(y)} \quad \text{where} \quad p(x) = \int K_\varepsilon(x,y)d\mu(y)$$

- Renormalized kernel

$$A_\varepsilon(x,y) = \frac{K^{(\alpha)}(x,y)}{\sqrt{d^{(\alpha)}(x)}\sqrt{d^{(\alpha)}(y)}} \quad \text{where} \quad d^{(\alpha)}(x) = \int K^{(\alpha)}(x,y)d\mu(y)$$

- $\alpha=1$ , Laplacian-Beltrami operator, separate geometry from density
- $\alpha=0$ , classical normalized graph Laplacian

# General Diffusion Map

- P.S.D. Radial basis kernel

$$K_\varepsilon(x,y) = h\left(\frac{\|x-y\|^2}{\varepsilon^2}\right)$$

- Normalize kernel

$$K^{(\alpha)}(x,y) = \frac{K_\varepsilon(x,y)}{p^\alpha(x)p^\alpha(y)} \quad \text{where} \quad p(x) = \int K_\varepsilon(x,y)d\mu(y)$$

- Markov kernel

$$a_\varepsilon^{(\alpha)}(x,y) = \frac{K^{(\alpha)}(x,y)}{d^{(\alpha)}(x)} \quad \text{where} \quad d^{(\alpha)}(x) = \int K^{(\alpha)}(x,y)d\mu(y)$$

- Diffusion Operator:

$$A_\varepsilon^{(\alpha)}f(x) = \int a_\varepsilon^{(\alpha)}(x,y)f(y)p(y)dy, \quad p(x) = \frac{\exp(-U(x))}{Z}$$

$$\Delta_\varepsilon^{(\alpha)} = \frac{I - A_\varepsilon^{(\alpha)}}{\varepsilon}$$

# Convergence of Diffusion Map

## [Coifman-Lafon 2005]

- Uniform sampling: Laplacian eigenmap converges to Laplacian-Beltrami operators [Belkin-Niyogi]
- Nonuniform sampling with  $p(x)$ 
  - $\alpha=1$ :  $\Delta_\varepsilon^{(1)} = \frac{I - A_\varepsilon^{(1)}}{\varepsilon} = \Delta_0 + O(\varepsilon^{1/2})$  where  $\Delta_0$  is Laplacian-Beltrami operator on Riemannian manifolds
  - $\alpha=1/2$ : backward Fokkar-Planck operator
  - $\alpha=0$ : classical normalized graph laplacian

# Convergence Theorem

## [Coifman-Lafon 2006]

**Theorem 7.1.** Let  $\mathcal{M} \in \mathbb{R}^p$  be a compact smooth submanifold,  $q(x)$  be a probability density on  $\mathcal{M}$ , and  $\Delta_{\mathcal{M}}$  be the Laplacian-Beltrami operator on  $\mathcal{M}$ .

$$(67) \quad \lim_{t \rightarrow 0} L_{t,\alpha} = \frac{\Delta_{\mathcal{M}}(fq^{1-\alpha})}{q^{1-\alpha}} - \frac{\Delta_{\mathcal{M}}(q^{1-\alpha})}{q^{1-\alpha}}.$$

This suggests that

- for  $\alpha = 1$ , it converges to the Laplacian-Beltrami operator  $\lim_{t \rightarrow 0} L_{t,1} = \Delta_{\mathcal{M}}$ ;
- for  $\alpha = 1/2$ , it converges to a Schrödinger operator whose conjugation leads to a forward Fokker-Planck equation;
- for  $\alpha = 0$ , it is the normalized graph Laplacian.

# Hessian LLE

- Laplacian LLE

$$f^T L f = \sum_{i \geq j} w_{ij} (f_i - f_j)^2 \geq 0 \sim \int \|\nabla_M f\|^2 = \int (\text{trace}(f^T \mathcal{H} f))^2$$

where  $\mathcal{H} = [\partial^2 / \partial_i \partial_j] \in \mathbb{R}^{d \times d}$  is the Hessian matrix.

- Hessian LLE

$$\min \int \|\mathcal{H} f\|^2, \quad \|f\| = 1$$

- Laplacian kernel: const + linear + bilinear
- Hessian kernel: const + linear functions

Note that:  $\Delta(f) = \text{trace}(H(f))$

# Hessian LLE Algorithm (I)

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## Algorithm 3: Hessian LLE Algorithm

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**Input:** A weighted undirected graph  $G = (V, E, d)$  such that

- 1  $V = \{x_i \in \mathbb{R}^p : i = 1, \dots, n\}$
- 2  $E = \{(i, j) : \text{if } j \text{ is a neighbor of } i, \text{ i.e. } j \in \mathcal{N}_i\}$ , e.g.  $k$ -nearest neighbors

**Output:** Euclidean  $k$ -dimensional coordinates  $Y = [y_i] \in \mathbb{R}^{k \times n}$  of data.

- 3 **Step 1:** Compute local PCA on neighborhood of  $x_i$ , for,

$$\tilde{X}^{(i)} = [x_{i_1} - \mu_i, \dots, x_{i_k} - \mu_i]^{p \times k} = \tilde{U}^{(i)} \tilde{\Sigma} (\tilde{V}^{(i)})^T, \quad x_{i_j} \in \mathcal{N}(x_i),$$

where  $\mu_i = \sum_{j=1}^k x_{i_j} = \frac{1}{k} X_i \mathbf{1}$ ,  $\tilde{U}^{(i)} = [\tilde{U}_1^{(i)}, \dots, \tilde{U}_k^{(i)}]$  is an approximate tangent space at  $x_i$ ;

Continued...

# Hessian LLE Algorithm (II)

4 **Step 2:** Hessian estimation, assumed  $d$ -dimension: define

$$M = [1, \tilde{V}_1, \dots, \tilde{V}_k, \tilde{V}_1 \tilde{V}_2, \dots, \tilde{V}_{d-1} \tilde{V}_d] \in \mathbb{R}^{k \times (1+d+\binom{d}{2})}$$

where  $\tilde{V}_i \tilde{V}_j = [\tilde{V}_{ik} \tilde{V}_{jk}]^T \in \mathbb{R}^k$  denotes the elementwise product (Hadamard product) between vector  $\tilde{V}_i$  and  $\tilde{V}_j$ . Now we perform a Gram-Schmidt Orthogonalization procedure on  $M$ , get

$$\tilde{M} = [1, \hat{v}_1, \dots, \hat{v}_k, \hat{w}_1, \hat{w}_2, \dots, \hat{w}_{\binom{d}{2}-1}] \in \mathbb{R}^{k \times (1+d+\binom{d}{2})}$$

Define Hessian by

$$[H^{(i)}]^T = [last \quad \binom{d}{2} \quad columns \quad of \quad \tilde{M}]_{k \times \binom{d}{2}}$$

as the first  $d + 1$  columns of  $\tilde{M}$  consists an orthonormal basis for the kernel of Hessian.

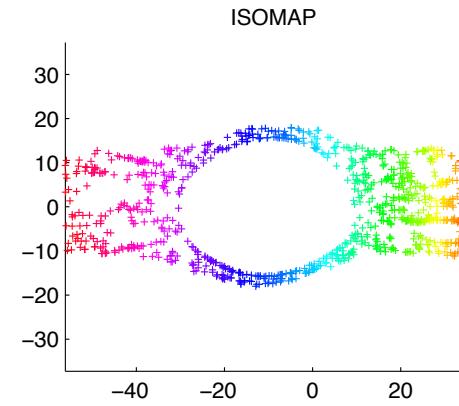
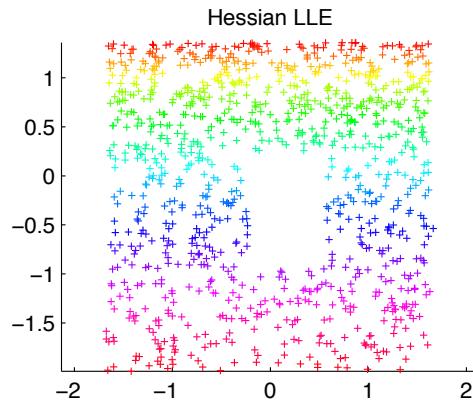
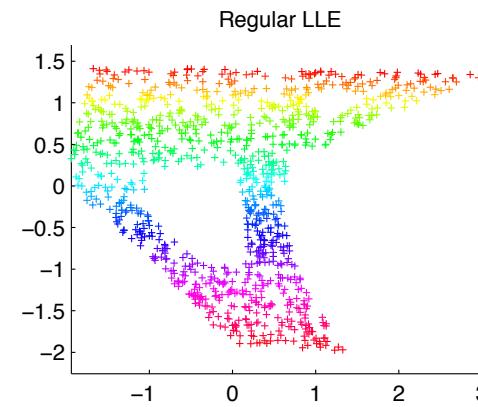
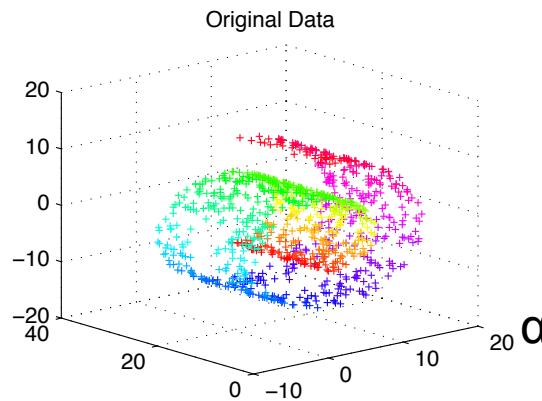
5 **Step 3:** Define

$$K = \sum_{i=1}^n S^{(i)} H^{(i)T} H^{(i)} S^{(i)T} \in \mathbb{R}^{n \times n}, \quad [x_1, \dots, x_n] S^{(i)} = [x_{i_1}, \dots, x_{i_k}],$$

find smallest  $d + 1$  eigenvectors of  $K$  and drop the smallest eigenvector, the remaining  $d$  eigenvectors will give rise to a  $d$ -embedding.

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# Comparisons on Swiss Roll with holes



# Two Assumptions on ISOMAP

- (ISO1)** *Isometry.* The mapping  $\psi$  preserves geodesic distances. That is, define a distance between two points  $m$  and  $m'$  on the manifold according to the distance travelled by a bug walking along the manifold  $M$  according to the shortest path between  $m$  and  $m'$ . Then the isometry assumption says that

$$G(m, m') = |\theta - \theta'|, \quad \forall m \leftrightarrow \theta, m' \leftrightarrow \theta',$$

where  $|\cdot|$  denotes Euclidean distance in  $\mathbb{R}^d$ .

- (ISO2)** *Convexity.* The parameter space  $\Theta$  is a convex subset of  $\mathbb{R}^d$ . That is, if  $\theta, \theta'$  is a pair of points in  $\Theta$ , then the entire line segment  $\{(1-t)\theta + t\theta' : t \in (0, 1)\}$  lies in  $\Theta$ .

**Convexity** is hard to meet: consider two balls in an image which never intersect, whose center coordinate space  $(x_1, y_1, x_2, y_2)$  must have a **hole**.

# Relaxations (Donoho-Grimes'2003)

- (LocISO1) *Local Isometry.* In a small enough neighborhood of each point  $m$ , geodesic distances to nearby points  $m'$  in  $M$  are identical to Euclidean distances between the corresponding parameter points  $\theta$  and  $\theta'$ .
- (LocISO2) *Connectedness.* The parameter space  $\Theta$  is a open connected subset of  $\mathbb{R}^d$ .

# Convergence of Hessian LLE (Donoho-Grimes)

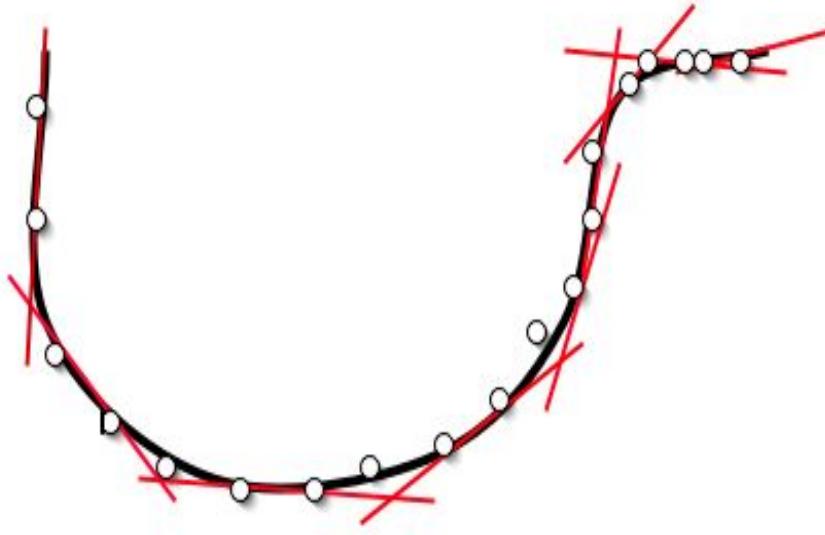
**Theorem 1** Suppose  $M = \psi(\Theta)$  where  $\Theta$  is an open connected subset of  $\mathbb{R}^d$ , and  $\psi$  is a locally isometric embedding of  $\Theta$  into  $\mathbb{R}^n$ . Then  $\mathcal{H}(f)$  has a  $d+1$  dimensional nullspace, consisting of the constant function and a  $d$ -dimensional space of functions spanned by the original isometric coordinates.

We give the proof in Appendix A.

**Corollary 2** Under the same assumptions as Theorem 1, the original isometric coordinates  $\theta$  can be recovered, up to a rigid motion, by identifying a suitable basis for the null space of  $\mathcal{H}(f)$ .

# Local Tangent Space Alignment

Local Tangent space approximation



$$\min_Y \sum_{i \sim j} \|y_i - U_i U_j^T y_j\|^2$$

where  $U_i$  is a local PCA basis for tangent space at point  $x_i \in \mathbb{R}^p$ .

# LTSA Algorithm (Zha-Zhang'05)

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## Algorithm 4: LTSA Algorithm

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**Input:** A weighted undirected graph  $G = (V, E, d)$  such that

- 1  $V = \{x_i \in \mathbb{R}^p : i = 1, \dots, n\}$
- 2  $E = \{(i, j) : \text{if } j \text{ is a neighbor of } i, \text{ i.e. } j \in \mathcal{N}_i\}$ , e.g.  $k$ -nearest neighbors

**Output:** Euclidean  $k$ -dimensional coordinates  $Y = [y_i] \in \mathbb{R}^{k \times n}$  of data.

- 3 **Step 1:** Compute local PCA on neighborhood of  $x_i$ ,  $x_{i_j} \in \mathcal{N}(x_i)$ ,

$$\tilde{X}^{(i)} = [x_{i_1} - \mu_i, \dots, x_{i_k} - \mu_i]^{p \times k} = \tilde{U}^{(i)} \tilde{\Sigma} (\tilde{V}^{(i)})^T,$$

where  $\mu_i = \sum_{j=1}^k x_{i_j} = \frac{1}{k} X_i \mathbf{1}$ ,  $\tilde{U}^{(i)} = [\tilde{U}_1^{(i)}, \dots, \tilde{U}_k^{(i)}]$  is an approximate tangent space at  $x_i$ . Define

$$G_i = [1/\sqrt{k}, \tilde{V}_1^{(i)}, \dots, \tilde{V}_d^{(i)}]^{k \times (d+1)};$$

- 4 **Step 2:** Alignment (kernel) matrix

$$K^{n \times n} = \sum_{i=1}^n S_i W_i W_i^T S_i^T, \quad W_i^{k \times k} = I - G_i G_i^T,$$

where selection matrix  $S_i^{n \times k} : [x_{i_1}, \dots, x_{i_k}] = [x_1, \dots, x_n] S_i^{n \times k}$ ;

- 5 **Step 3:** Find smallest  $d + 1$  eigenvectors of  $K$  and drop the smallest eigenvector, the remaining  $d$  eigenvectors will give rise to a  $d$ -embedding.
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# From LTSA to Connection Laplacian

LTSA (Zhang-Zha'05):

$$\min_Y \sum_{i \sim j} \|y_i - U_i U_j^T y_j\|^2$$

where  $U_i$  is a local PCA basis for tangent space at point  $x_i \in \mathbb{R}^p$ .

Vector Connection Laplacian (Singer-Wu'11):

$$\min_Y \sum_{i \sim j} \|y_i - O_{ij} y_j\|^2, \quad O_{ij} = \arg \min_O \|U_i - O_{ij} U_j\|^2$$

where  $U_i$  is a local PCA basis for tangent space at point  $x_i \in \mathbb{R}^p$ .

# Comparisons of Manifold Learning Techniques

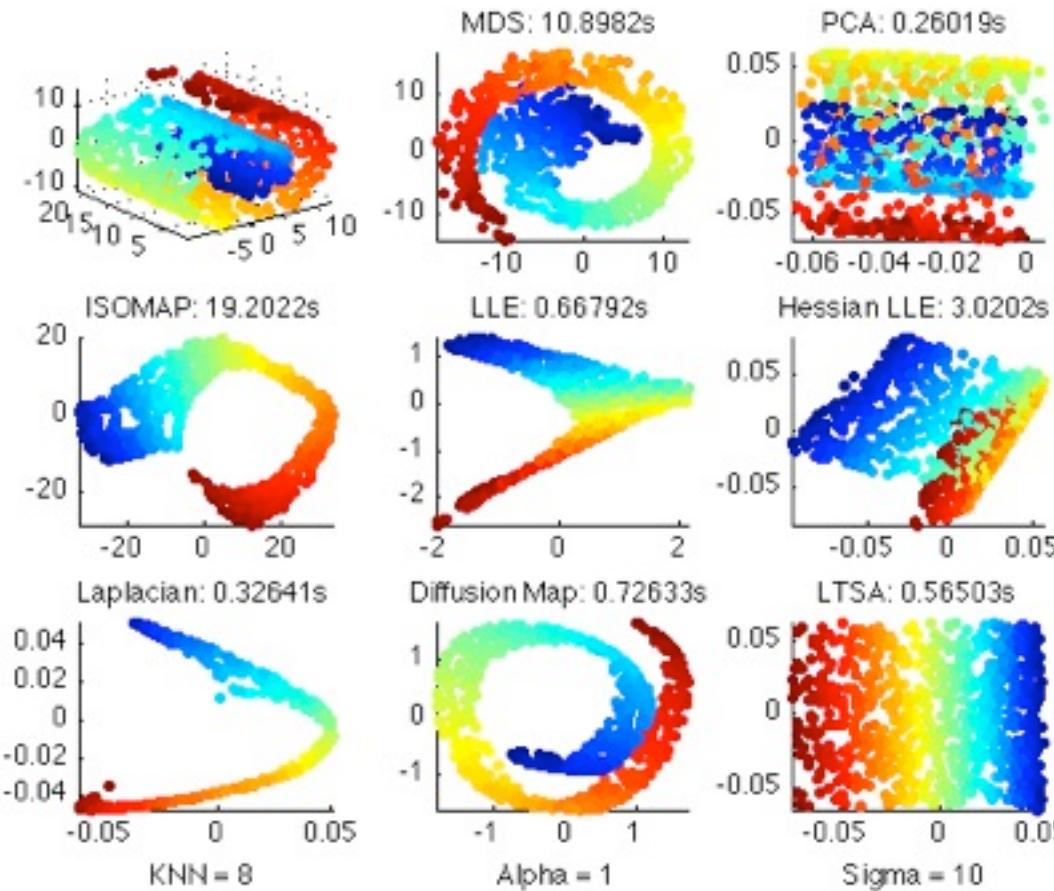
- MDS
- PCA
- ISOMAP
- LLE
- Hessian LLE
- Laplacian LLE
- Diffusion Map
- Local Tangent Space Alignment
- Matlab codes: mani.m

Courtesy of Todd Wittman

# How To Compare

- Speed
- Manifold Geometry
- Non-convexity
- Curvature
- Corners
- High-Dimensional Data: *Can the method process image manifolds?*
- Sensitivity to Parameters
  - K Nearest Neighbors: *Isomap, LLE, Hessian, Laplacian, KNN Diffusion*
  - Sigma: *Diffusion Map, KNN Diffusion*
- Noise
- Non-uniform Sampling
- Sparse Data
- Clustering

# Speed on Swiss Roll



Now go to Todd Wittman's slides, page 13th...

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