Advanced Introduction to Machine Learning, CMU-10715

Manifold Learning

Barnabás Póczos



Motivation

 Find meaningful low-dimensional structures hidden in high-dimensional observations.

The human brain confronts the same problem in perception: 30,000 auditory nerve fibers 10⁶ optic nerve fibers

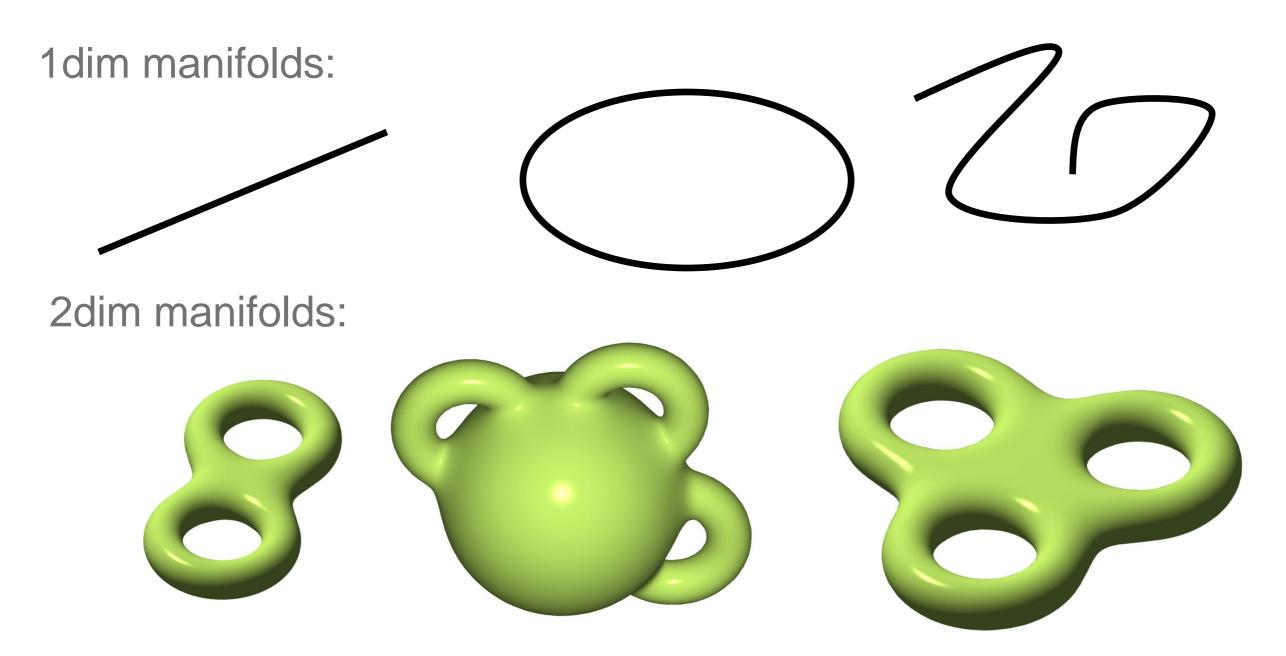
⇒ extract small number of perceptually relevant features.

 Difficult to visualize data in dimensions greater than three.

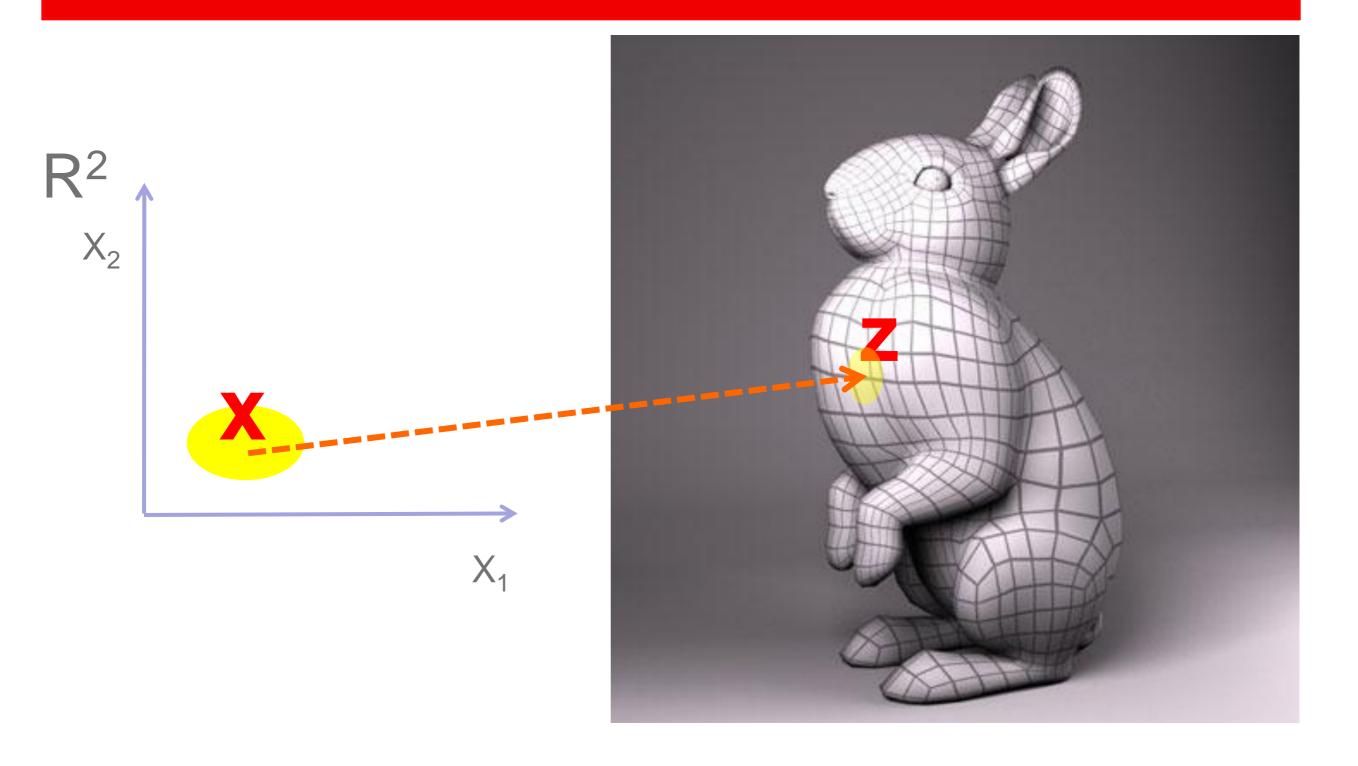
Manifolds

Informal definition:

Manifold = any object which is nearly "flat" on small scales.



Manifold Learning

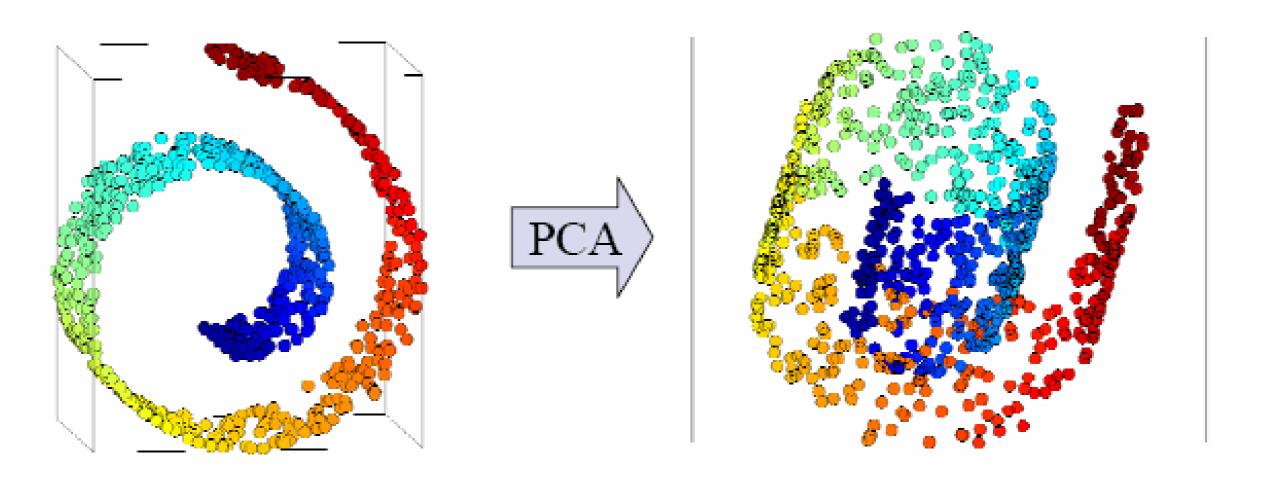


Algorithms

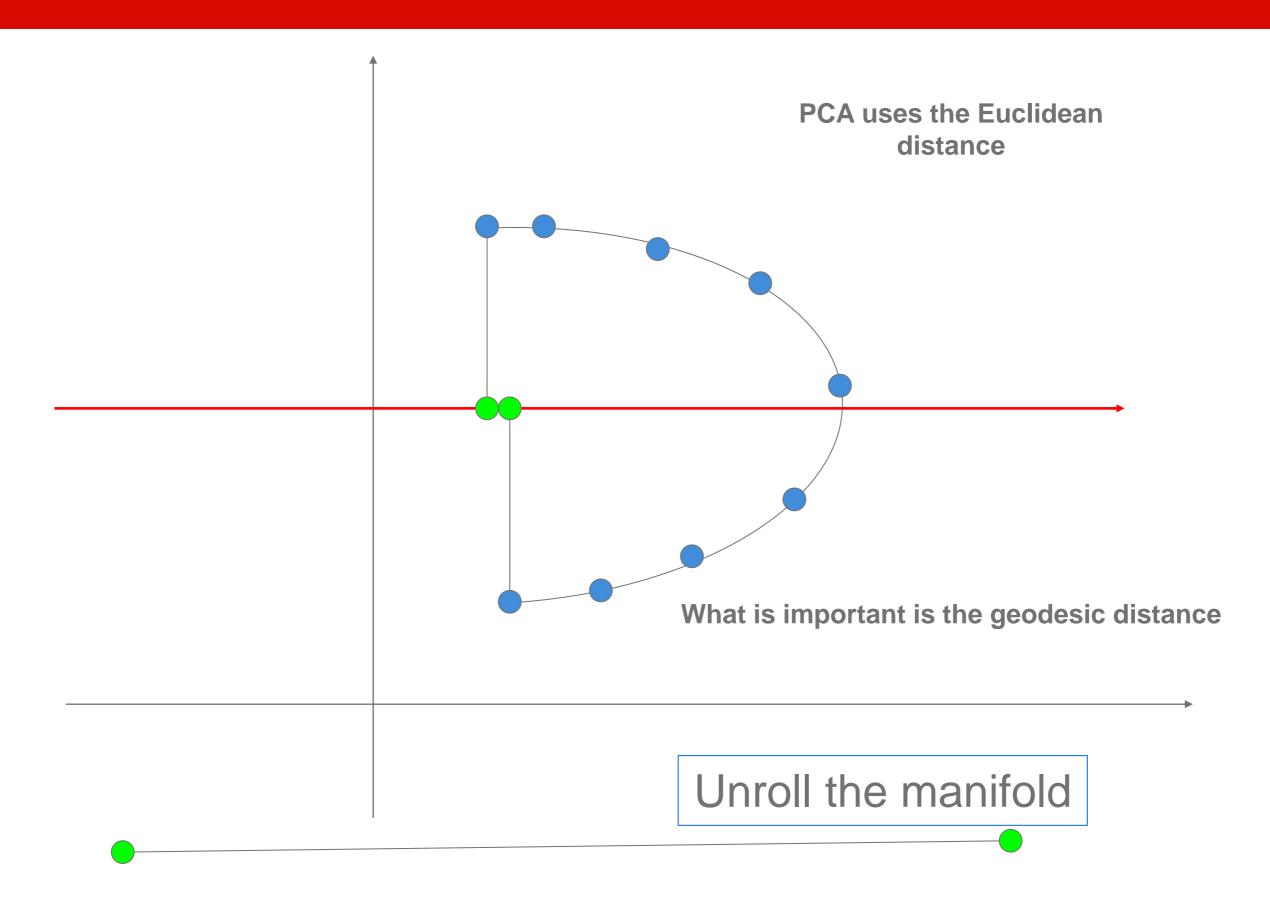
- PCA (1901), kernel PCA
- Multi-dimensional Scaling (1952)
- Maximum Variance Unfolding, Colored MVU
- Mixture of PCA, Mixture of Factor Analyzers
- Local Linear Embedding (2000)
- Isomap (2000), C-Isomap
- Hessian Eigenmaps
- Laplacian Eigenmaps (2003)
- Local Tangent Space Alignment
- ... and many more

PCA

PCA is a linear method: it fails to find the nonlinear structure in the data



Issues with PCA



Multi-dimensional Scaling

Multi-dimensional Scaling

☐ In PCA we are given a set of points

$$X = [x_1, \dots, x_n] \in \mathbb{R}^{l \times n}$$

☐ In MDS we are given pairwise distances instead

of the actual data points.

Question: If we only preserve the pairwise distances do we preserve the structure?

From Distances to Inner Products

$$d_{ij}^2 = d_{ki}^2 + d_{kj}^2 - 2d_{ki}d_{kj}cos(\alpha)$$

$$b_{ij} = d_{ki}d_{kj}cos(\alpha)$$

$$A_{ij}$$

$$A_{ki}$$

$$A_{kj}$$

$$A_{kj}$$

$$A_{kj}$$

$$A_{kj}$$

$$b_{ij} = \frac{1}{2}(d_{ki}^2 + d_{kj}^2 - d_{ij}^2) = \langle X_i - X_k, X_j - X_k \rangle$$

From Distances to Inner Products

Similarly:

Center the data and then calculate $\langle x_i, x_j \rangle$

$$\langle x_i, x_j \rangle = G_{ij} = -\frac{1}{2} \left[d_{ij}^2 - \frac{1}{n} \sum_{l=1}^n d_{il}^2 - \frac{1}{n} \sum_{m=1}^n d_{mj}^2 + \frac{1}{n^2} \sum_{o=1}^n \sum_{p=1}^n d_{op}^2 \right]$$

MDS cost function:

$$J_{MDS}(y_1,\ldots,y_n) = \sum_{i,j} (\langle x_i,x_j\rangle - \langle y_i,y_j\rangle)^2$$

From Distances to Inner Products

MDS algorithm:

Step 1: Build a Gram matrix of inner products

$$X = [x_1, \dots, x_n] \in \mathbb{R}^{l \times n}$$
$$G = \{\langle x_i, x_j \rangle\}_{i,j} = X^T X \in \mathbb{R}^{n \times n}$$

Step 2: Find the top k eigenvectors of G

$$[\psi_1,\ldots,\psi_k] \in \mathbb{R}^{n \times k}$$

with the top k eigenvalues: $\Lambda = diag(\lambda_1, \dots, \lambda_k) \in \mathbb{R}^{k \times k}$

Step 3:
$$[y_1,\ldots,y_n]= \Lambda^{1/2}[\psi_1,\ldots,\psi_k]^T \in \mathbb{R}^{k\times n}$$

Metric MDS = PCA

Observation: If the data is centered, then the Gram matrix can be found this way:

$$S_{ij} = ||x_i - x_j||^2 \quad u = \frac{1}{\sqrt{n}} [1, \dots, 1]^T$$
$$G = -\frac{1}{2} (I - uu^T) S (I - uu^T)$$

PCA operates on $\frac{1}{n}XX^T \in \mathbb{R}^{l \times l}$

MMD operates on $G = X^T X \in \mathbb{R}^{n \times n}$

Though based on a somewhat different geometric intuition, metric MDS is closely related to PCA.

There are many different versions of MDS...

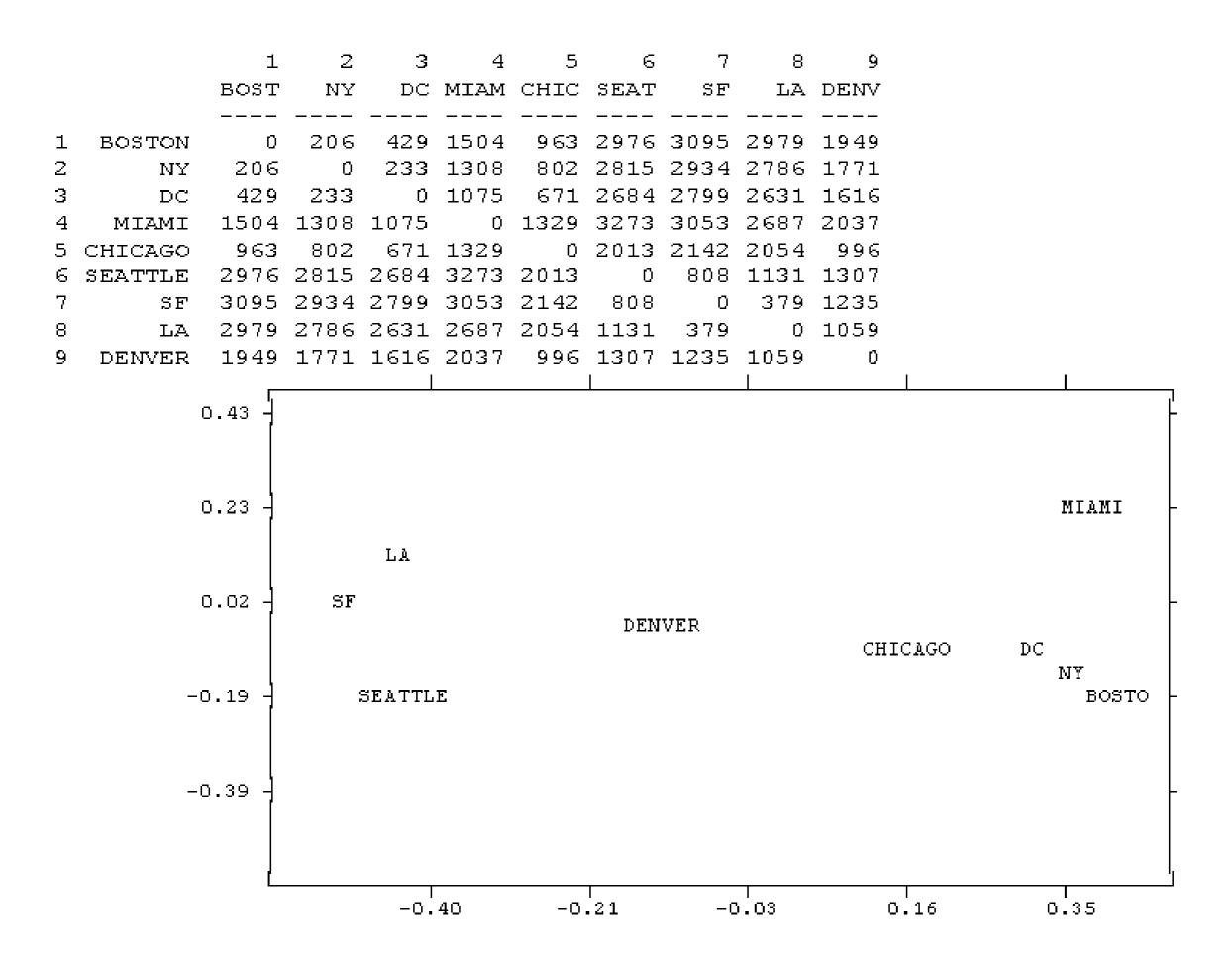


Table 1 Flying Mileages Between 10 American Cities

Atlanta	Chicago	Denver	Houston	Los Angeles	Mianii	New York	San Francisco	Seattle	Washington, DC	
0	587	1212	701	1936	604	748	2139	2182	543	Atlanta
5B7	0	920	940	1745	1188	713	1858	1737	597	Chicago
1212	920	0	879	831	1726	1631	949	1021	1494	Denver
701	940	879	Û	1374	968	1420	1645	1891	1220	Houston
1936	1745	831	1374	0	2339	2451	347	959	2300	Los Angeles
604	1188	1726	968	2339	O	1092	2594	2734	923	Miami
748	713	1631	1420	2451	1092	0	2571	2408	205	New York
2139	1858	949	1645	347	2594	2571	0	678	2442	San Francisco
2182	1737	1021	1891	959	2734	2408	678	0	2329	Scattle
543	597	1494	1220	2300	923	205	2442	2329	0	Washington, DC

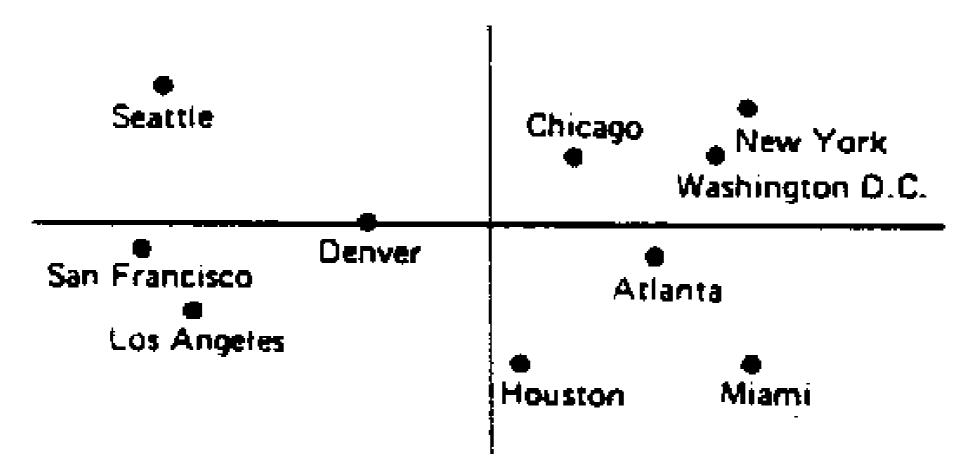


Figure 1 CMDS of flying mileages between 10 American cities.

Isomap

A Global Geometric Framework for Nonlinear Dimensionality Reduction

J. B. Tenenbaum, V. de Silva and J. C. Langford Science 290 (5500): 2319-2323, 22 December 2000

ISOMAP

Comes from Isometric feature mapping

Step1: Take a data matrix as input.

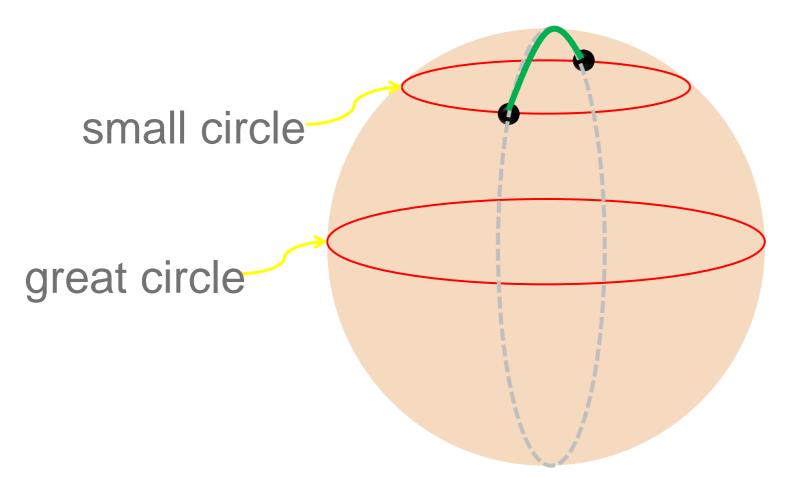
Step2: Estimate geodesic distance between any two points by "a chain of short paths". Approximate the geodesic distance by Euclidean distances.

Step3: Perform MDS

Differential Geometry

Geodesic: the shortest curve on a manifold that connects two points on the manifold

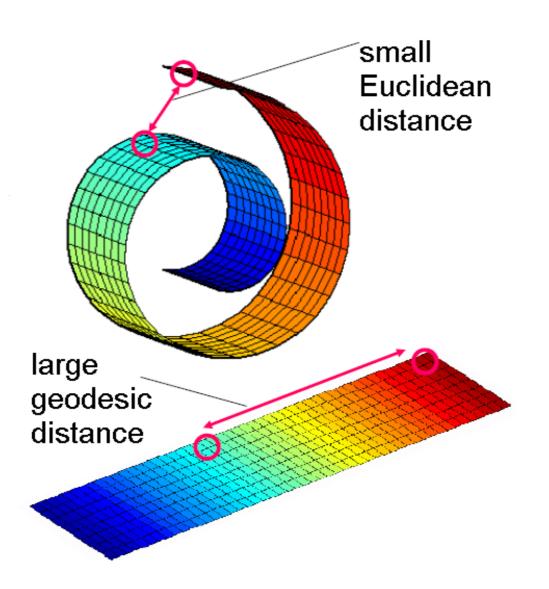
Example (3D sphere)



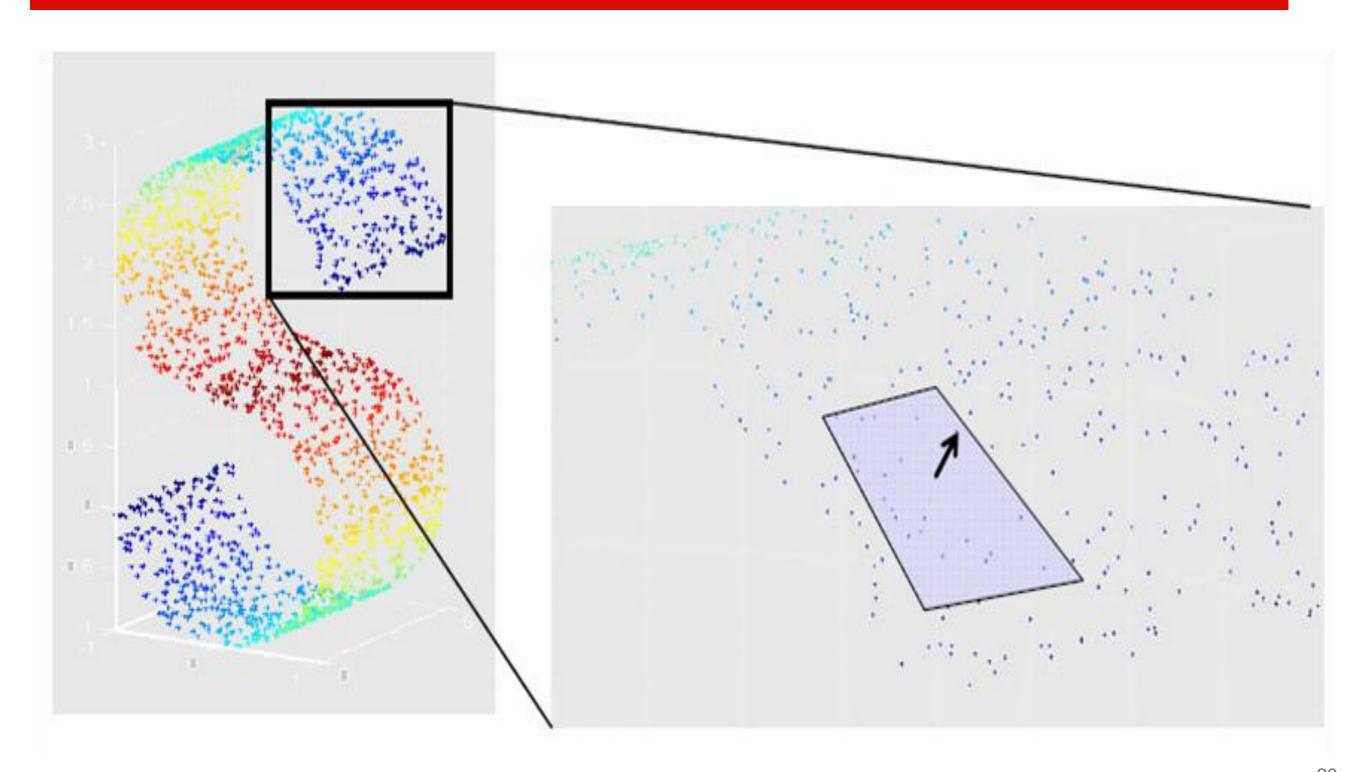
Geodesic distance

Euclidean distance needs not be a good measure between two points on a manifold

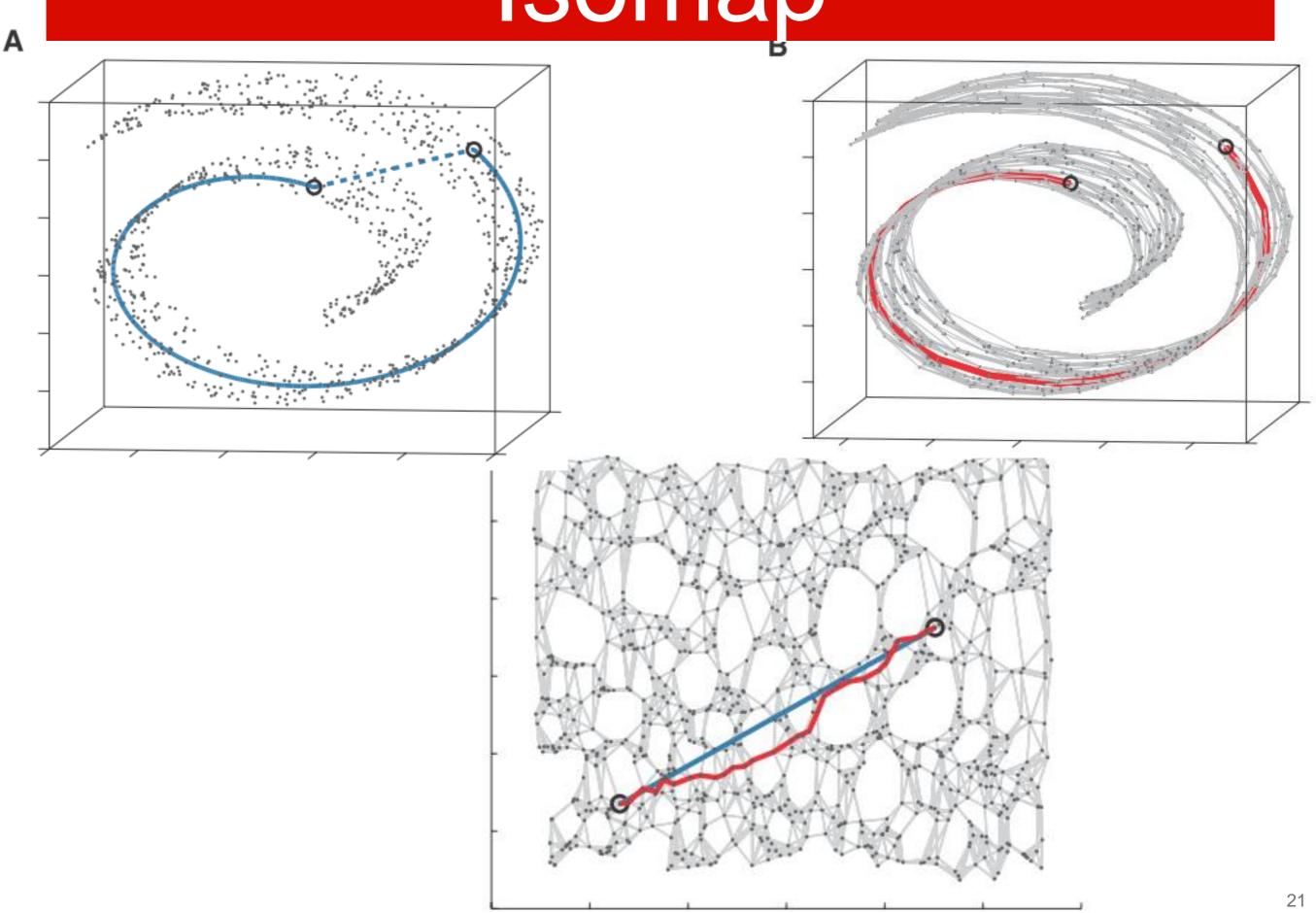
Length of geodesic is more appropriate

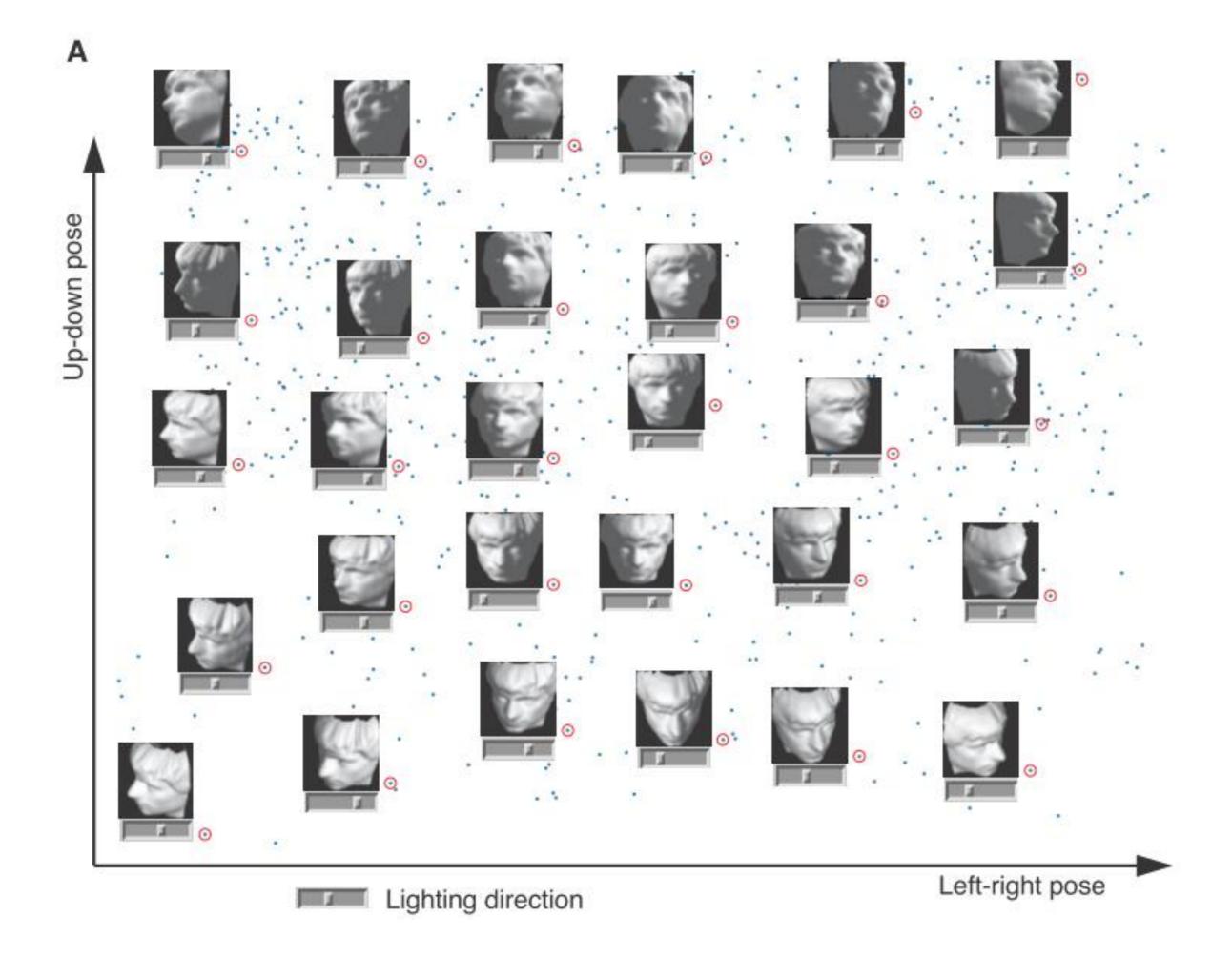


The Swiss-role Dataset



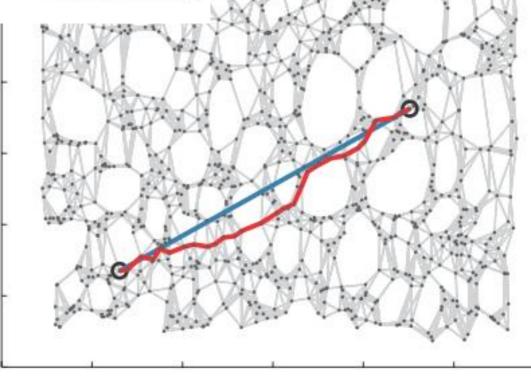
Isomap



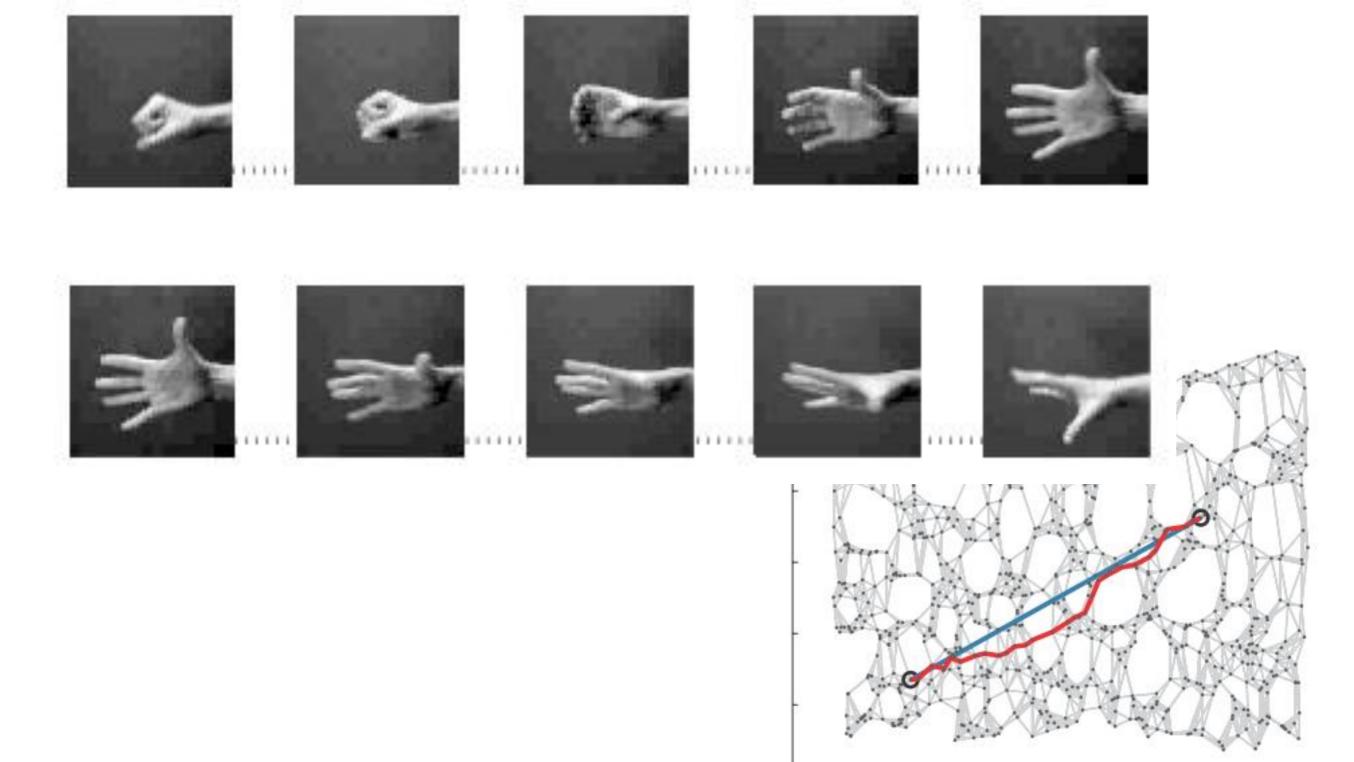


ISOMAP Interpolation



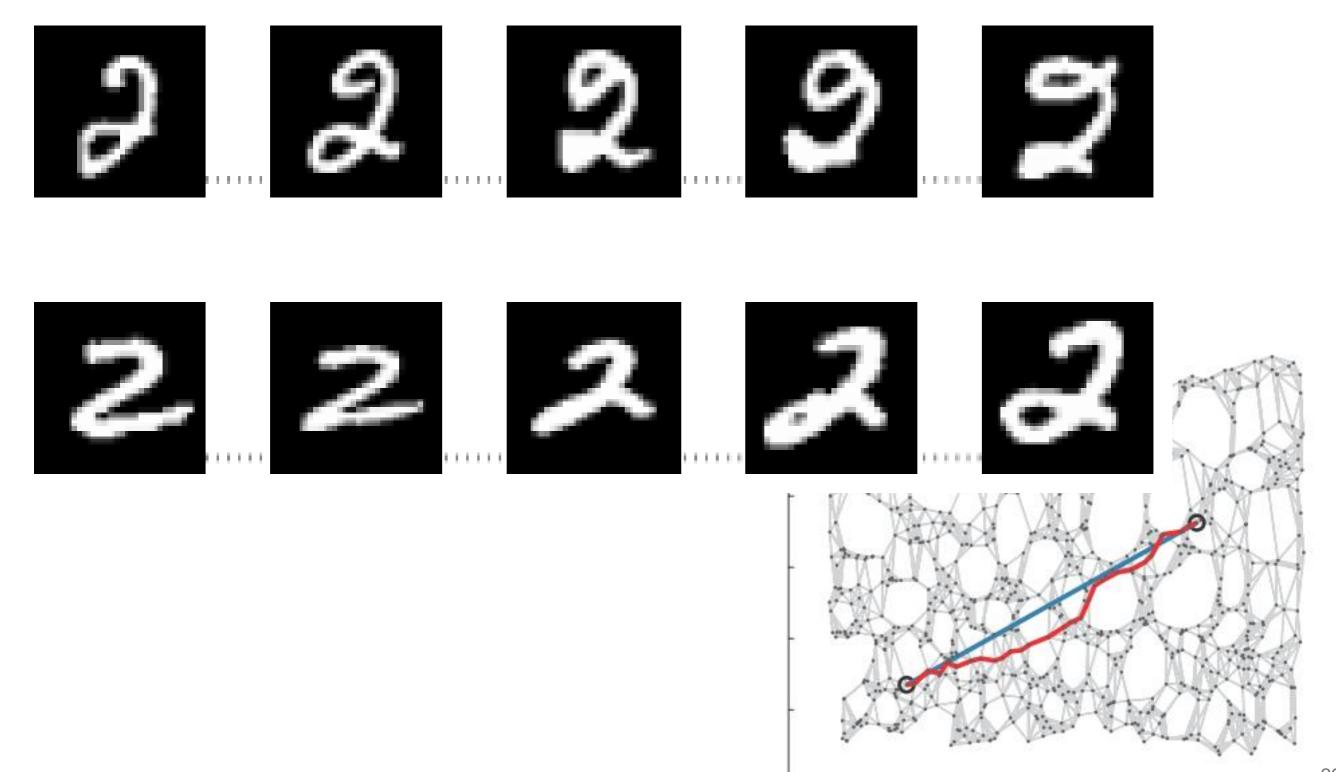


ISOMAP Interpolation



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ISOMAP Interpolation



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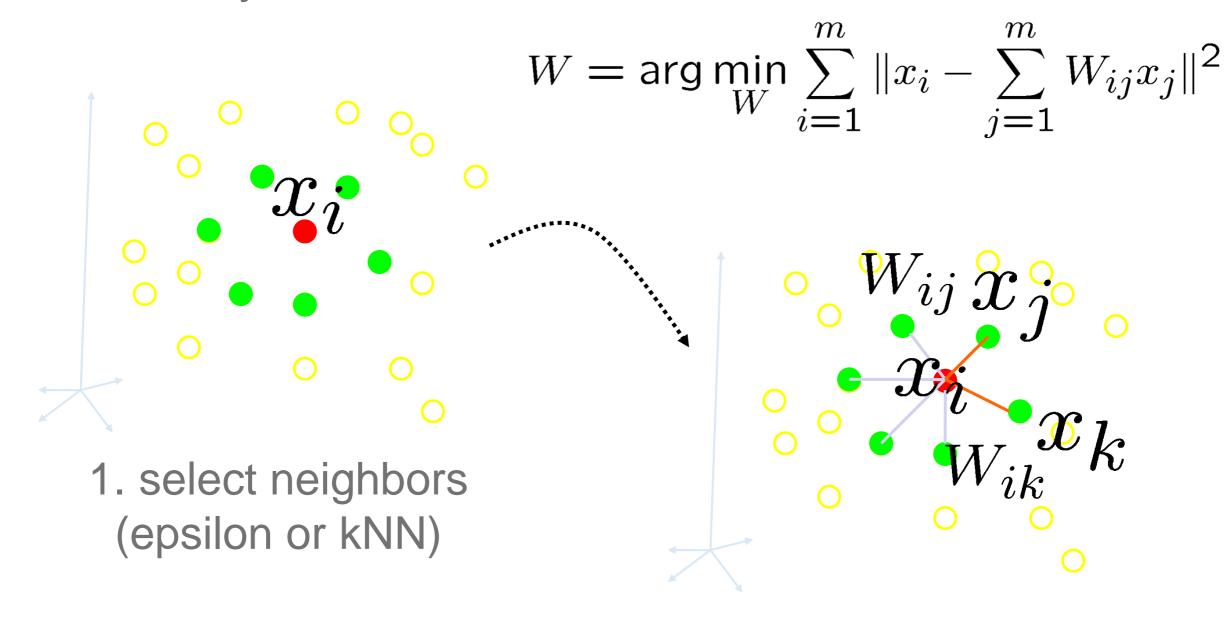
ISOMAP Summary

- ☐ Build graph from kNN or epsilon neighbors
- ☐ Run MDS
- ☐ Since MDS is slow, ISOMAP will be very slow.
- Need estimate of k or epsilon.
- ☐ Assumes data set is convex (no holes).

Nonlinear dimensionality reduction by locally linear embedding.

Sam Roweis & Lawrence Saul. *Science*, v.290 no 5500, Dec.22, 2000. pp.2323--2326.

Assumption: manifold is approximately "linear" when viewed locally. Data: $X = [x_1, \dots, x_m] \in \mathbb{R}^{D \times m}$



2. reconstruct with linear weights

☐ Step 1.

$$W = \arg\min_{W} \sum_{i=1}^{m} ||x_i - \sum_{j=1}^{m} W_{ij} x_j||^2$$

Subject to $\sum_{j} W_{ij} = 1$, $\forall i$, and $W_{ij} = 0$ if x_j is not neighbor of x_i .

Without the constraints the weights that minimize the reconstruction errors are invariant to rotation, rescaling and translation of the data points.

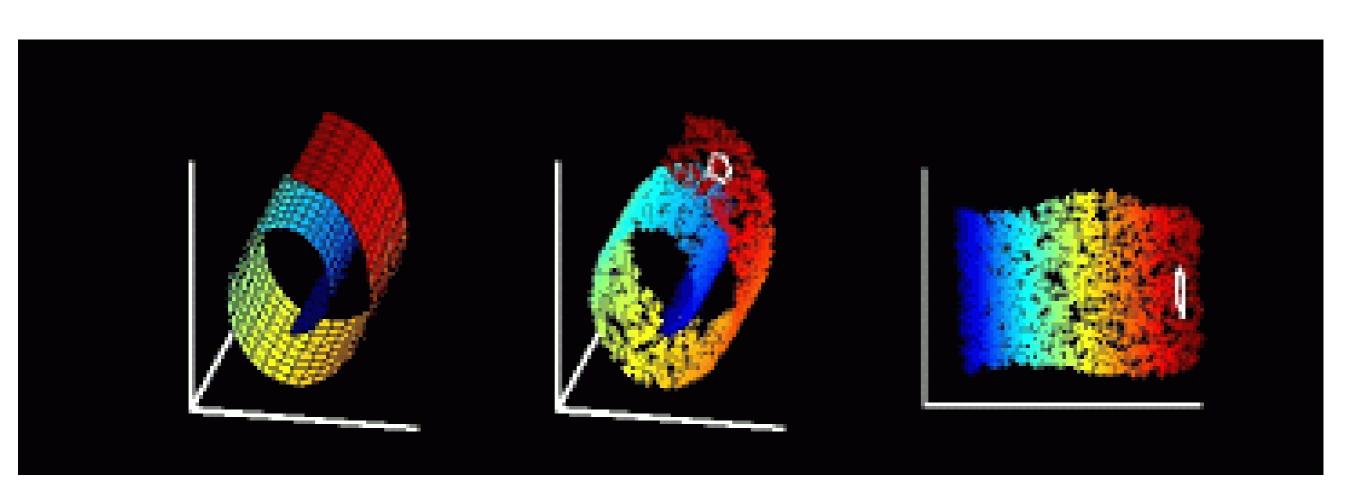
☐ Step 2. Given the weights W, find the embedded points:

$$[z_1, \dots, z_m] = \arg \min_{[z_1, \dots, z_m]} \sum_{i=1}^m ||z_i - \sum_{j=1}^m W_{ij} z_j||^2$$

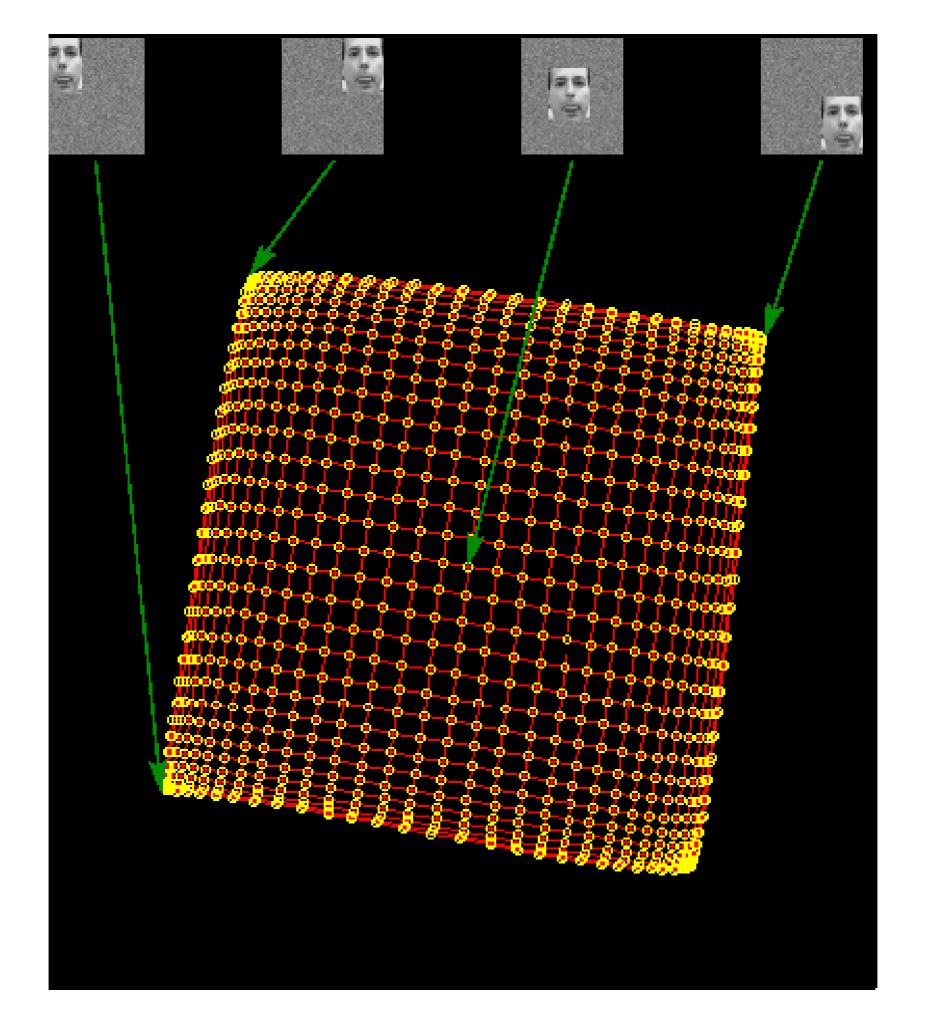
Subject to $\sum_i z_i = 0$ and unit covariance matrix.

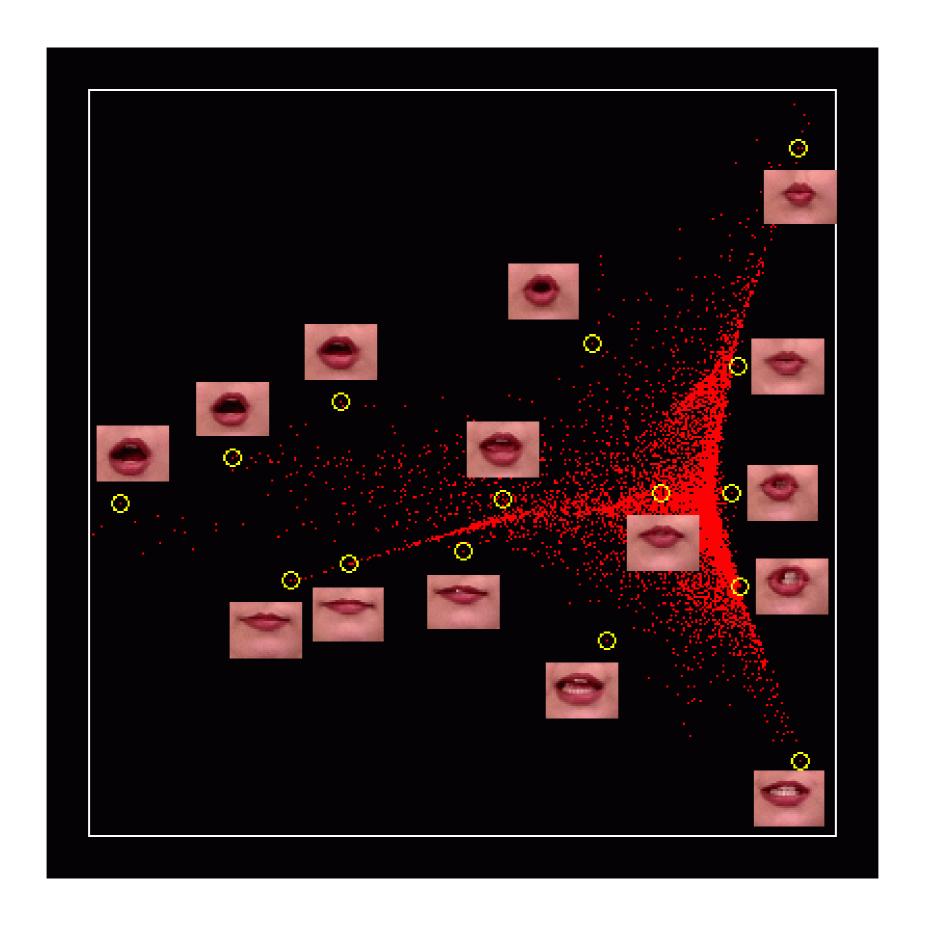
The same weights that reconstruct the data points in D dimensions should also reconstruct the points in d dimensions.

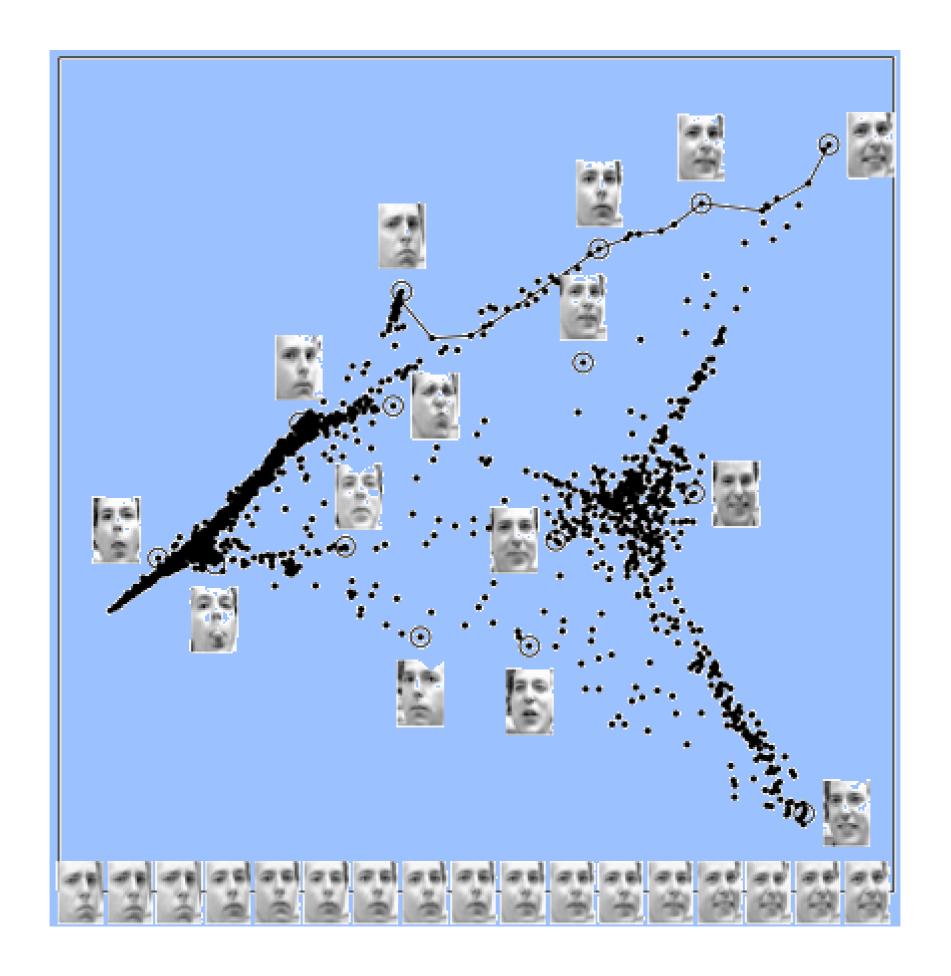
The weights characterize the intrinsic geometric properties of each neighborhood.



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Maximum Variance Unfolding

K. Q. Weinberger and L. K. Saul.
Unsupervised learning of image manifolds by semidefinite programming.

International Journal of Computer Vision, Volume 70 Issue 1, October 2006, Pages 77 - 90

Build a graph from kNN or epsilon neighbors.

Given x_1, \ldots, x_T find y_1, \ldots, y_T such that $\|x_i - x_j\| = \|y_i - y_j\|$ for all $(i, j) \in E$ neighborhood graph and var(y) is as large as possible.

Formally,

$$\max_{y} tr(cov(y))$$

s.t. $\|x_i - x_j\| = \|y_i - y_j\|$ for all $(i, j) \in E$ neighborhood graph

Here
$$tr(cov(y)) = \frac{1}{T} \sum_{i=1}^{T} ||y_i - \bar{y}||^2$$
, where $\bar{y} = \frac{1}{T} \sum_{i=1}^{T} y_i$

$$X=[x_1,\ldots,x_T]\in\mathbb{R}^{D imes T},\ Y=[y_1,\ldots,y_T]\in\mathbb{R}^{d imes T}$$

Let $P=X^TX$, $Q=Y^TY\succeq 0$.

Our goal is to find $Q \succeq 0$. Then with PCA we can find y_1, \ldots, y_T from Q.

Consider the constraint $||x_i - x_j|| = ||y_i - y_j||$

From this, we have
$$\|x_i-x_j\|^2=\|y_i-y_j\|^2$$

$$x_i^Tx_i-2x_i^Tx_j+x_j^Tx_j=y_i^Ty_i-2y_i^Ty_j+y_j^Ty_j$$

$$Q_{ii}-2Q_{ij}+Q_{jj}=P_{ii}-2P_{ij}+P_{jj}$$

Consider the cost function:

$$cov(y) = \frac{1}{T} \sum_{i=1}^{T} (y_i - \bar{y})(y_i - \bar{y})^T$$
$$= \frac{1}{T} \sum_{i=1}^{T} y_i y_i^T - \bar{y} \bar{y}^T$$
$$= \frac{1}{T} YY^T - \frac{1}{T^2} Y \mathbf{1} \mathbf{1}^T Y^T$$

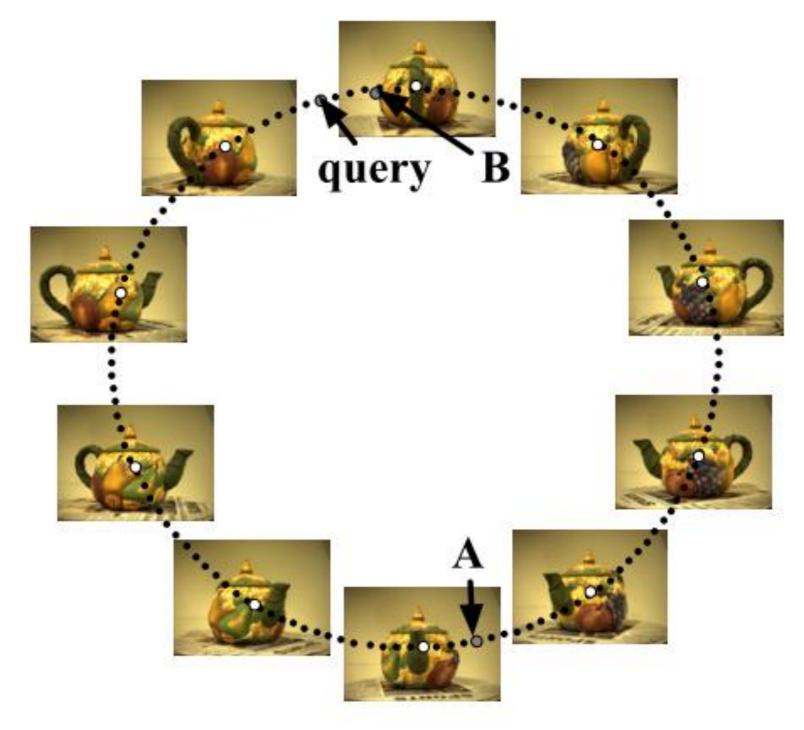
$$tr(cov(y)) = \frac{1}{T}tr(YY^T) - \frac{1}{T^2}tr(Y\mathbf{1}\mathbf{1}^TY^T)$$
$$= \frac{1}{T}tr(YY^T) - \frac{1}{T^2}tr(Y^TY\mathbf{1}\mathbf{1}^T)$$
$$= \frac{1}{T}tr(Q) - \frac{1}{T^2}tr(Q\mathbf{1}\mathbf{1}^T)$$

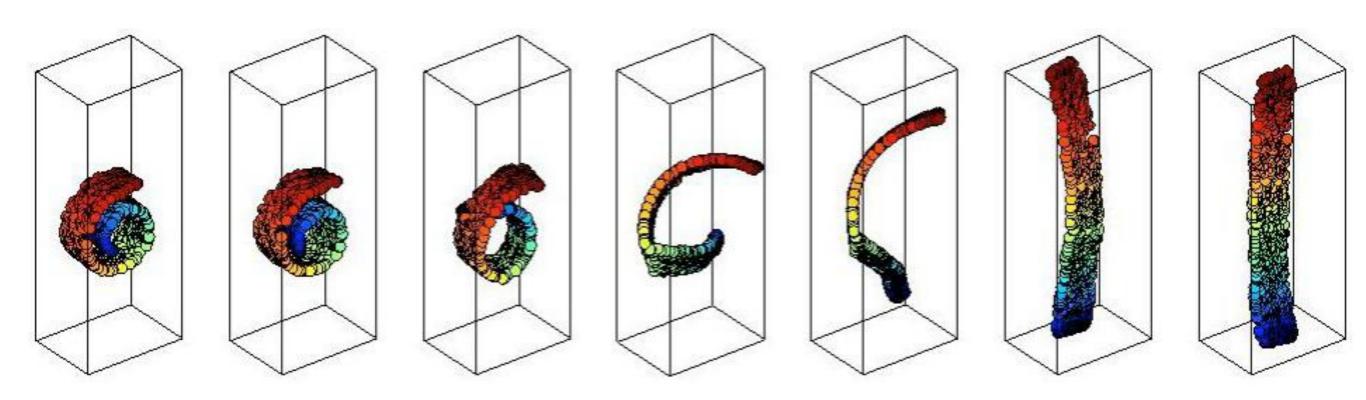
The final problem is a semi-definite problem (SDP):

$$\max_{Q} \frac{1}{T} tr(Q) - \frac{1}{T^2} tr(Q \mathbf{1} \mathbf{1}^T)$$

s.t.
$$Q_{ii} - 2Q_{ij} + Q_{jj} = P_{ii} - 2P_{ij} + P_{jj}$$
 for all $(i, j) \in E$, $Q \succ 0$

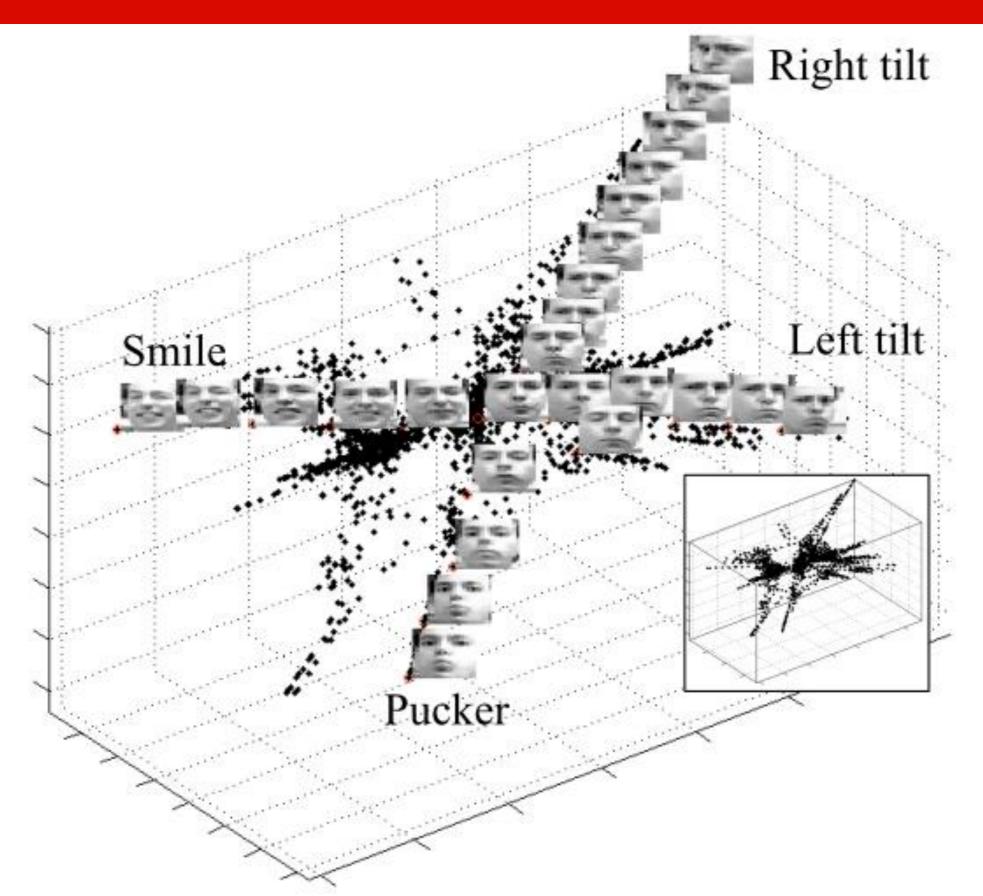
D= 76*101*3 d=3 N=400 images





Swiss roll "unfolded" by maximizing variance subject to constraints that preserve local distances and angles.

The middle snap-shots show various feasible (but non-optimal) intermediate solutions.



M. Belkin and P. Niyogi. "Laplacian eigenmaps for dimensionality reduction and data representation," *Neural Comput.*,15(6):1373–1396, 2003.

Data: $X = [x_1, \dots, x_n] \in \mathbb{R}^{l \times n}$

Step 1. Build graph from kNN or epsilon neighbors

Step 2. Choose weights:

$$W_{ij} = \exp(-\frac{1}{t}||x_i - x_j||^2)$$
 if $(i, j) \in E$
 $W_{ij} = 0$ Otherwise

Special case: $t = \infty$, then $W_{ij} = 1$ if $(i, j) \in E$

Step 3. Assume the graph is connected, otherwise proceed with Step 3 for each connected component:

$$D_{ii} = \sum_{j=1}^{n} W_{ij}$$

$$L = D - W \in \mathbb{R}^{n \times n} \text{ Laplacian matrix}$$

Lemma: L is symmetric, positive semi-definite matrix.

Solve the eigenvector problem:

$$Lf = \lambda Df$$

Solve the eigenvector problem:

$$Lf = \lambda Df \quad f \in \mathbb{R}^n$$

The first m+1 smallest eigenvalues:

$$Lf_0 = \lambda_0 Df_0$$
 $0 = \lambda_0, f_0 = [1, ..., 1]^T \in \mathbb{R}^n$
 $Lf_1 = \lambda_1 Df_1$
:

$$Lf_m = \lambda_m Df_m \quad 0 = \lambda_0 \le \lambda_1 \le \dots \le \lambda_m$$

The embedding:

$$\mathbb{R}^l \ni x_i \to [f_1(i), \dots f_m(i)]^T \in \mathbb{R}^m$$

Laplacian Eigenmap (Explanation)

Let us embed the neighborhood graph to 1 dim first.

A reasonable cost function is:

$$\min_{y_1,...y_n} \sum_{i,j=1}^n (y_i - y_j)^2 W_{ij}$$

subject to appropriate constraints to avoid y=0.

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

Proof: $\sum_{i,j=1}^{n} (y_i - y_j)^2 W_{ij} = \sum_{i,j=1}^{n} (y_i^2 + y_j^2 - 2y_i y_j) W_{ij}$
 $= \sum_{i} y_i^2 D_{ii} + \sum_{j} y_j^2 D_{jj} - 2 \sum_{i,j} y_i y_j W_{ij} = 2y^T L y$

Laplacian Eigenmap (Explanation)

Therefore, our minimization problem is

$$\min_{y=[y_1,...y_n]^T} y^T L y$$

Subject to:

 $y^T D y = 1$ to fix the scaling.

 $y^T D \mathbf{1} = 0$ to avoid the trivial $y = [1, ..., 1]^T$ solution.

Embedding the neighborhood graph to m dimension:

$$\min_{Y^T = [y_1, \dots, y_n] \in \mathbb{R}^{d \times n}} tr(Y^T L Y)$$

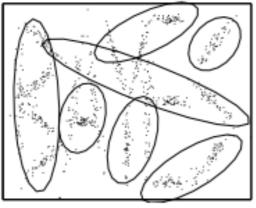
Subject to: $Y^TDY = I$

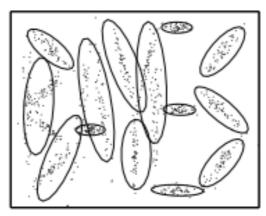
Solution: $LY = \lambda DY$

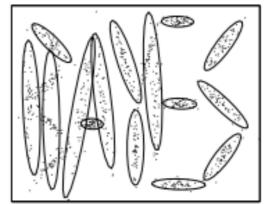
Variational Variational Inference for Bayesian Mixtures of Factor Analysers

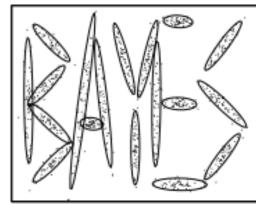
Zoubin Ghahramani, Matthew J. Beal, NIPS 1999

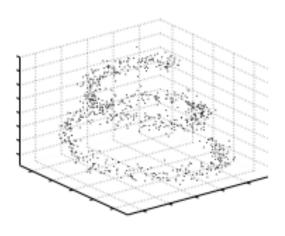


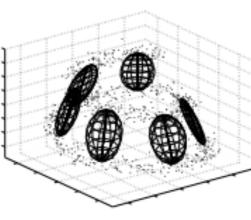


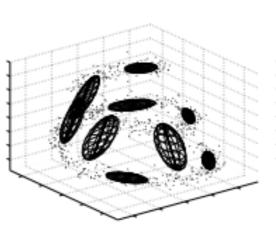


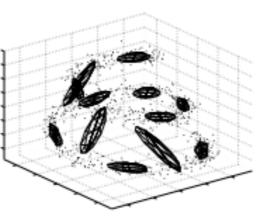


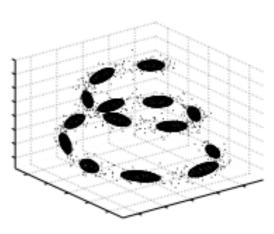








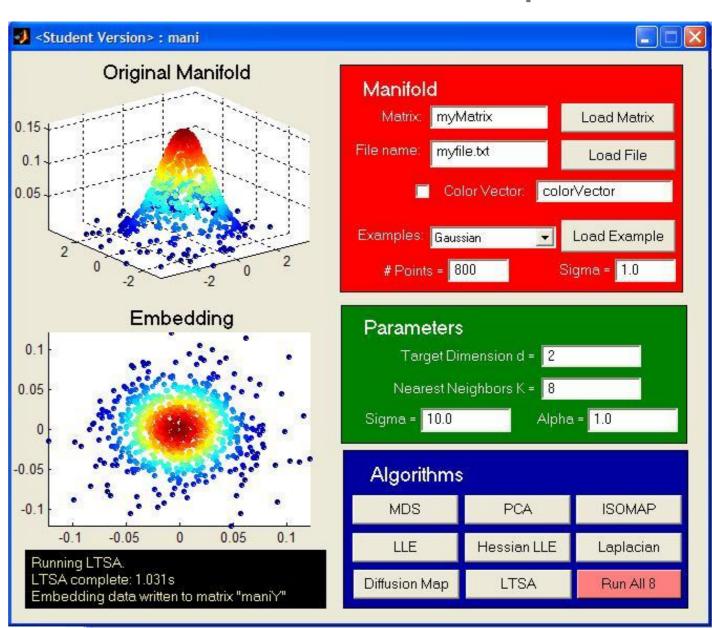




MANI Matlab demo

Todd Wittman: MANIfold learning demonstration GUI Contains a couple of methods and examples.

http://www.math.ucla.edu/~wittman/mani



The following results are taken from Todd Wittman

How do we compare the methods?

- □ Speed
 □ Manifold Geometry
 □ Non-uniform Sampling
 □ Curvature
 □ Corners
 □ Clustering
- ☐ 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

Testing Examples

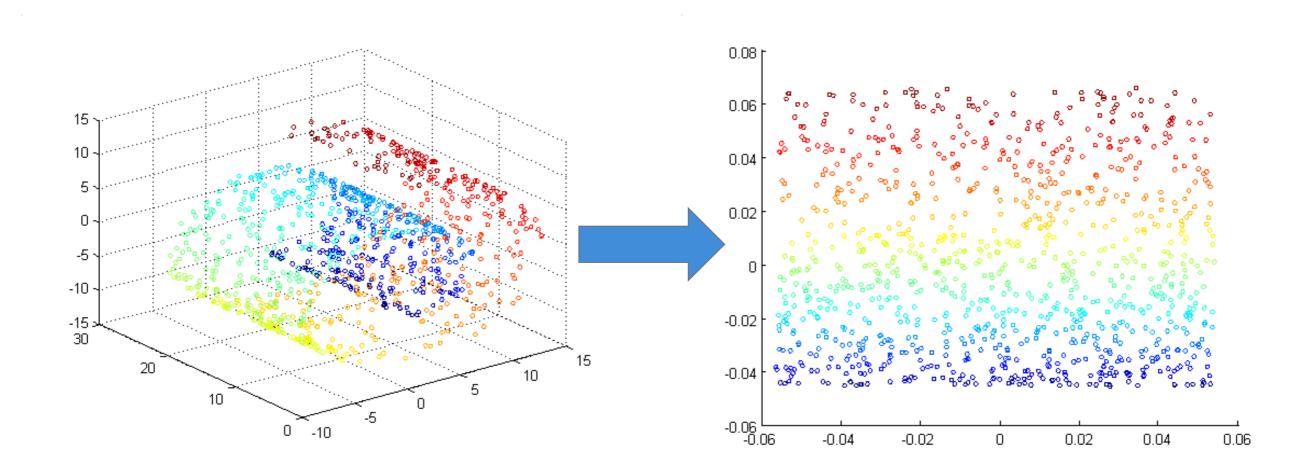
- □ Swiss Roll
- Swiss Hole
- Punctured Sphere
- Corner Planes
- □ 3D Clusters

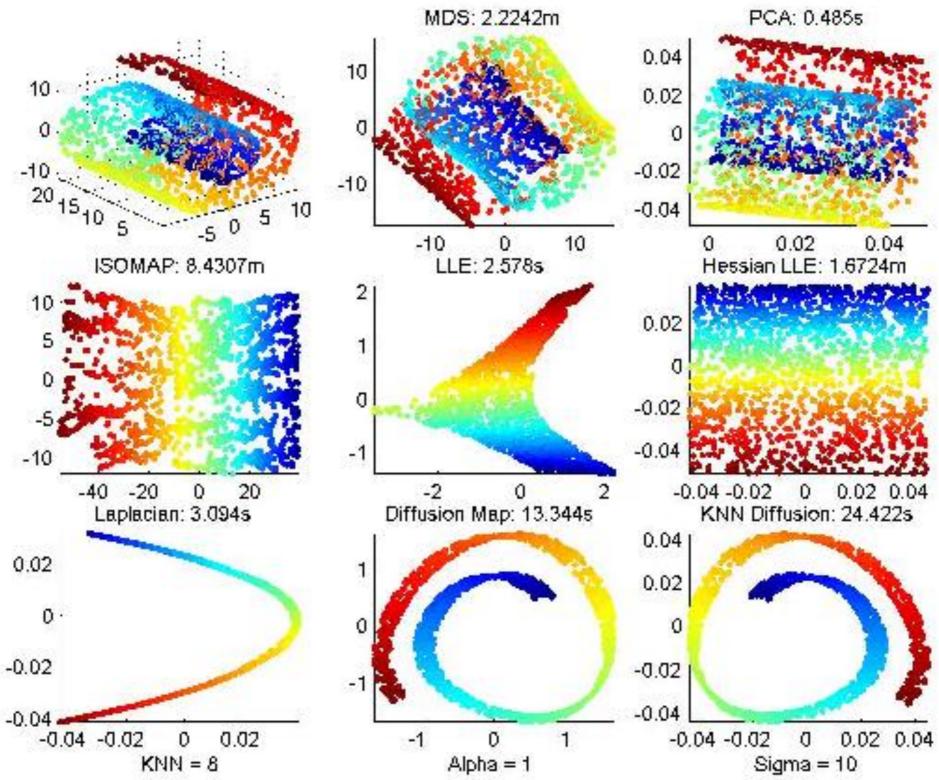
- Twin Peaks
- ☐ Toroidal Helix
- ☐ Gaussian
- □ Occluded Disks

We'll compare the speed and sensitivity to parameters throughout.

Manifold Geometry

First, let's try to unroll the Swiss Roll. We should see a plane.





Hessian LLE is pretty slow, MDS is very slow, and ISOMAP is extremely slow.

MDS and PCA don't can't unroll Swiss Roll, use no manifold information.

LLE and Laplacian can't handle this data.

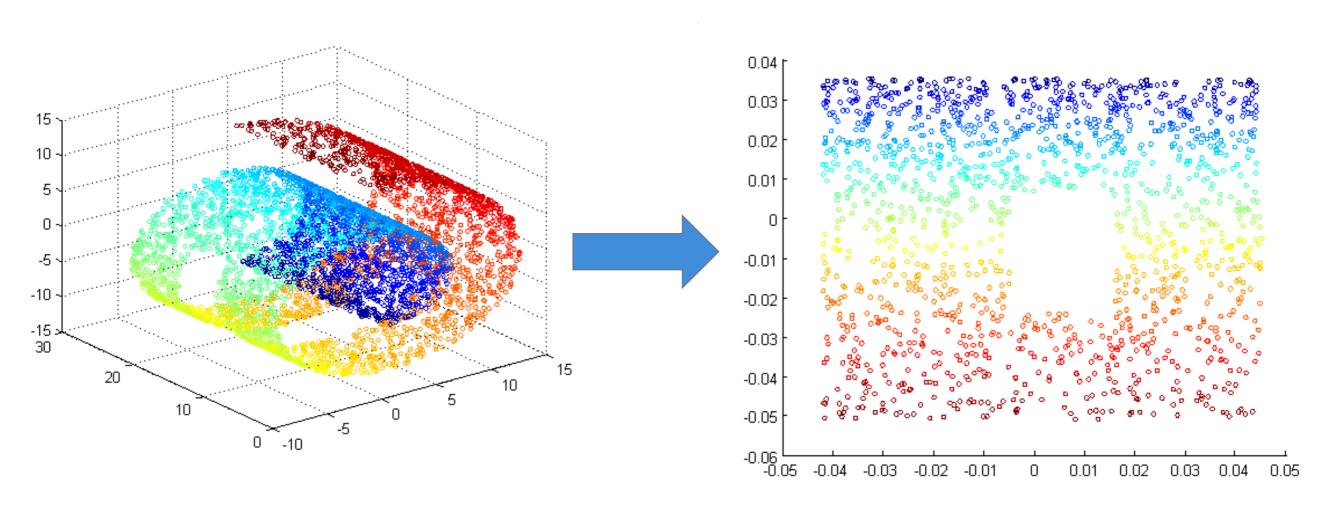
Diffusion Maps could not unroll Swiss Roll for any value of Sigma.

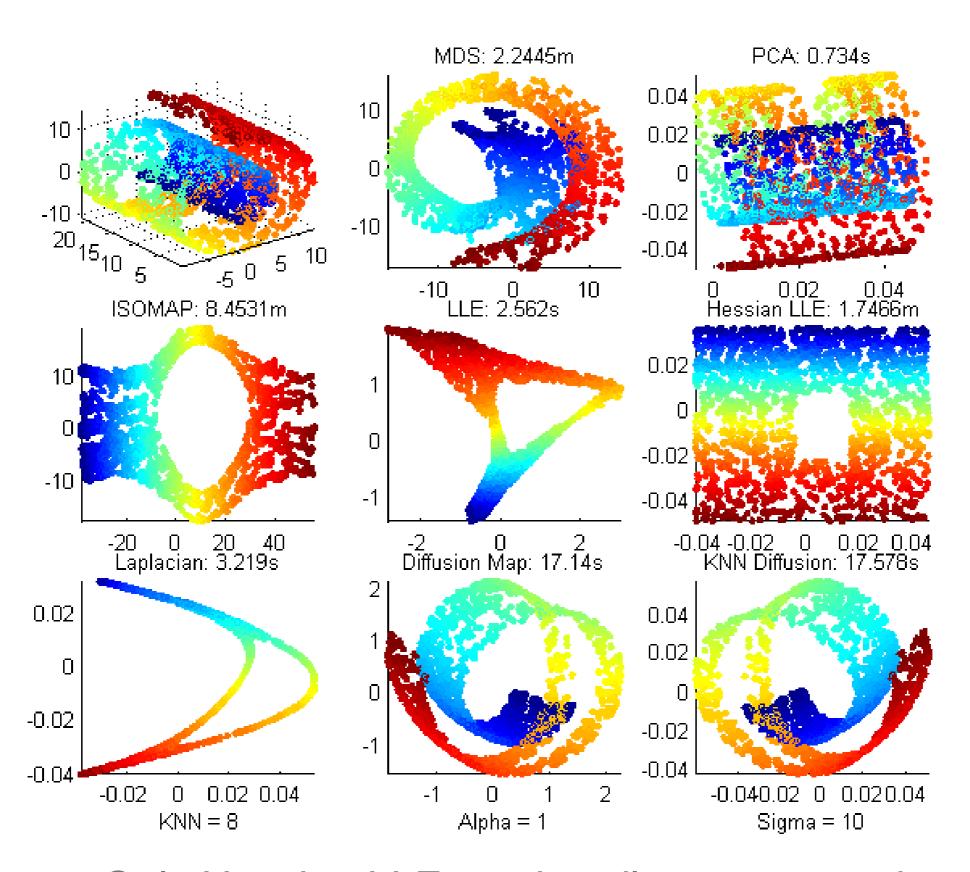
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Non-Convexity

Can we handle a data set with a hole?

Swiss Hole: Can we still unroll the Swiss Roll when it has a hole in the middle?



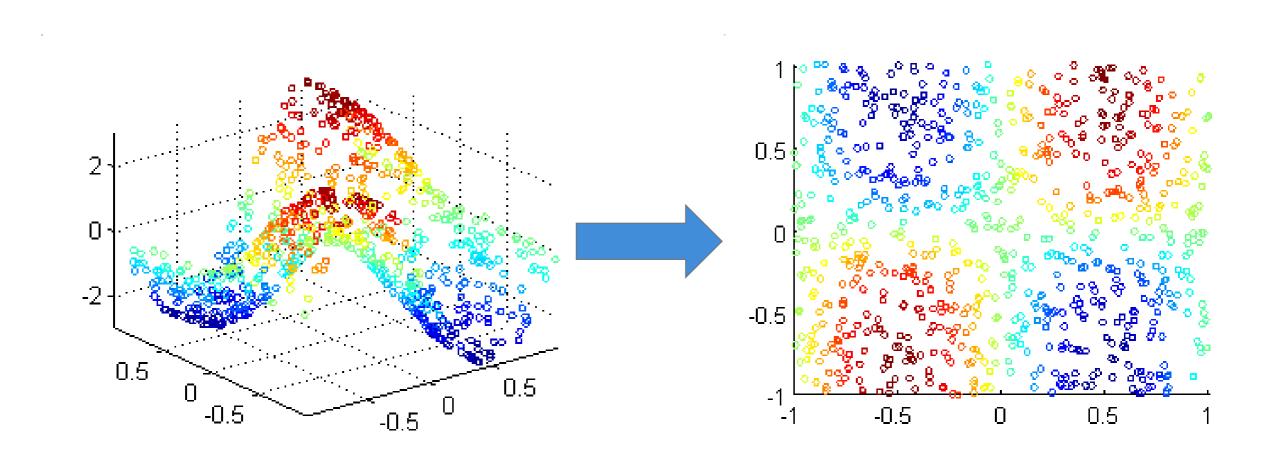


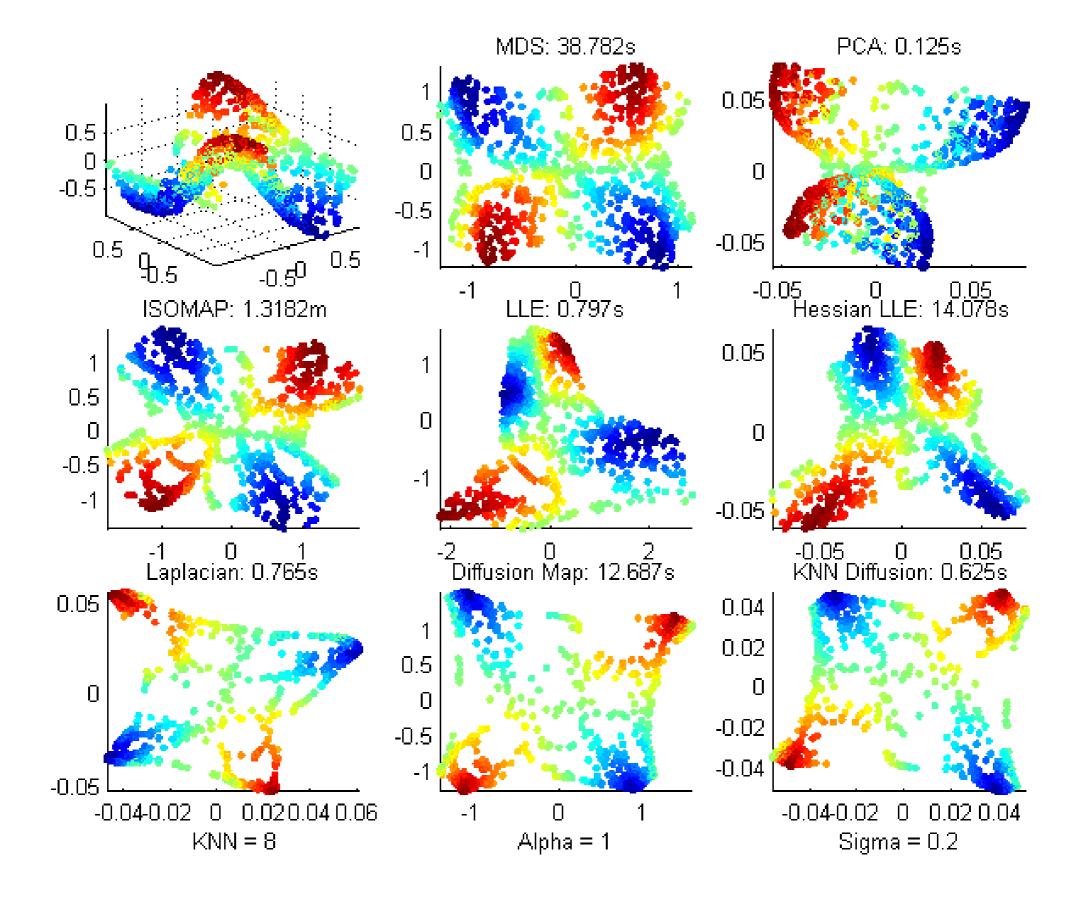
Only Hessian LLE can handle non-convexity. ISOMAP, LLE, and Laplacian find the hole but the set is distorted. 57

Manifold Geometry

Twin Peaks: fold up the corners of a plane.

LLE will have trouble because it introduces curvature to plane.





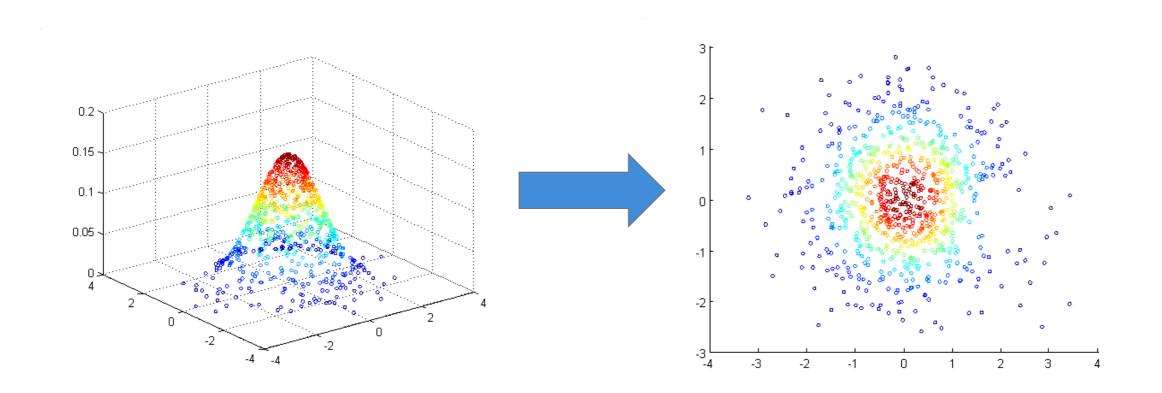
PCA, LLE, and Hessian LLE distort the mapping the most.

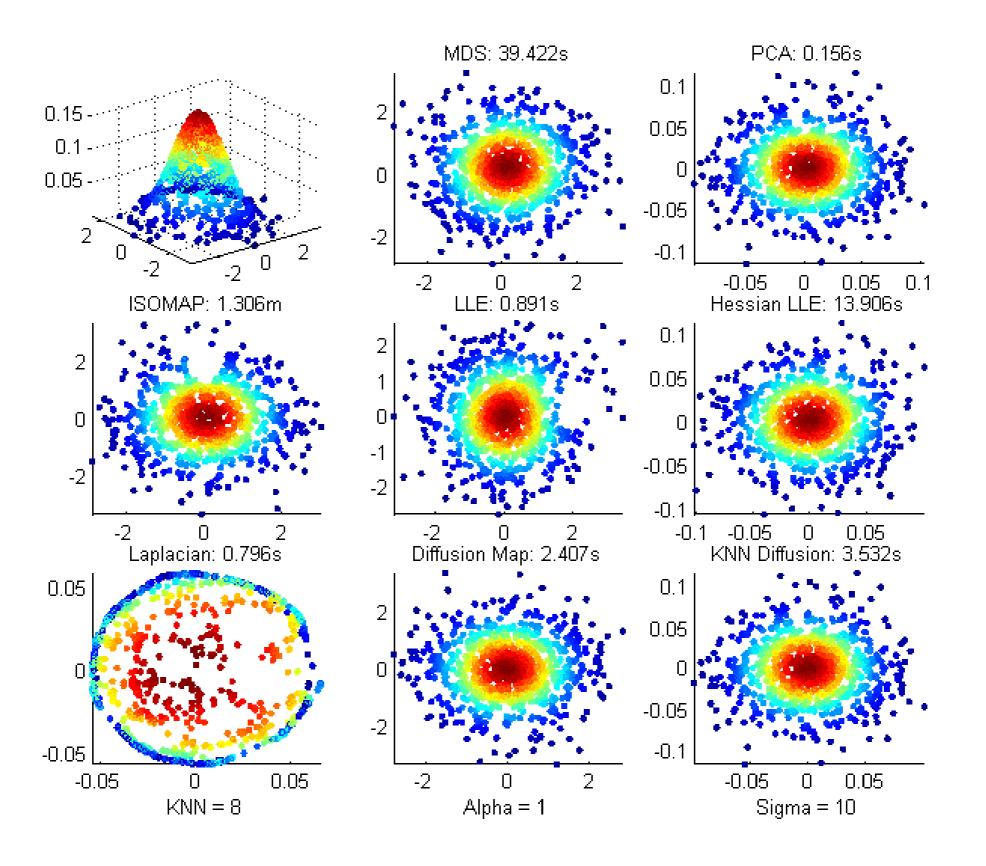
Curvature & Non-uniform Sampling

Gaussian: We can randomly sample a Gaussian distribution.

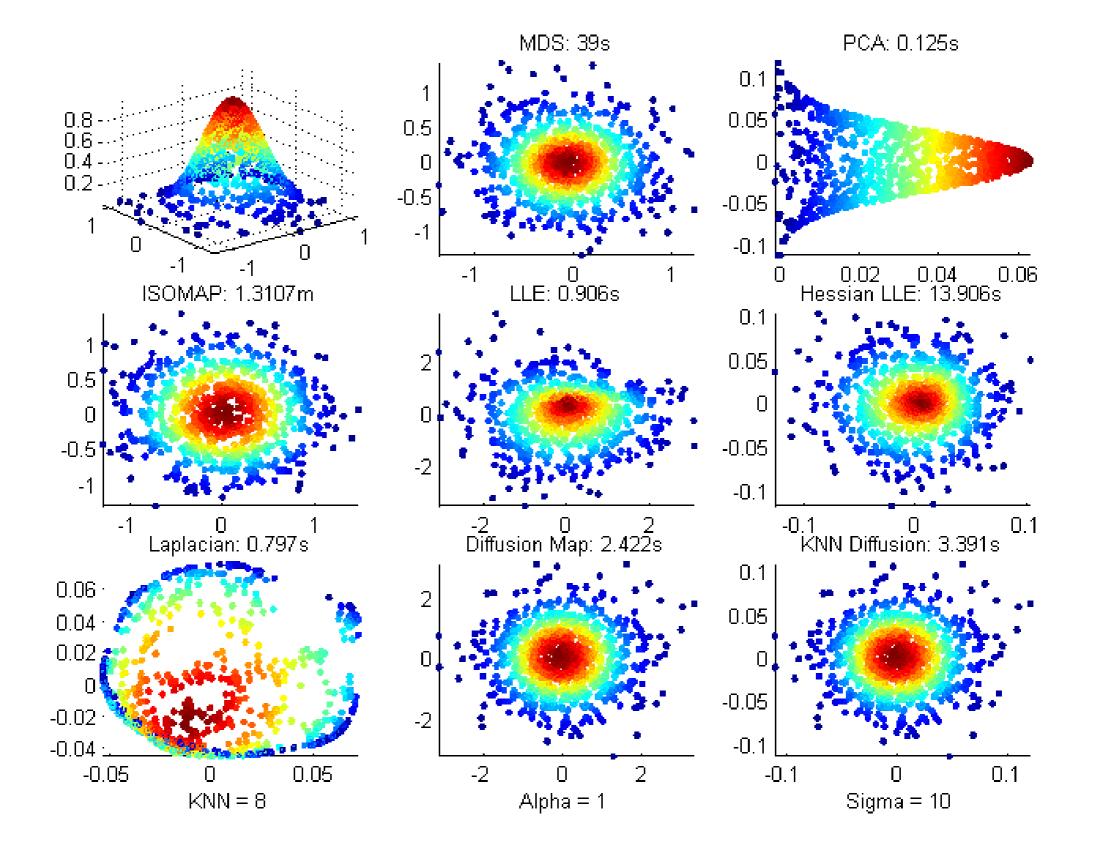
We increase the curvature by decreasing the standard deviation.

Coloring on the z-axis, we should map to concentric circles.



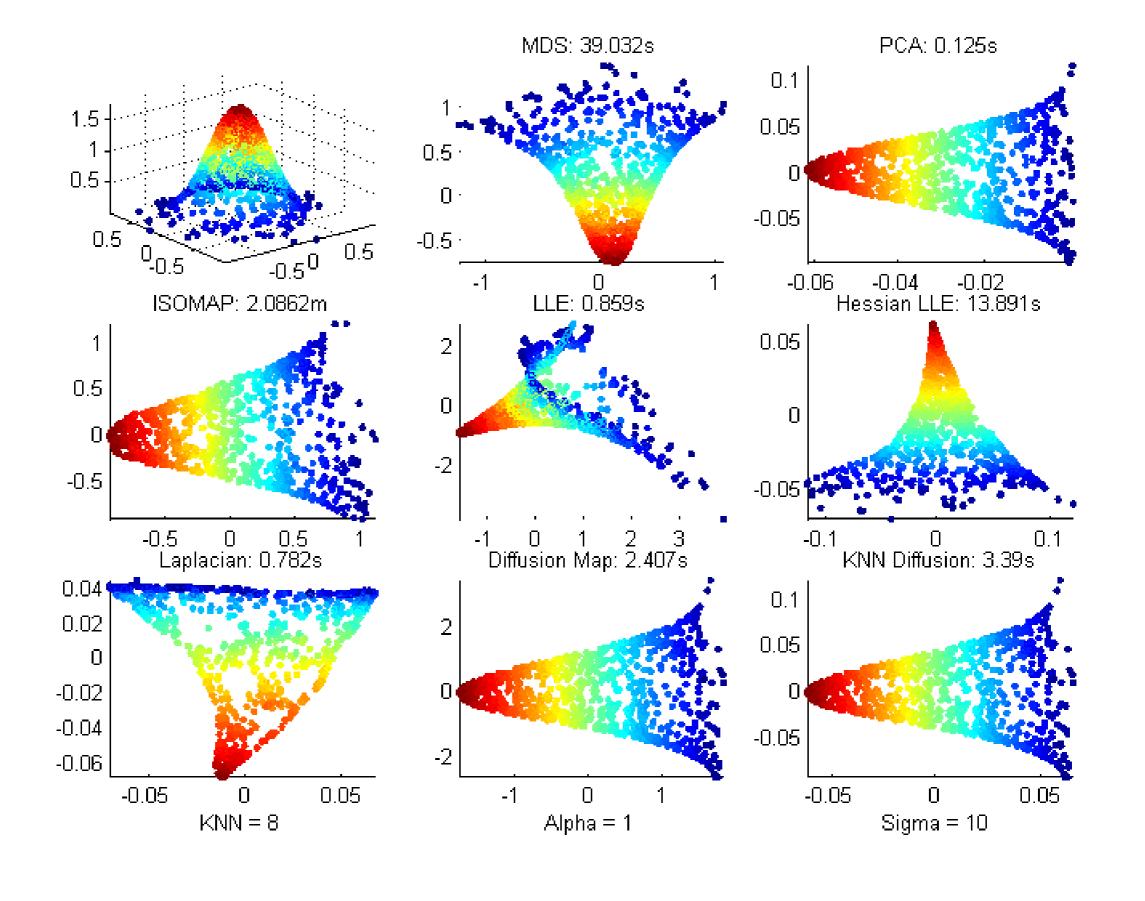


For std = 1 (low curvature), MDS and PCA can project accurately. Laplacian Eigenmap cannot handle the change in sampling.



For std = 0.4 (higher curvature), PCA projects from the side rather than top-down.

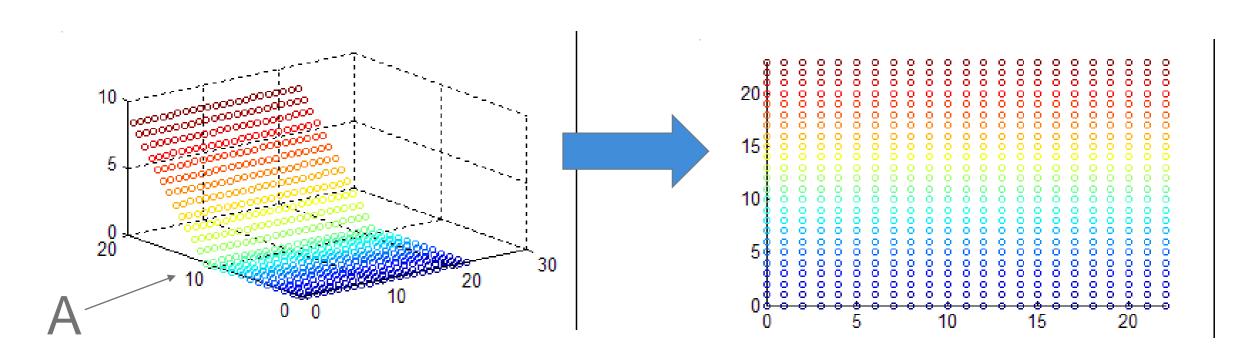
Laplacian looks even worse.



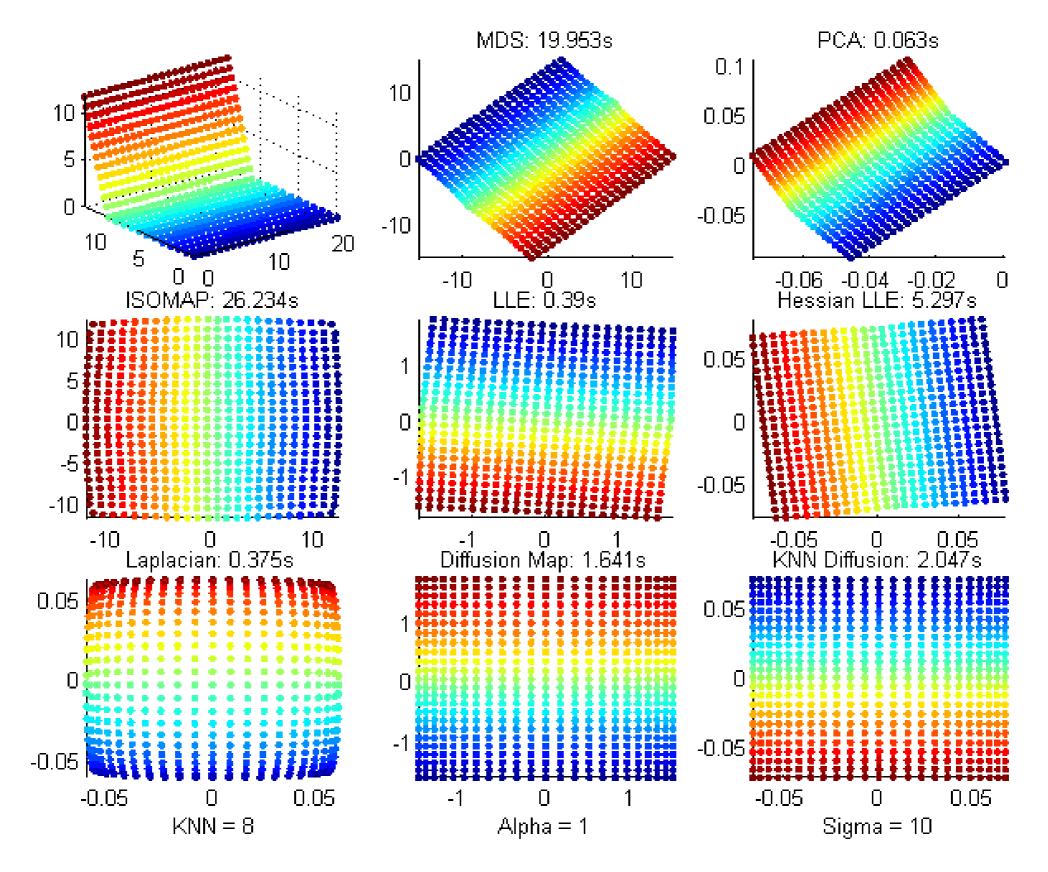
For std = 0.3 (high curvature), none of the methods can project correctly.

Corners

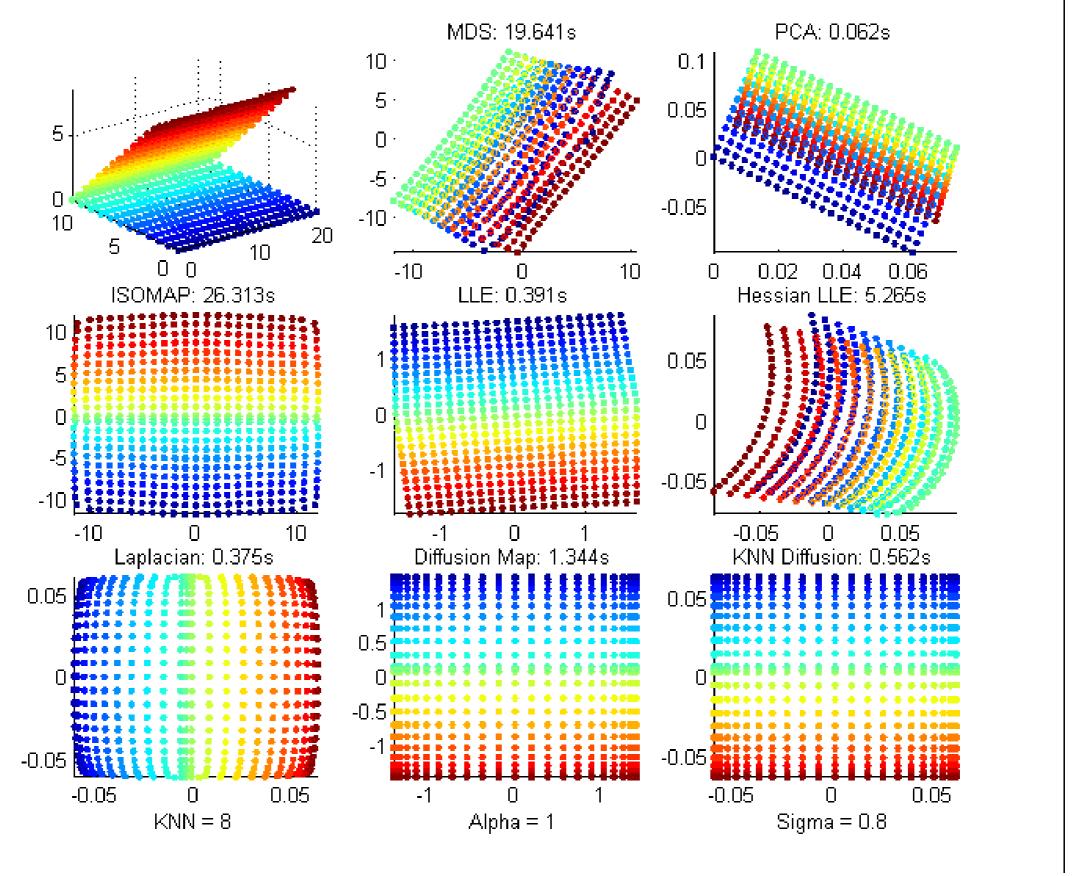
Corner Planes: We bend a plane with a lift angle A. We want to bend it back down to a plane.



If A > 90, we might see the data points written on top of each other.



For angle A=75, we see some disortions in PCA and Laplacian.



For A = 135, MDS, PCA, and Hessian LLE overwrite the data points.

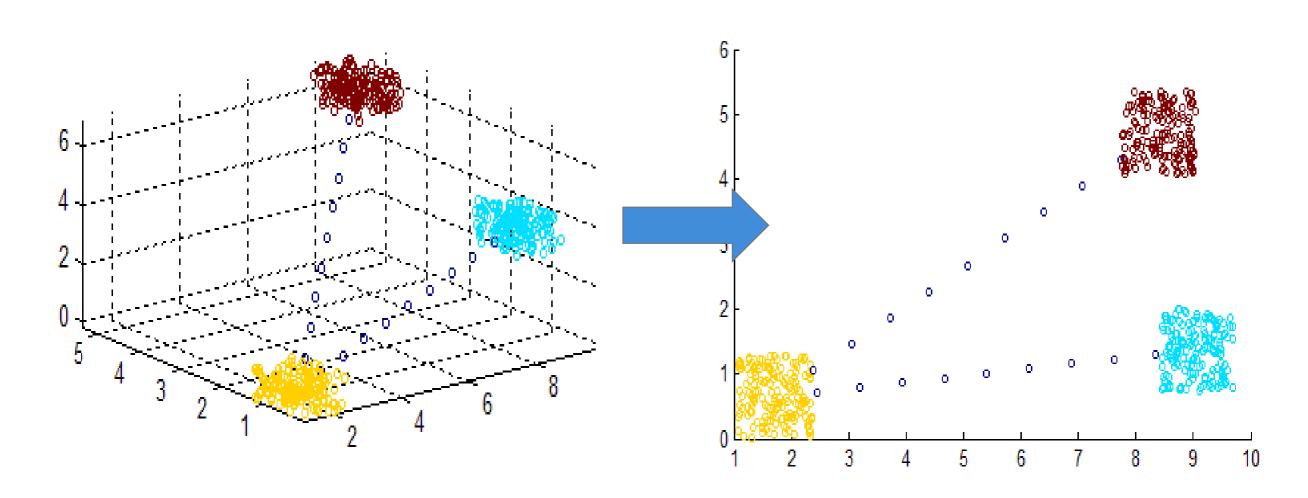
Diffusion Maps work very well for Sigma < 1.

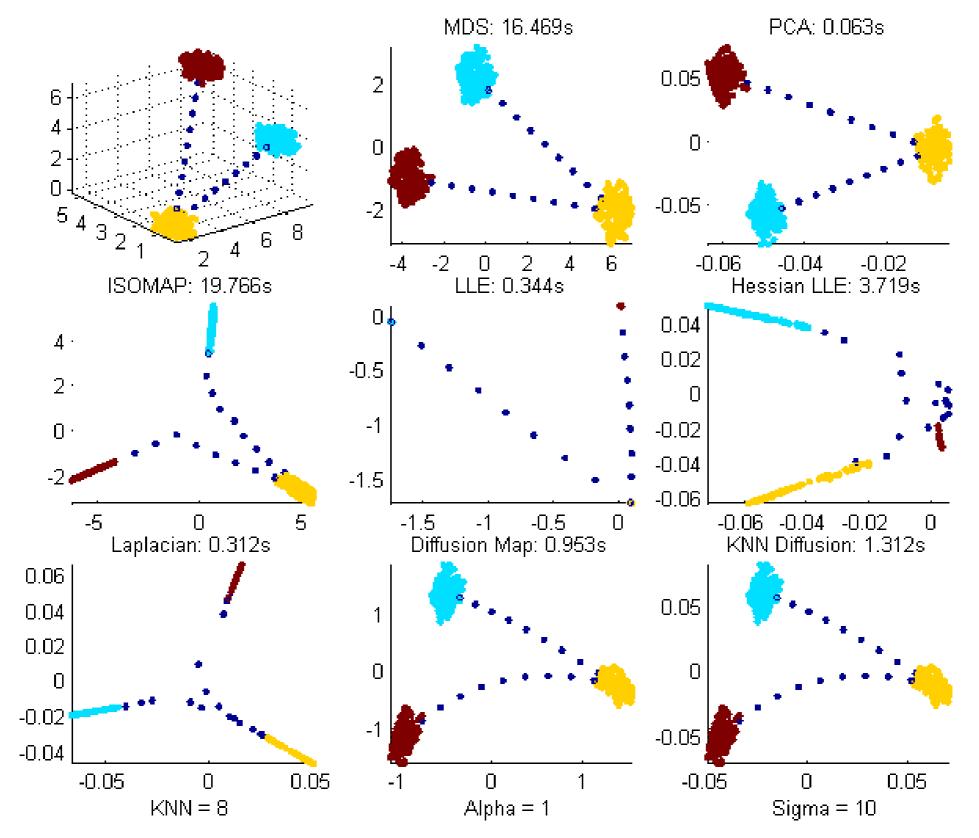
LLE handles corners surprisingly well.

Clustering

A good mapping should preserve clusters in the original data set.

3D Clusters: Generate M non-overlapping clusters with random centers. Connect the clusters with a line.



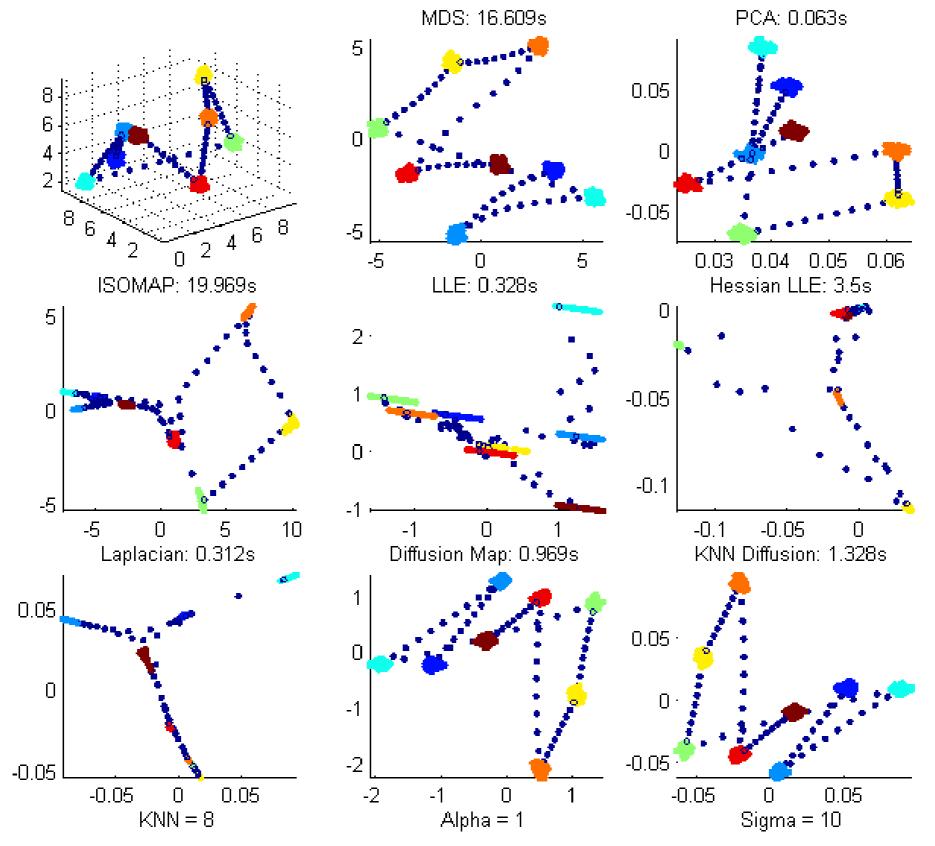


For M = 3 clusters, MDS and PCA can project correctly.

Diffusion Maps work well with large Sigma.

LLE compresses each cluster into a single point.

Hessian LLE has trouble with the sparse connecting lines.



For M=8 clusters, MDS and PCA can still recover.

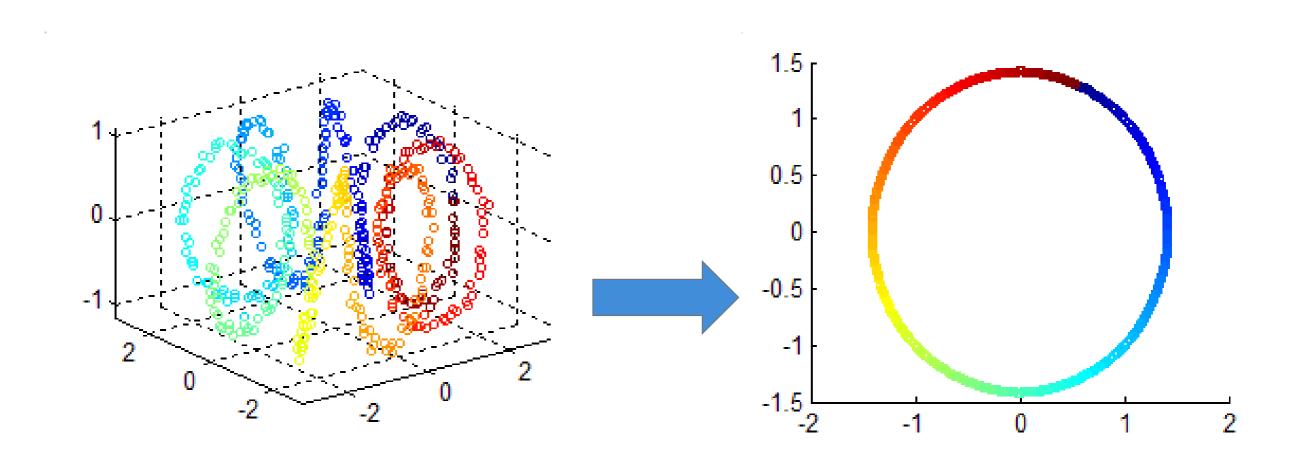
Diffusion Maps do quite well.

LLE and ISOMAP are decent, but Hessian and Laplacian fail.

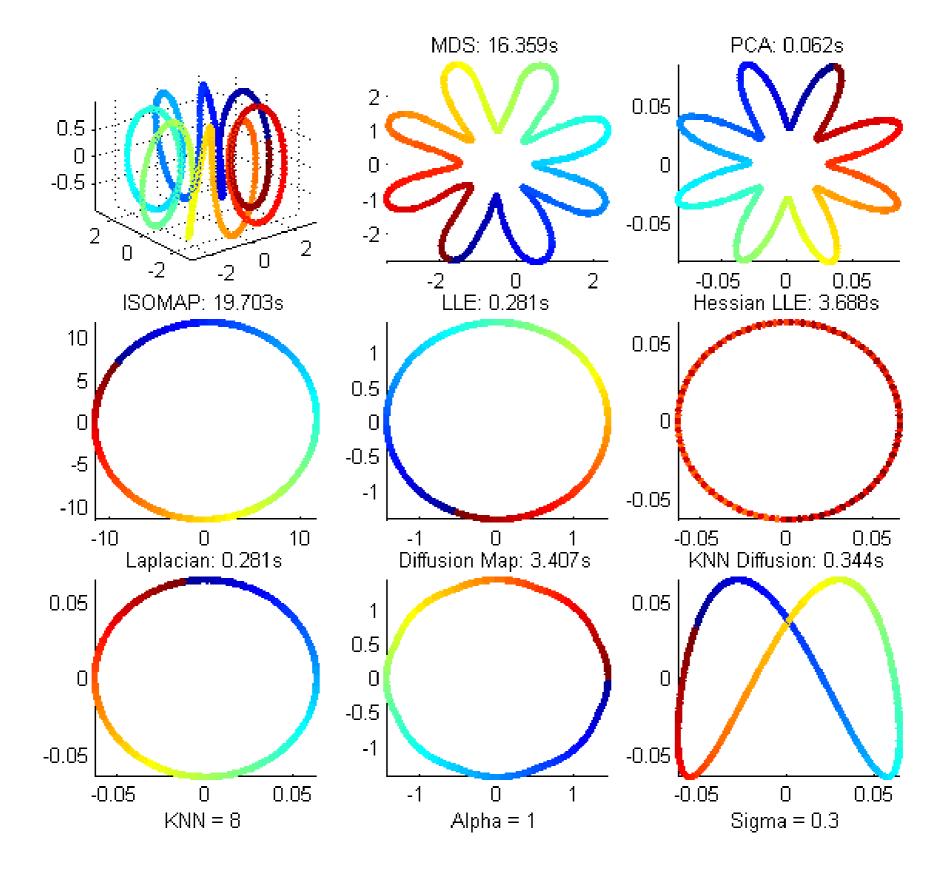
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Noise & Non-uniform Sampling

Can the method handle changes from dense to sparse regions? Toroidal Helix should be unraveled into a circle parametrized by t.



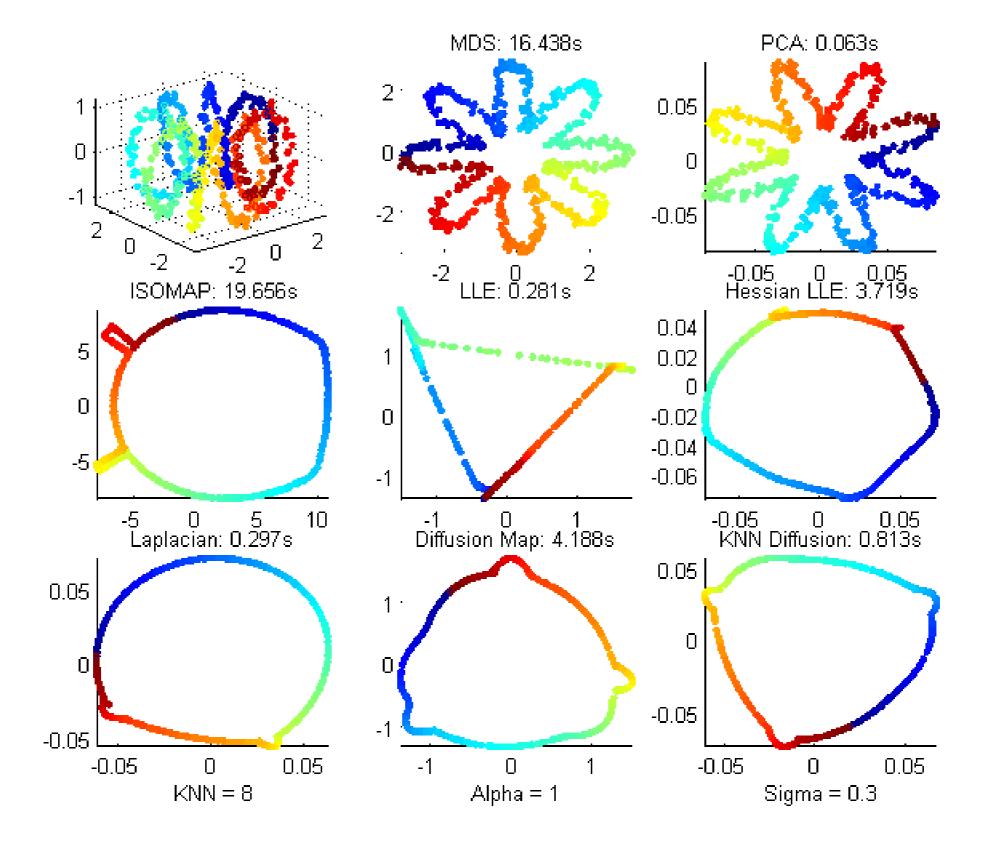
We can change the sampling rate along the helix by changing the exponent R on the parameter t and we can add some noise.



With no noise added, ISOMAP, LLE, Laplacian, and Diffusion Map are correct.

MDS and PCA project to an asterisk.

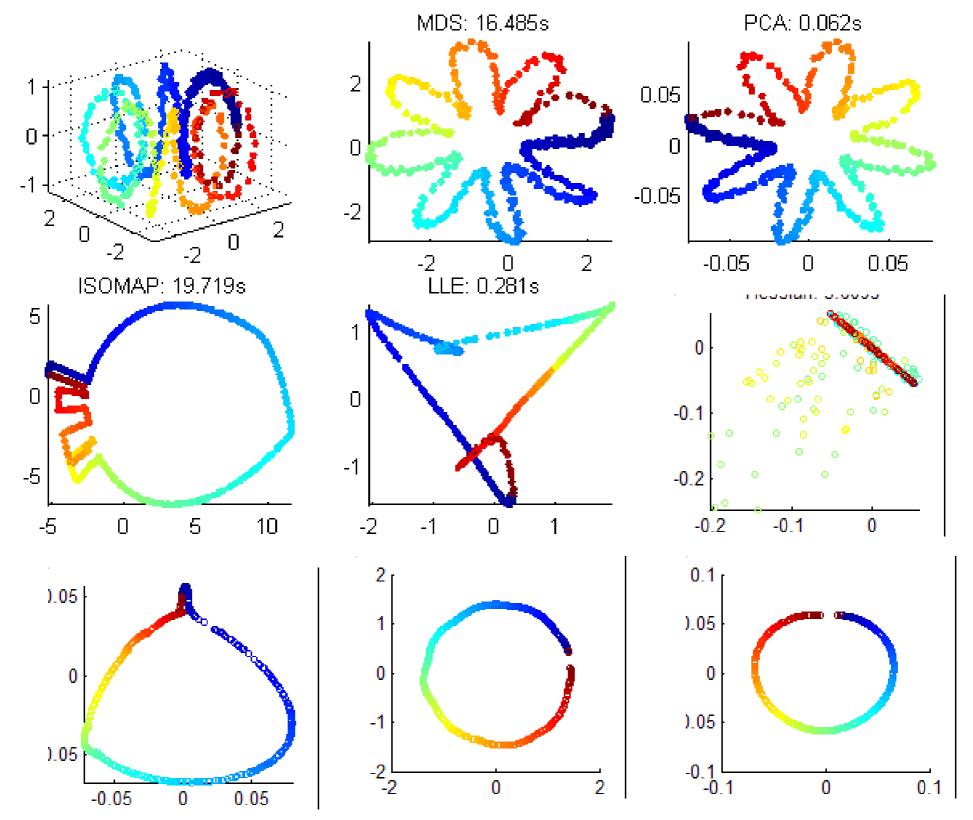
What's up with Hessian and KNN Diffusion?



Adde noise to the Helix sampling.

LLE cannot recover the circle.

ISOMAP emphasizes outliers more than the other methods.



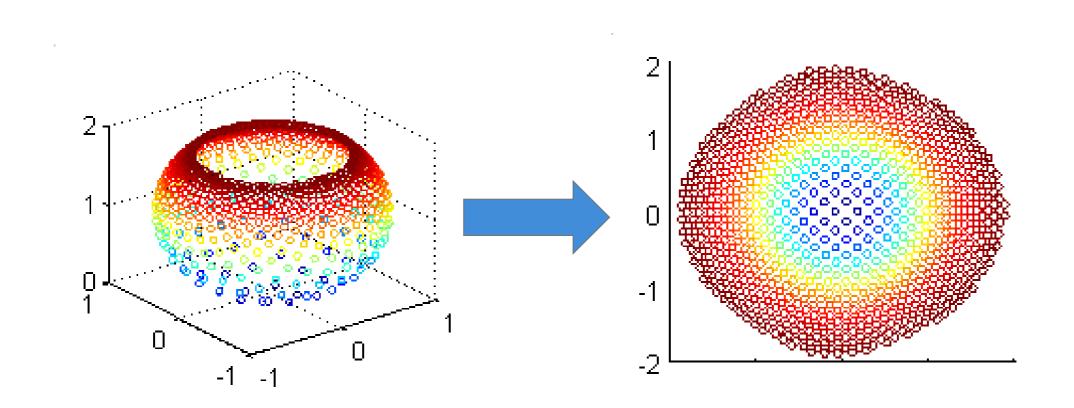
When the sampling rate is changed along the torus, Laplacian starts to mess up and Hessian is completely thrown off.

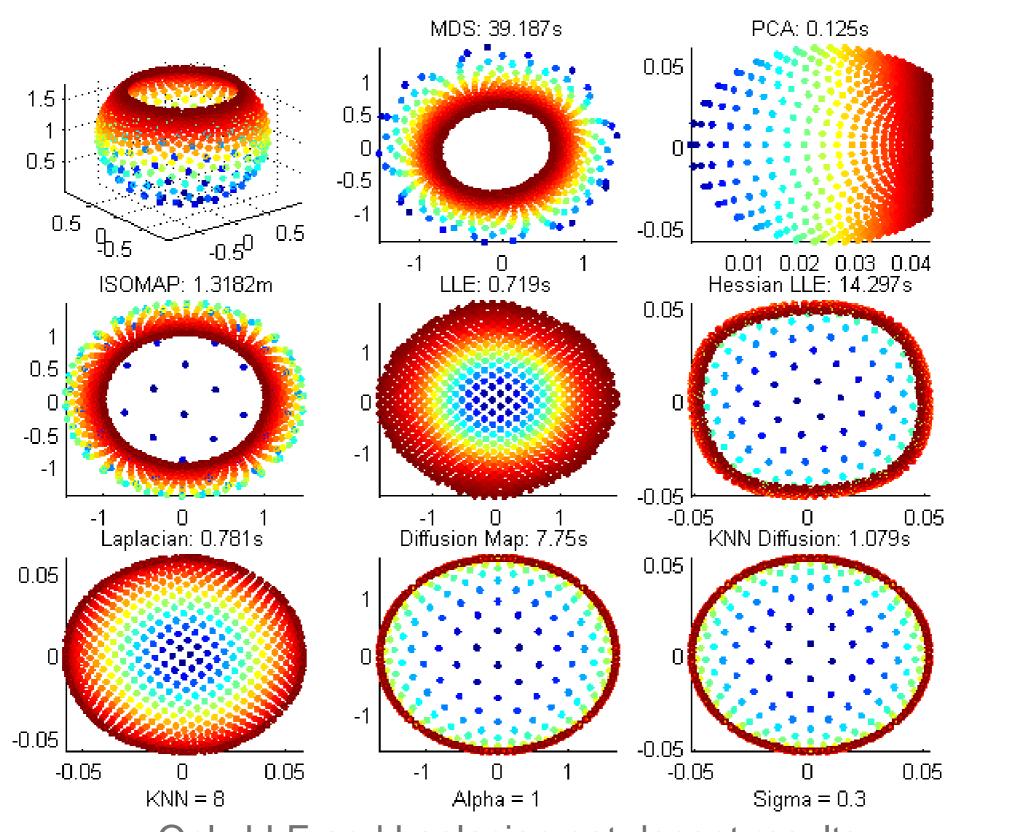
Hessian LLE code crashed frequently on this example.

Diffusion maps handle it quite well for carefully chosen Sigma=0.3.

Sparse Data & Non-uniform Sampling

Of course, we want as much data as possible. But can the method handle sparse regions in the data? Punctured Sphere: the sampling is very sparse at the bottom and dense at the top.





Only LLE and Laplacian get decent results.

PCA projects the sphere from the side. MDS turns it inside-out.

Hessian and Diffusion Maps get correct shape, but give too much emphasis to the sparse region at the bottom of the sphere.

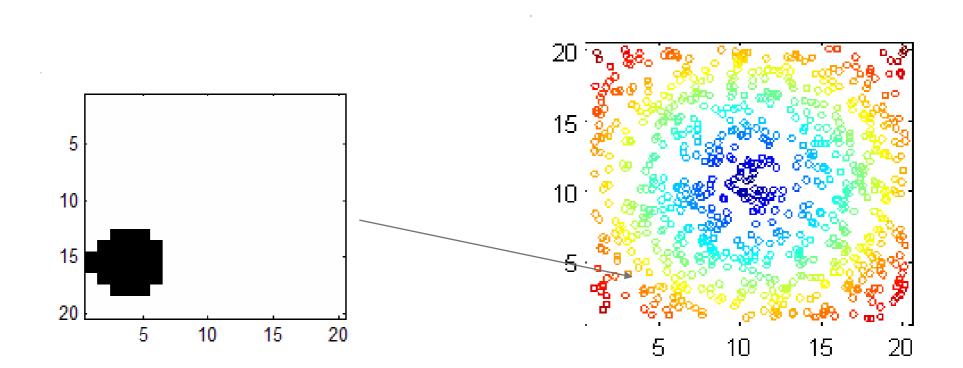
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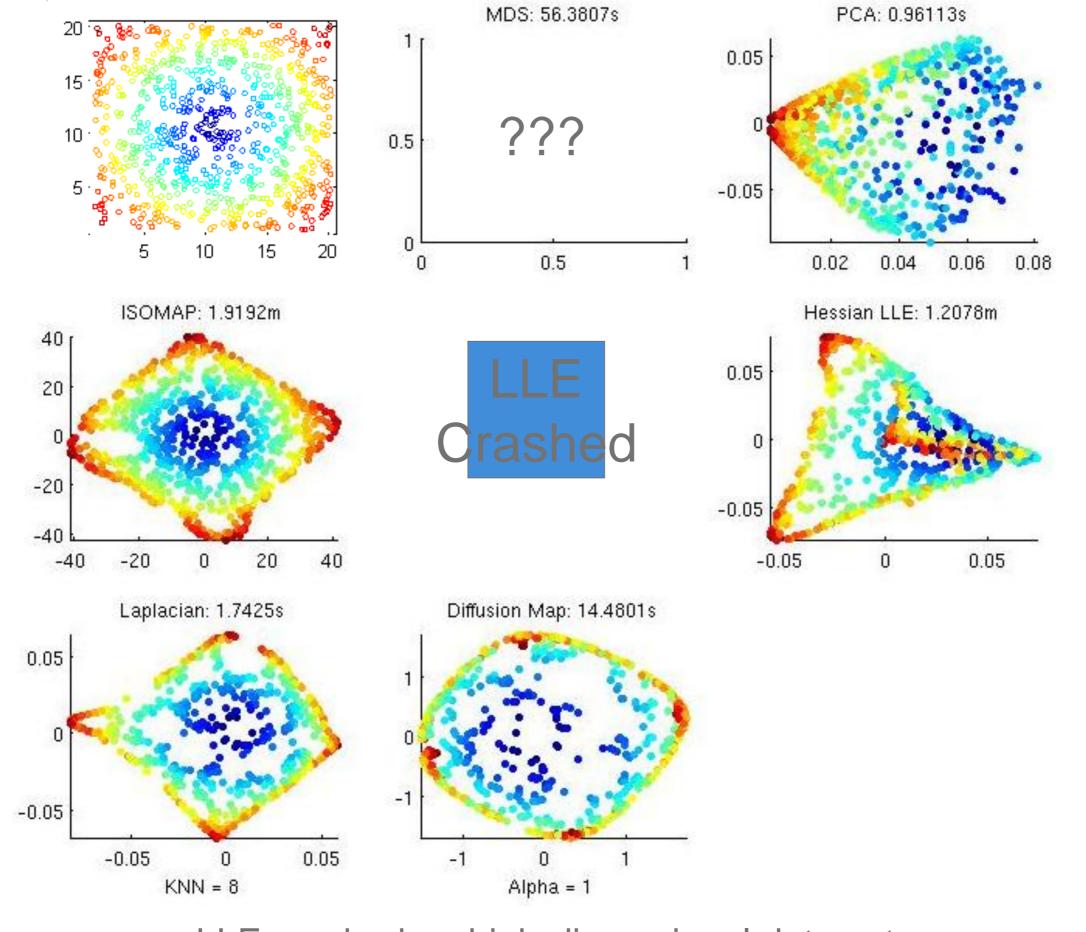
High-Dimensional Data

All of the examples so far have been 3D. But can the data handle high-dimensional data sets, like images?

Disks: Create 20x20 images with a disk of fixed radius and random center.

We should recover the centers of the circles.



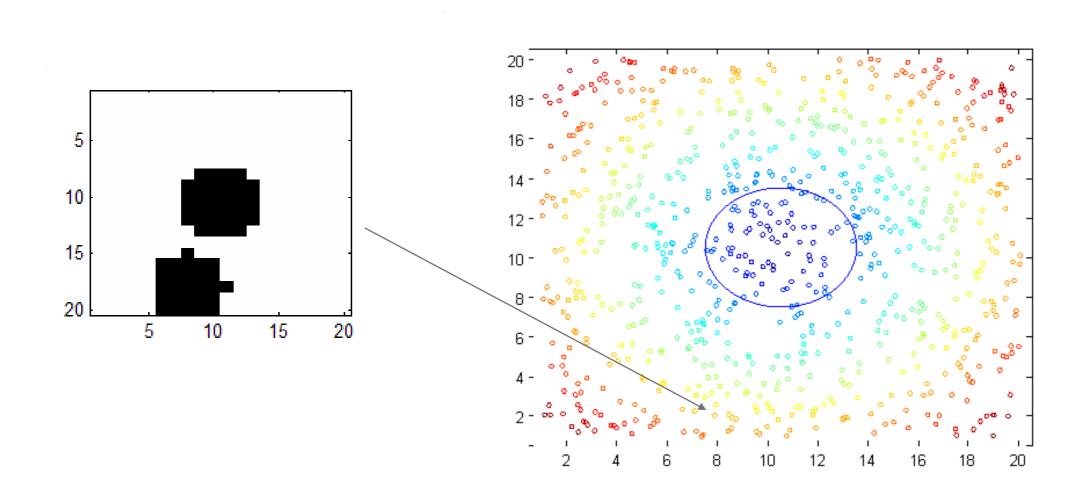


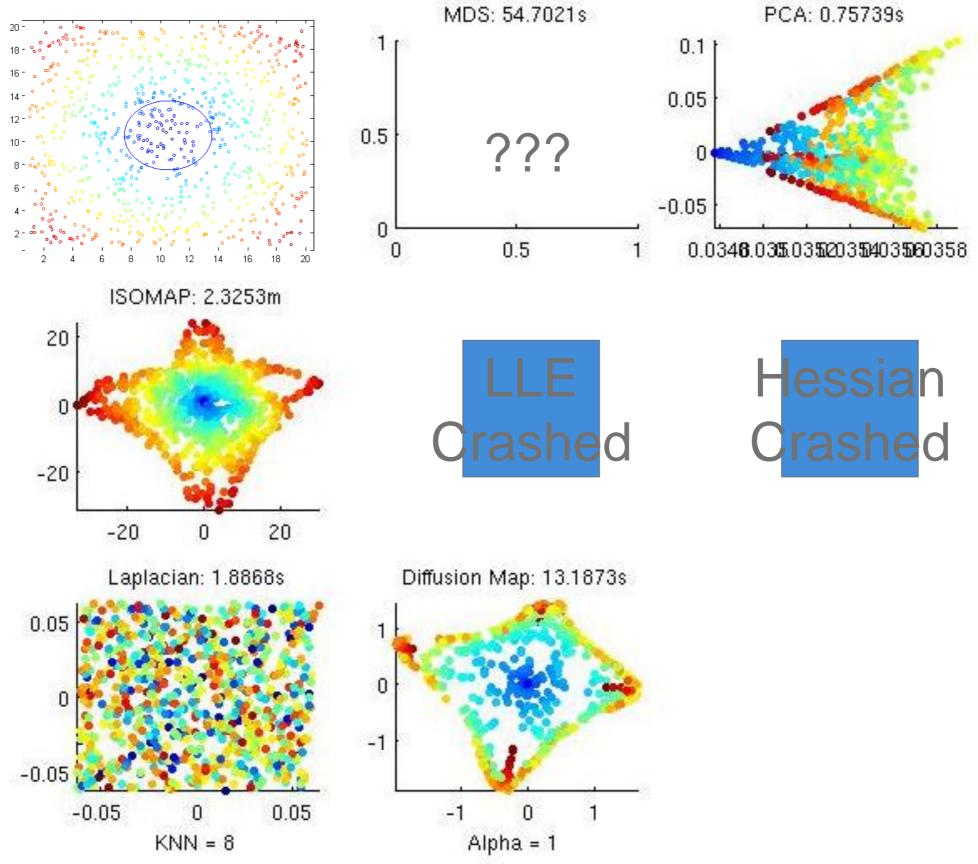
LLE crashed on high-dimensional data set.

Number of images was not high enough, but ISOMAP did a very good job.

Occluded Disks

We can add a second disk of radius R in the center of every image.





Both LLE and Hessian crashed, possibly # points is too small.

Laplacian failed completely.

Is ISOMAP the best for high-dimensional data?

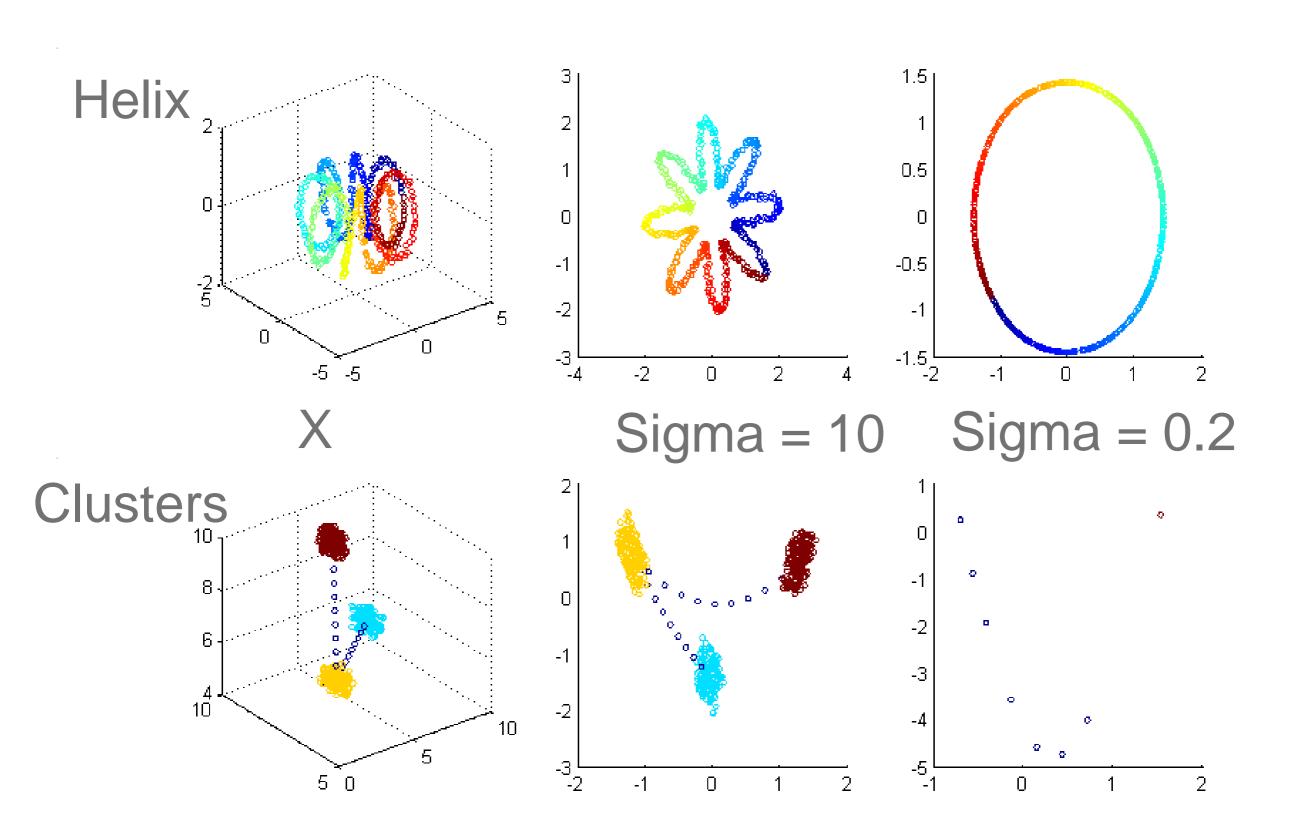
Sensitivity to Parameters

When the number of points is small or the data geometry is complex, it is important to set K appropriately, neither too big nor small.

But if the data set is dense enough, we expect K around 8 or 10 to suffice.

For Diffusion Maps, the method is very sensitive to the Sigma in Gaussian kernel. Varies from example to example.

Diffusion Map Sigma depends on manifold.



So what have you learned, Dorothy?

	MDS	PCA	ISOMAP	LLE	Hessian	Laplacian	Diffusion Map	KNN Diffusion
Speed	Very slow	Extremely fast	Extremely slow	Fast	Slow	Fast	Fast	Fast
Infers geometry?	NO	NO	YES	YES	YES	YES	MAYBE	MAYBE
Handles non-convex?	NO	NO	NO	MAYBE	YES	MAYBE	MAYBE	MAYBE
Handles non- uniform sampling?	YES	YES	YES	YES	MAYBE	NO	YES	YES
Handles curvature?	NO	NO	YES	MAYBE	YES	YES	YES	YES
Handles corners?	NO	NO	YES	YES	NO	YES	YES	YES
Clusters?	YES	YES	YES	YES	NO	NO	YES	YES
Handles noise?	YES	YES	MAYBE	NO	YES	YES	YES	YES
Handles sparsity?	YES	YES	YES	YES	NO may crash	YES	NO	NO
Sensitive to parameters?	NO	NO	YES	YES	YES	YES	VERY	VERY 82

Some Notes on using MANI

- ☐ Hard to set K and Sigma just right.
- ☐ MDS and ISOMAP are very slow.
- □ Hessian LLE is pretty slow. Since Hessian needs a dense data set, this means it takes even longer when the # points is large.
- □ Occluded Disks is 400-dimensional data, which takes a long time and a lot of data points to correctly map.

☐ Matlab GUIs seem to run better on PC than Linux.

Credits

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Thanks for your attention ©