# A geometric (and partial) introduction to Dimensionality Reduction

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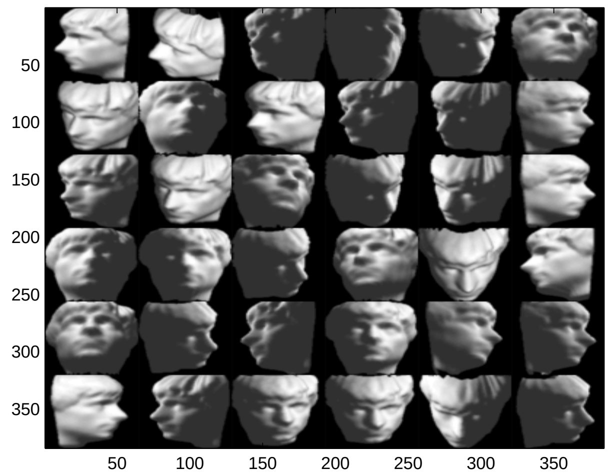
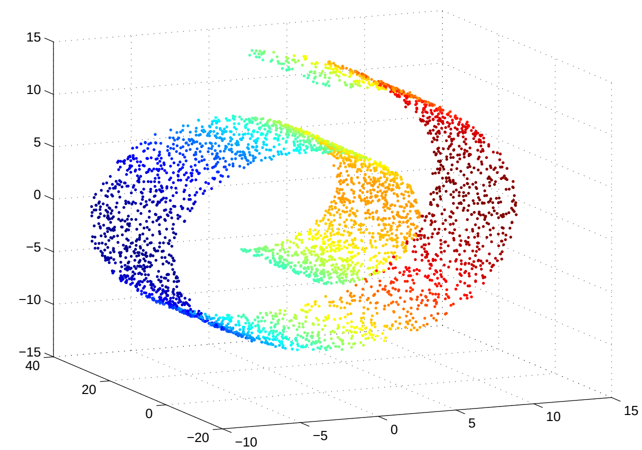
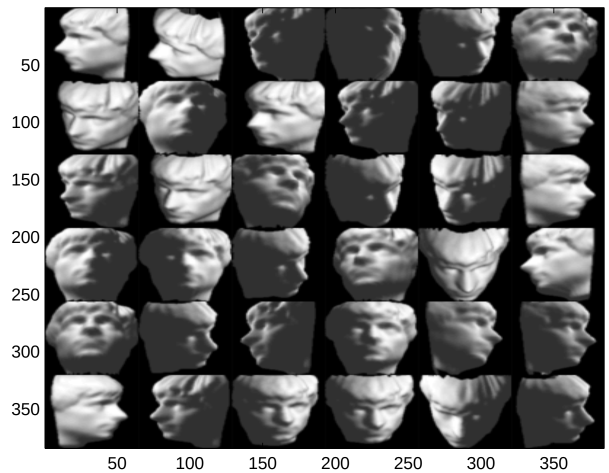
# Introduction

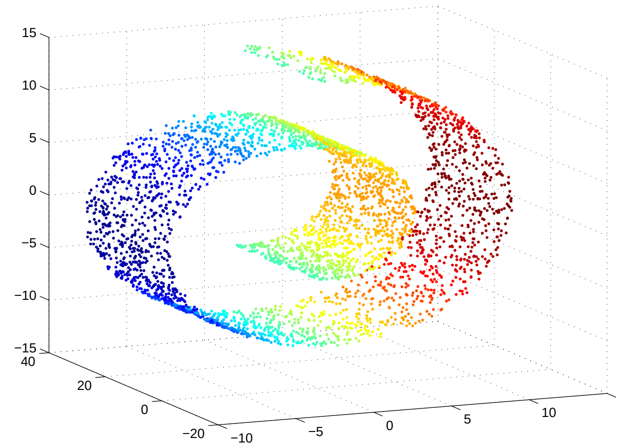



- More and more available data represented by point clouds in high dimensional spaces:
  - measurement and data storage capacities are growing very fast,
  - e.g. images databases, astronomic data,...
- Data often depends upon a small numbers of “independant” parameters (e.g. number of degrees of freedom of an observed system):
  - data sampled around low dimensional shapes (manifolds).
  - underlying manifolds may be highly non linear.

# Introduction




- Need to analyze and visualize these data.
- Dimensionality reduction methods intend to embedded the data in low dimensional spaces while preserving as well as possible (some of) their geometric properties. $\Rightarrow$ many different approaches that gave rise to a huge literature in the last decade...
- In this talk:
  - a very incomplete and partial introduction to dimensionality reduction,
  - a focus on a small set of geometric-motivated methods (trying to avoid as most as possible technical details).

# Preliminaries and notations

The following notations and assumptions are used all along the talk.

- Data: $X = \{x_1, x_2, \cdots, x_N\} \subset \mathbb{R}^D$ a finite point cloud with mean vector

$$\overline{x} = \sum_{n=1}^{N} x_i \in \mathbb{R}^D$$

$$X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1D} \\ x_{21} & x_{22} & \cdots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{ND} \end{pmatrix}$$

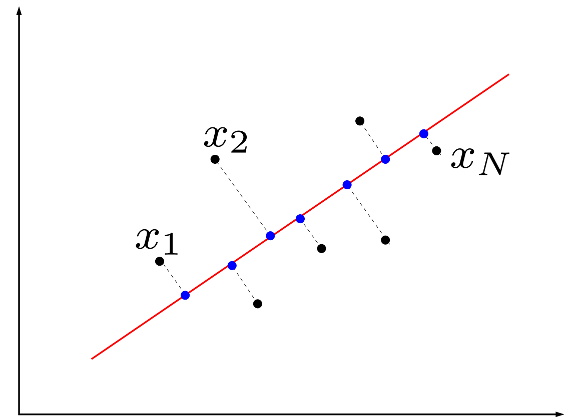
- $N$: number of data points
- $D$: ambient dimension
- Underlying/latent manifold: $M \subset \mathbb{R}^D$ is a $d$-dimensional submanifold of $\mathbb{R}^D$. The points of $X$ are assumed to be sampled on or around $M$.

# Preliminaries and notations

- Two “equivalent” points of view:
  1. $M \subset \mathbb{R}^D$ is a submanifold and one intends to find an embedding $Y$ of $X$ in some low dimensional space such that the “geometry” of $Y$ is as similar as possible as the one of $M$ in some sense,
  2. $M = f(N)$ where $N$ is some $d$-dimensional manifold (the latent manifold - in general $N$ is expected to be an open subset of $\mathbb{R}^d$) and $f : N \to \mathbb{R}^D$ an embedding with some specified properties (isometry, conformal,...). One then intends to find $Y$ such that $X = f(Y)$. The coordinates of $Y$ are known as the latent variables.
  3. In some statistical/probabilistic approaches (not considered in this talk): $X = f(Y) + \varepsilon(Y)$ where $\varepsilon$ is some noise model.

# PCA

Find the $d$-dimensional subspace of $\mathbb{R}^D$ that best approximates $X$ in a least square sense (and then project $X$ on this subspace)




- Let $V$ be a $d$-dimensional subspace of $\mathbb{R}^D$ and let $\mathbf{u}_1, \cdots \mathbf{u}_D$ be an orthonomal basis such that $\mathbf{u}_1, \cdots \mathbf{u}_d$ is a basis of $\vec{V}$.
- Approximate each point $x_n$ by

$$\tilde{x}_n = \sum_{i=1}^{d} \alpha_{ni} \mathbf{u}_i + \sum_{i=d+1}^{D} b_i \mathbf{u}_i$$

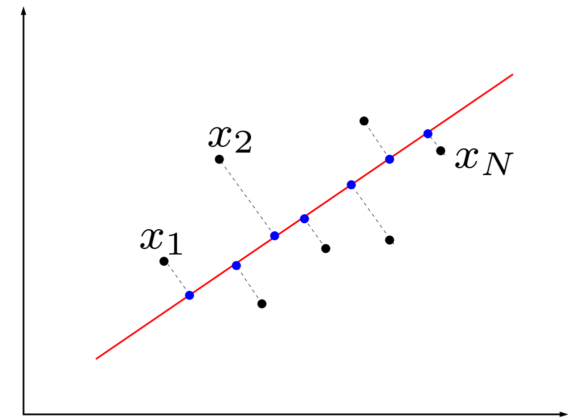
- Minimize

$$E = \frac{1}{N} \sum_{i=1}^{N} \|x_n - \tilde{x}_n\|^2$$

# PCA

$$\tilde{x}_n = \sum_{i=1}^{d} \alpha_{ni} \mathbf{u}_i + \sum_{i=d+1}^{D} b_i \mathbf{u}_i$$

$$E = \frac{1}{N} \sum_{i=1}^{N} \|x_n - \tilde{x}_n\|^2$$




- Minimizing $E$ with respect to $\alpha_{ni}$ and $b_i$ leads to

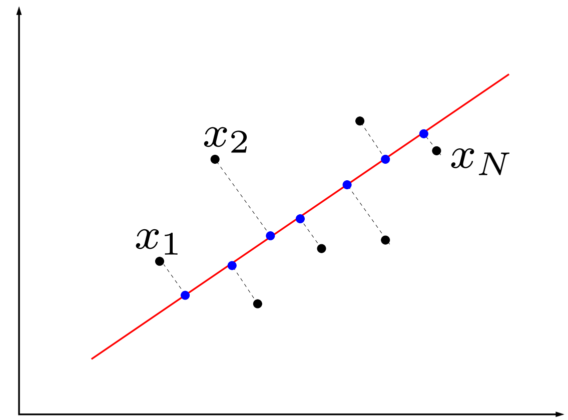
$$x_n - \tilde{x}_n = \sum_{i=d+1}^{D} \{(x_n - \overline{x})^T \mathbf{u}_i\} \mathbf{u}_i$$

$\Rightarrow$ Given $\vec{V}$ the best affine subspace $V$ is the one passing through $\overline{x}$ and $\tilde{x}_n$ is the orthogonal projection on $V$.

# PCA

$$E = \frac{1}{N} \sum_{i=1}^{N} \|x_n - \tilde{x}_n\|^2$$

$$x_n - \tilde{x}_n = \sum_{i=d+1}^{D} \{(x_n - \overline{x})^T \mathbf{u}_i\} \mathbf{u}_i$$




- Now $E$ only depends on $\mathbf{u}_i$:

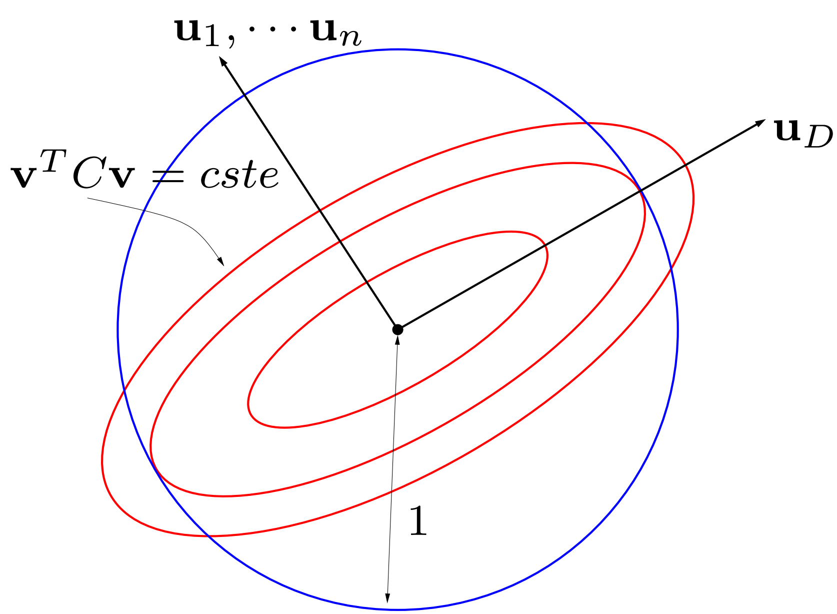
$$E = \frac{1}{N} \sum_{n=1}^{N} \sum_{i=d+1}^{D} (x_n^T \mathbf{u}_i - \overline{x}^T \mathbf{u}_i)^2 = \sum_{i=d+1}^{D} \mathbf{u}_i^T C \mathbf{u}_i$$

where

$$C = \frac{1}{N} \sum_{n=1}^{N} (x_n - \overline{x})(x_n - \overline{x})^T$$ is the covariance matrix of $X$

# PCA

**Proposition:** The minimum of $E$ is obtained for the space spanned by the $d$ eigenvectors of $C$ corresponding to the $d$ largest eigenvalues.




**"Proof":** For simplicity, assume that $d = D - 1$.

- minimize $E = \mathbf{u}_D^T C \mathbf{u}_D$ under the constraint $\mathbf{u}_D^T \mathbf{u}_D = 1$.
- "Lagrange multipliers":
  minimization of $\mathbf{u}_D C \mathbf{u}_D + \lambda(1 - \mathbf{u}_D^T \mathbf{u}_D)$
  derivative with respect to $\mathbf{u}_D$: $2C\mathbf{u}_D - 2\lambda \mathbf{u}_D$ is equal to $0$ if $C\mathbf{u}_D = \lambda \mathbf{u}_D$.

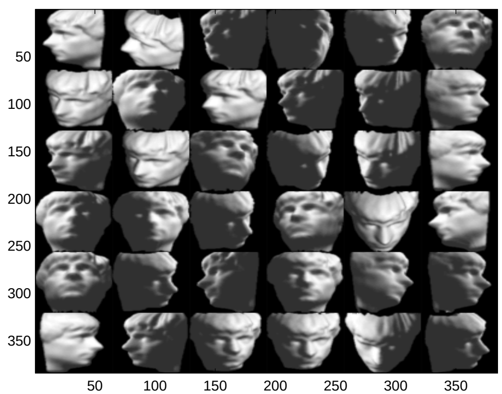
# PCA: remarks

- (A) Find the $d$-dimensional subspace of $\mathbb{R}^D$ that best approximates $X$ in a least square sense (and then project $X$ on this subspace)

  $$\Longleftrightarrow$$

  (B) Find the $d$-dimensional subspace of $\mathbb{R}^D$ onto which the projected data has maximum variance.
- There exist other more probabilistic/statistical formulations of the problem that lead to the same solution.

# PCA: example

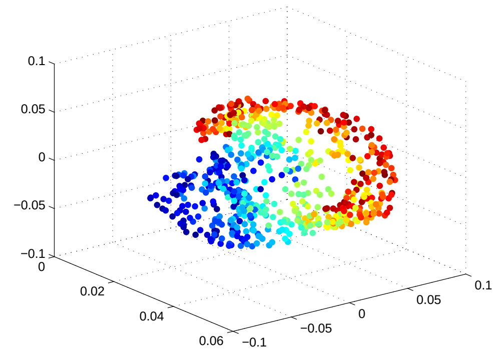



Dimension: $64 * 64 = 4096$.

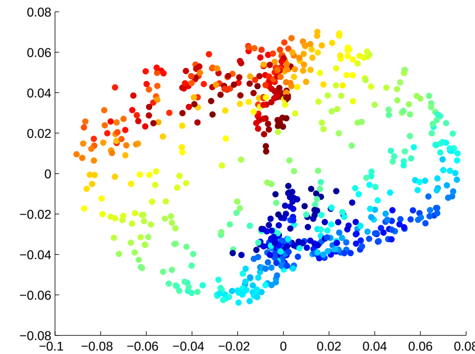
$N = 698$

3 free parameters:

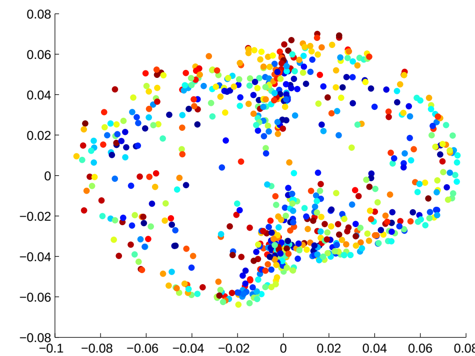
- left-right pose,
- up-down pose,
- light pose.




3D-proj: light




2D-proj: pose 1

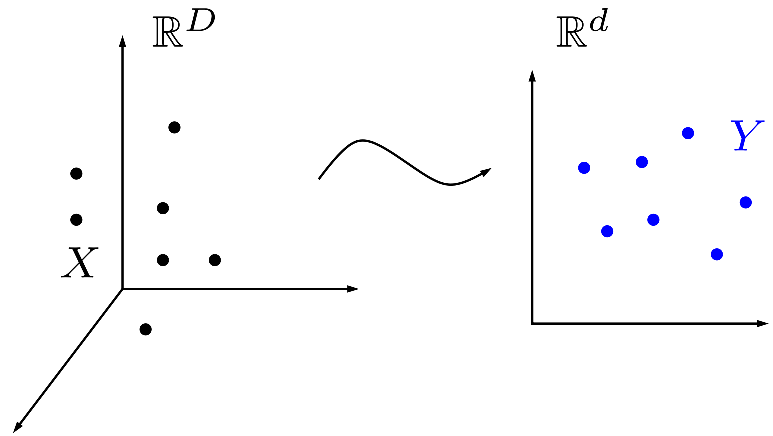



2D-proj: pose 2

# Multidimensional Scaling (MDS)

Find a low dimensional "projection" $Y \subset \mathbb{R}^d$ of the data $X$ such as to preserve, as closely as possible, the pairwise distances between data points.

Without loss of gen. we assume that $\overline{x} = 0$ (and $\overline{y} = 0$).




- The $N \times N$ matrix of squared pairwise distance: $D = D_X = (\|x_i - x_j\|^2)$
- The $N \times N$ Gram matrix: $G = G_X = (x_i^T x_j) = XX^T$
- Relationship between $D$ and $G$ (exercise):

$$G = -\frac{1}{2} JDJ \text{ where } J = Id_N - \frac{1}{N}\mathbf{1}\mathbf{1}^T = (\delta_{ij} - \frac{1}{N})$$

- **Goal:** Find $Y = \{y_1, \cdots y_N\} \subset \mathbb{R}^d$ minimizing

$$\rho(D_X, D_Y) = \|G_X - G_Y\|_2^2 = \|\frac{1}{2} J(D_X - D_Y)J\|_2^2$$

# Multidimensional Scaling (MDS)

$$\rho(D_X, D_Y) = \|G_X - G_Y\|_2^2 = \|\frac{1}{2}J(D_X - D_Y)J\|_2^2$$

**Solution:**

- Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N \geq 0$ be the eigenvalues of $G_X$ and $\{\mathbf{v}_1, \cdots \mathbf{v}_N\} \subset \mathbb{R}^N$ an orthonormal eigenbasis.
- $Y \subset \mathbb{R}^d$ minimizing $\rho(D_X, D_Y)$ is given by the columns of the $d \times N$ matrix

$$Y = \begin{pmatrix} \sqrt{\lambda_1}\mathbf{v}_1^T \\ \sqrt{\lambda_2}\mathbf{v}_2^T \\ \vdots \\ \sqrt{\lambda_d}\mathbf{v}_d^T \end{pmatrix}$$

# Multidimensional Scaling (MDS)

**Justification:**

$$
\begin{aligned}
\min_Y \|G_X - G_Y\|_2^2 &= \min_Y \|XX^T - YY^T\|^2 \\
&= \min_Y \sum_{i=1}^{N}\sum_{j=1}^{N}(x_i^T x_j - y_i^T y_j)^2 \\
&= \min_Y Tr((XX^T - YY^T)^2)
\end{aligned}
$$

$XX^T$ and $YY^T$ are semidefinite positive: $XX^T = V\Lambda V^T$ and $YY^T = W\Lambda' W^T$ where
- $VV^T = WW^T = Id_N$,
- $\Lambda = Diag(\lambda_1, \cdots, \lambda_N)$ is diagonal with $\lambda_1 \geq \lambda_2 \cdots \geq \lambda_N$,
- $\Lambda' = Diag(\lambda'_1, \cdots \lambda'_d, 0, \cdots, 0)$ is diagonal with $\lambda'_1 \geq \cdots \geq \lambda'_d \geq 0$ because $Y \subset \mathbb{R}^d$.

$$
\begin{aligned}
\min_Y Tr((XX^T - YY^T)^2) &= \min_{W,\Lambda'} Tr(\Lambda - V^T W \Lambda' W^T V)^2 \quad \text{(use } Tr(AB) = Tr(BA)\text{)} \\
&= \min_{Q,\Lambda'} Tr(\Lambda - Q\Lambda' Q^T)^2 \quad \text{with} \quad Q = V^T W \\
&= \min_{Q,\Lambda'} Tr(\Lambda^2) + Tr(Q\Lambda' Q^T Q\Lambda' Q^T) - 2Tr(\Lambda Q\Lambda' Q^T)
\end{aligned}
$$

# Multidimensional Scaling (MDS)

## Justification:

$$
\begin{aligned}
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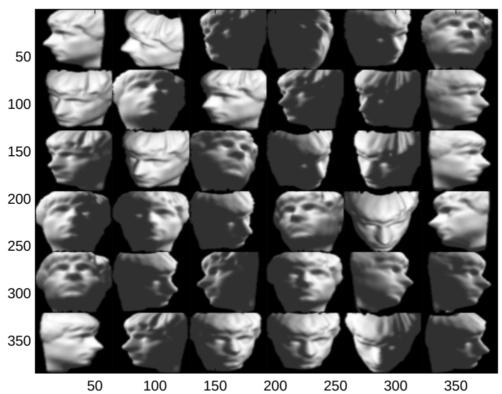
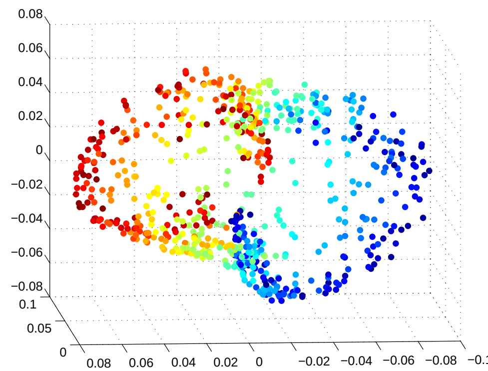
&= \min_{Q,\Lambda'} Tr(\Lambda^2) + Tr(Q\Lambda' Q^T Q \Lambda' Q^T) - 2Tr(\Lambda Q \Lambda' Q^T) \\
&= \min_{\Lambda'} Tr(\Lambda^2 + \Lambda'^2 - 2\Lambda\Lambda') \\
&= \min_{\Lambda'} Tr(\Lambda - \Lambda')^2
\end{aligned}
$$

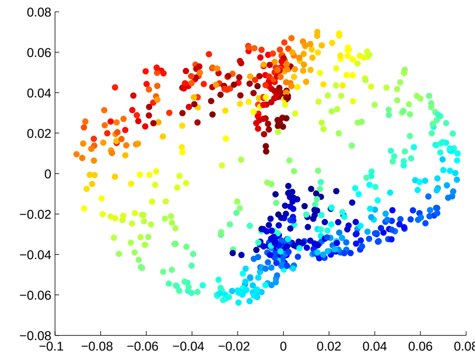
- The minimum is thus obtain for $\Lambda' = Diag(\lambda_1, \cdots, \lambda_d, 0, \cdots, 0)$ and one can choose $Q = V^T W = Id_N$ ($\Rightarrow W = V$).
- Since $YY^T = W\Lambda' W^T$, one has $Y = W\Lambda'^{\frac{1}{2}} = V\Lambda'^{\frac{1}{2}}$.

# MDS: example




3D-proj: light

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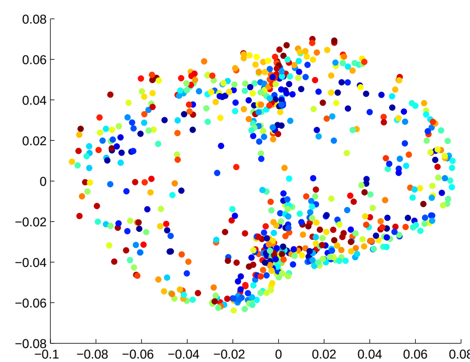



2D-proj: pose 2

# MDS: remarks

- Let $v \in \mathbb{R}^D$ be an eigenvector of $C$ with eigenvalue $\lambda$. One has

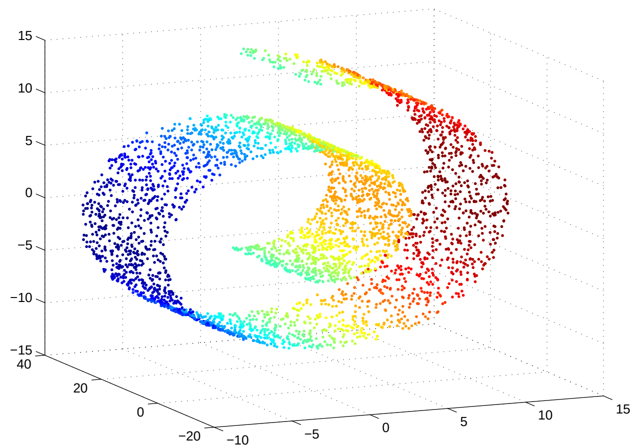
$$GXv = XX^T Xv = XCv = \lambda Xv$$

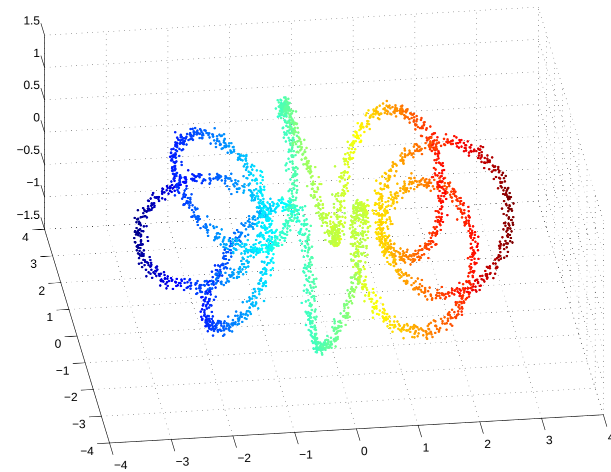
so $Xv \in \mathbb{R}^N$ is an eigenvector of $G$ with eigenvalue $\lambda$. Equivalently if $w \in \mathbb{R}^N$ is an eigenvector of $G$ with eigenvalue $\mu$, $X^T w \in \mathbb{R}^D$ is an eigenvector of $C$ with eigenvalue $\mu$.

- IMPORTANT: MDS does not require the knowledge of the coordinates of the points of $X$. If only the matrix $D$ of the pairwise squared distances between the data points is known, one can still apply MDS by first “double centering” $D$: $G = -\frac{1}{2}JDJ$.
- IMPORTANT: If $D$ is not obtained from a point cloud $X \subset \mathbb{R}^D$, one can still apply MDS but $G$ may have negative eigenvalues (indeed negative eigenvalues signify that $D$ is non Euclidean). The $d$-dimensional embedding $Y_{MDS}$ given by MDS is the one that have the Gram matrix that best approximates $G == -\frac{1}{2}JDJ$ (Eckart and Young ’36): for any $Y \subset \mathbb{R}^d$,

$$\|Y_{MDS}Y_{MDS}^T - G\| \leq \|YY^T - G\|$$

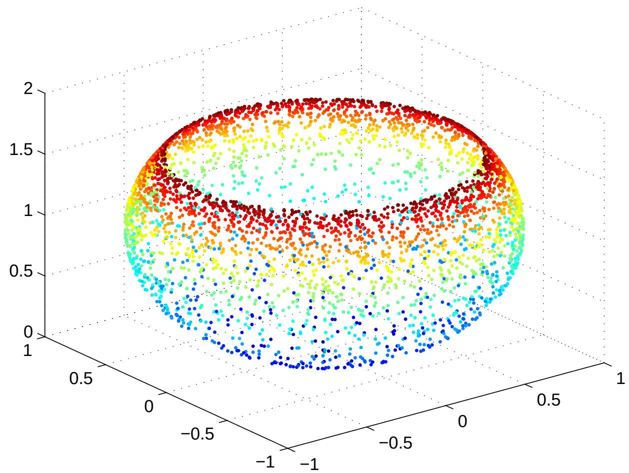
# Turning non linear

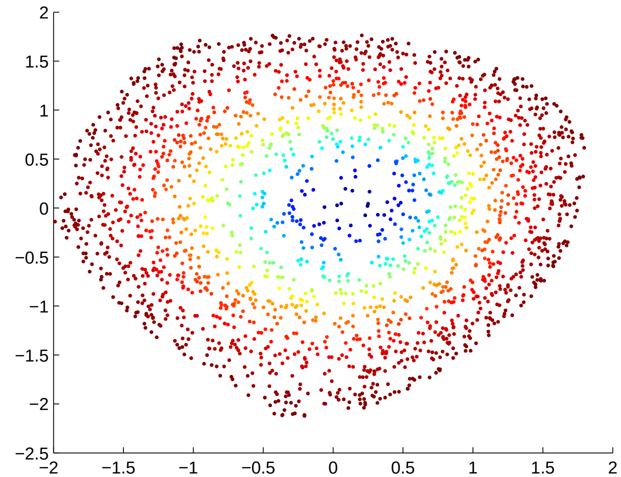



- (Classical) PCA and MDS become inefficient when the data is located around highly non linear manifolds.
- From now on we assume that the observed data lie on or are close to a $d$-dimensional submanifold $M \subset \mathbb{R}^D$.

# Locally Linear Embedding (L. Saul and S Roweis ’00)

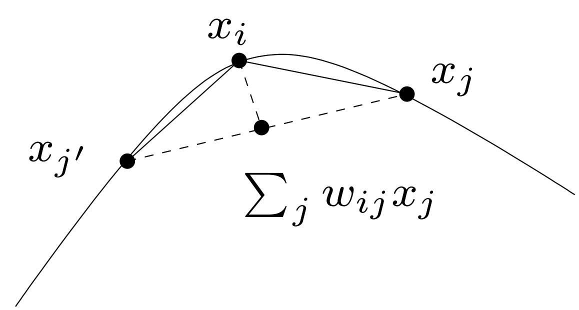



- Preservation of the local geometry of the data: LLE intends to find an embedding of the data $X \subset \mathbb{R}^D$ such that
  - nearby points remain nearby in the target low dimensional space,
  - nearby points remain similarly co-located in the target low dimensional space.

# LLE: overview of the algorithm

1. Build a neighborhood graph $\mathcal{G}$ with vertex set $X$ (e.g. $k$-NN or Rips graph). Compute weights $w_{ij}$ that best reconstruct each data point $x_i$ from its neighbors by minimizing the cost function




2. $$E(W) = \sum_i \|x_i - \sum_j w_{ij} x_j\|^2$$

   with the constraints that $w_{ij} = 0$ if $x_i$ and $x_j$ are not connected in $\mathcal{G}$ and that $\sum_j w_{ij} = 1$.

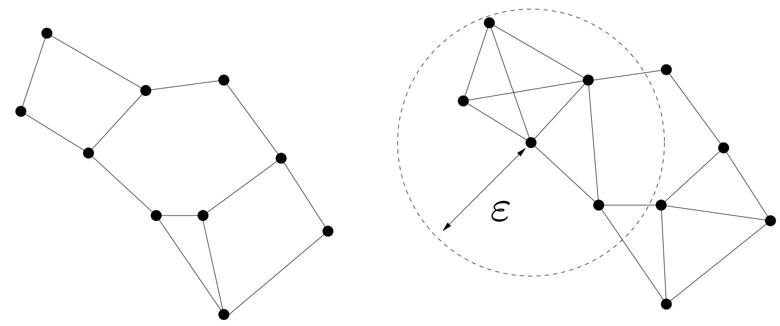
3. Compute the vectors $y_i$ minimizing the quadratic cost

$$\Phi(Y) = \sum_i \|y_i - \sum_j w_{ij} y_j\|^2$$

# LLE: step 1

- $k$-NN graph (depends on an interger parameter $k$): $x_i x_j$ is an edge of $\mathcal{G}$ iff $x_j$ is one of the $k$ nearest neighbours of $x_i$ (and vice-versa).

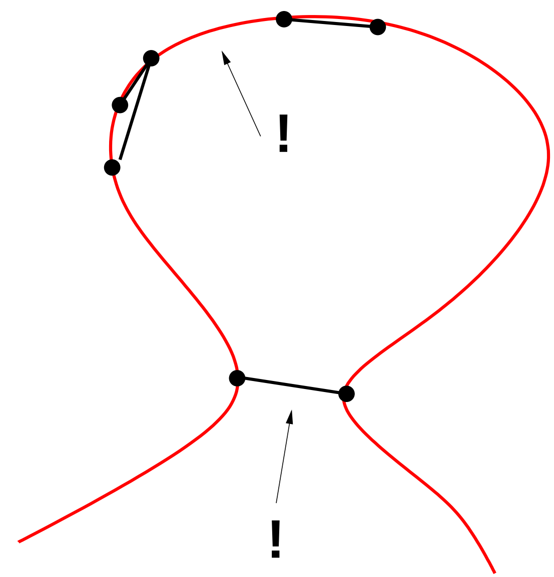
- Rips graph (depends on a real parameter $\varepsilon > 0$): $x_i x_j$ is an edge of $\mathcal{G}$ iff $d(x_i, x_j) \leq \varepsilon$.




3–NN

Rips graph

Take care that choosing the right neighborhood size may be problematic:



# LLE: step 2

Minimization of

$$E(W) = \sum_{i=1}^{N} \|x_i - \sum_{j \in N_{\mathcal{G}}(x_i)} w_{ij} x_j\|^2$$

with the constraints:

- $w_{ij} = 0$ if $x_i$ and $x_j$ are not connected in $\mathcal{G}$,
- $\sum_j w_{ij} = 1$.

- The weights $w_{ij}$ are invariant under rotation, scaling and translation (translation invariance commes from the 2nd constraint).
- The minimization boils down to $N$ quadratic minimizations under constraints. Let $x \in X$, let $x_j$ be its neighbors in $\mathcal{G}$ and let $w_j = w_{ij}$:

$$\varepsilon = \|x - \sum_{j \in N_{\mathcal{G}}(x)} w_j x_j\|^2 = \|\sum_j w_j (x - x_j)\|^2 = \sum_{j,k} w_j w_k G_{jk}$$

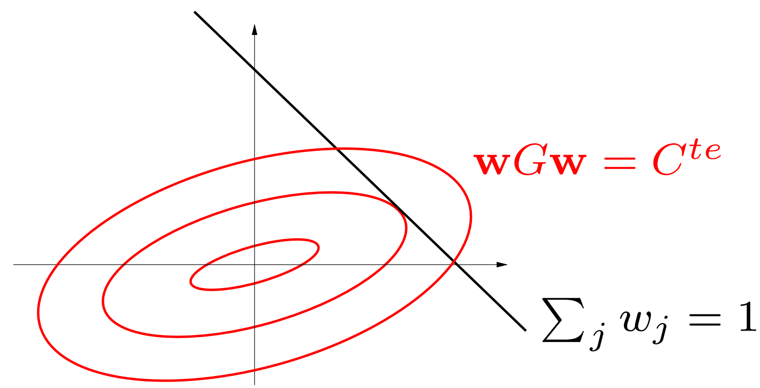
where $G = (G_{jk}) = ((x - x_j)^T (x - x_k))$ is the “local” Gram matrix.

# LLE: step 2

$$\varepsilon = \|x - \sum_{j \in N_{\mathcal{G}}(x)} w_j x_j\|^2 = \|\sum_j w_j (x - x_j)\|^2 = \sum_{j,k} w_j w_k G_{jk}$$

where $G = (G_j k) = ((x - x_j)^T (x - x_k))$ is the “local” Gram matrix.

- $G$ being semipositive definite, the minimization of $\varepsilon$ admits a closed form solution:
  - Solve the linear system $G\mathbf{w} = (1, 1, \cdots, 1)^T$
  - Rescale the $w_j$ such that they sum to $1$.




- Warning: if $G$ is singular or nearly singular (e.g. if the number of neighbors is greater than $D$), it may need to be regularized by adding a small multiple of the identity matrix ($\Rightarrow$ penalize large weigths).

# LLE: step 3

This step no longer requires the points $x_i$. Compute vectors $y_i$ minimizing the quadratic cost

$$\Phi(Y) = \sum_i \|y_i - \sum_j w_{ij} y_j\|^2 = \sum_i \left( y_i^T y_i - 2 \sum_j w_{ij} y_i^T y_j + \sum_{k,l} w_{ik} w_{il} y_k^T y_l \right) = \sum_{ij} M_{ij} y_i^T y_j$$

where $M_{ij} = \delta_{ij} - w_{ij} - w_{ji} + \sum_k w_{ki} w_{kj}$ (note that $M = (I - W)^T (I - W)$).

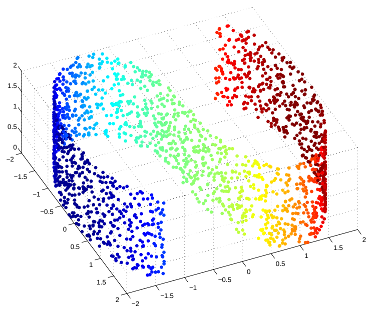
**Constraints:**

- remove translational degree of freedom: $\overline{y} = \sum_i y_i = 0$
- remove rotational degree of freedom: $\frac{1}{N} \sum_i y_i y_i^T = Id_d$

## Solution:

- compute the $(d+1)$ eigenvectors $\mathbf{v}_0, \cdots \mathbf{v}_d$ of $M$ corresponding to the $(d+1)$ smallest eigenvalues $\lambda_0 \leq \cdots \leq \lambda_d$ and discard $\mathbf{v}_0$.
- the $y_i$ are given by the lines of the matrix $(\mathbf{v}_1 \mathbf{v}_2 \cdots \mathbf{v}_d)$.

# LLE: examples



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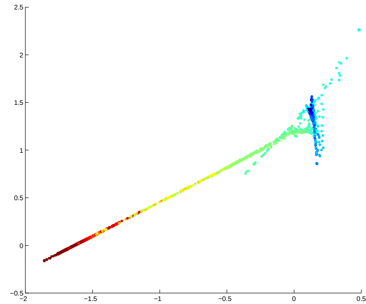
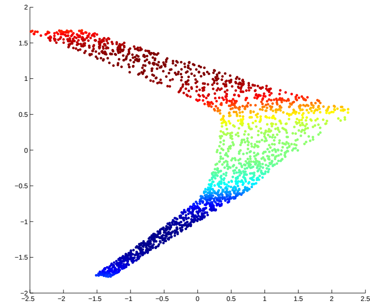
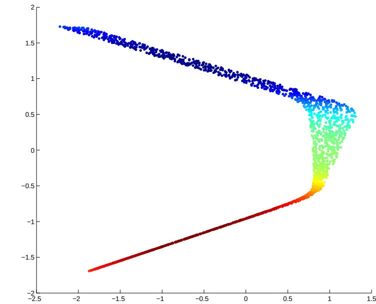


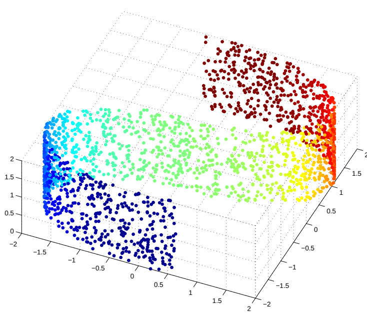
$k = 5NN$



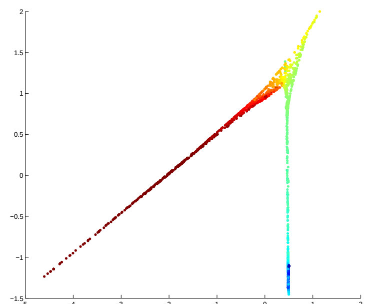
$k = 12NN$



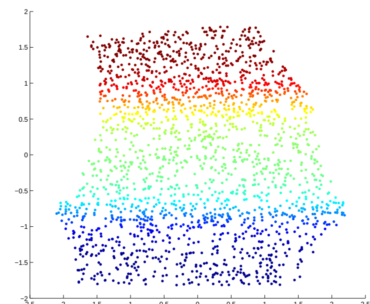
$k = 30NN$



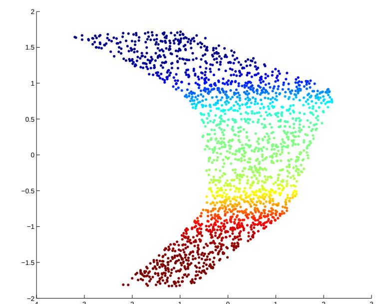
$S'$



$k = 5NN$

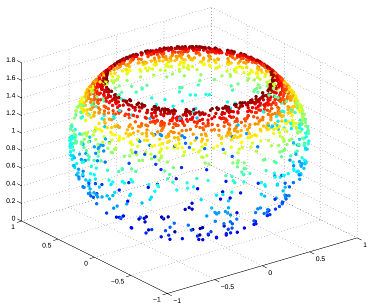


$k = 12NN$

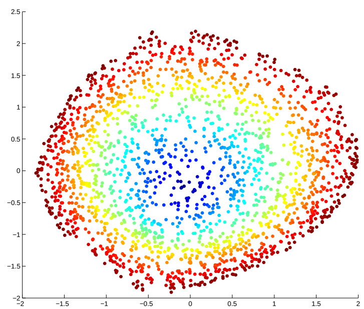


$k = 30NN$

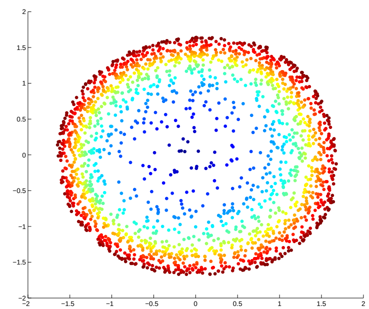
# LLE: examples



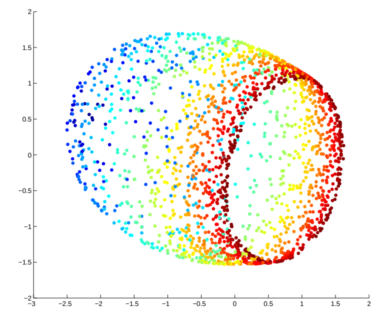
Fishbowl



$k = 12NN$

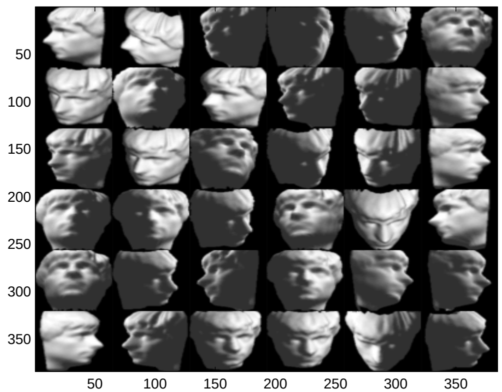


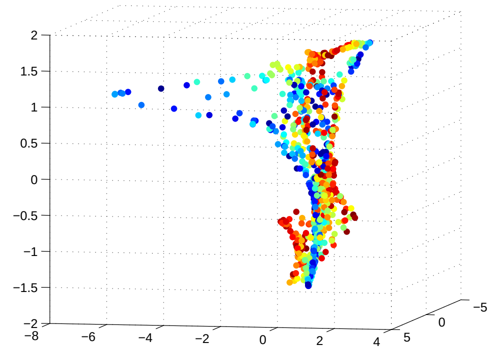
$k = 30NN$



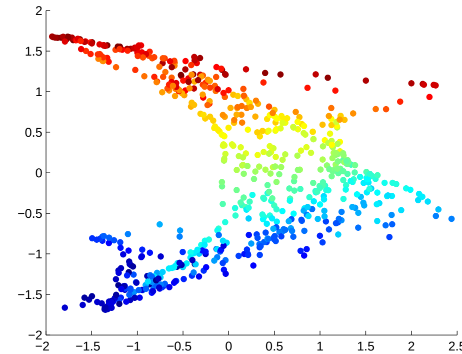
$k = 80NN$

# LLE: examples




3D-proj: light



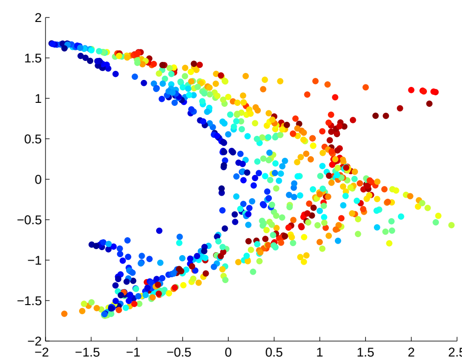

2D-proj: pose 1

Dimension: $64 * 64 = 4096$.

$N = 698$

3 free parameters:

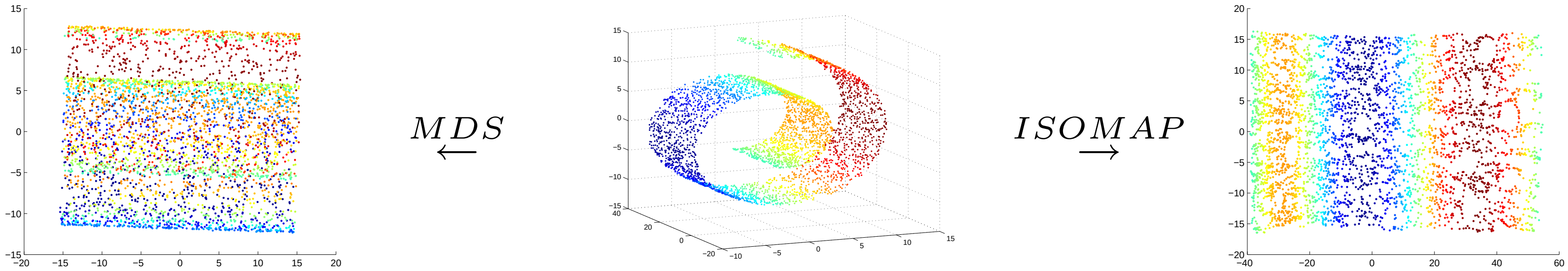
- left-right pose,
- up-down pose,
- light pose.




2D-proj: pose 2

$k = 6$ NN

# ISOMAP (de Silva, Tenenbaum, Langford ’00)




Variant of MDS where the matrix of Euclidean distances between data points is replaced by the matrix of the geodesic distances between data points.

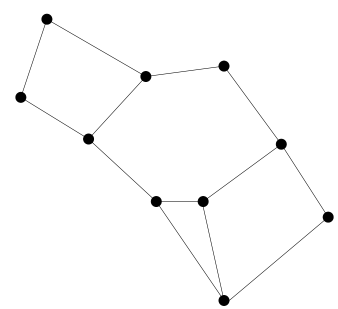
## Algorithm:

1. Build a neighborhood graph $\mathcal{G}$ with vertex set $X$ such that the geodesic distances on $\mathcal{G}$ approximates the geodesic distances on $M$.
2. Build the matrix $D_{\mathcal{G}} = (d_{\mathcal{G}}(x_i, x_j))$ of the pairwise squared distances in $\mathcal{G}$.
3. Apply MDS to $D_{\mathcal{G}}$.

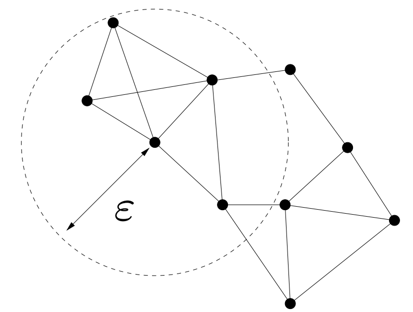
# Geodesic distance approximation

- $k$-NN graph (depends on an interger parameter $k$): $x_i x_j$ is an edge of $\mathcal{G}$ iff $x_j$ is one of the $k$ nearest neighbours of $x_i$ (and vice-versa).

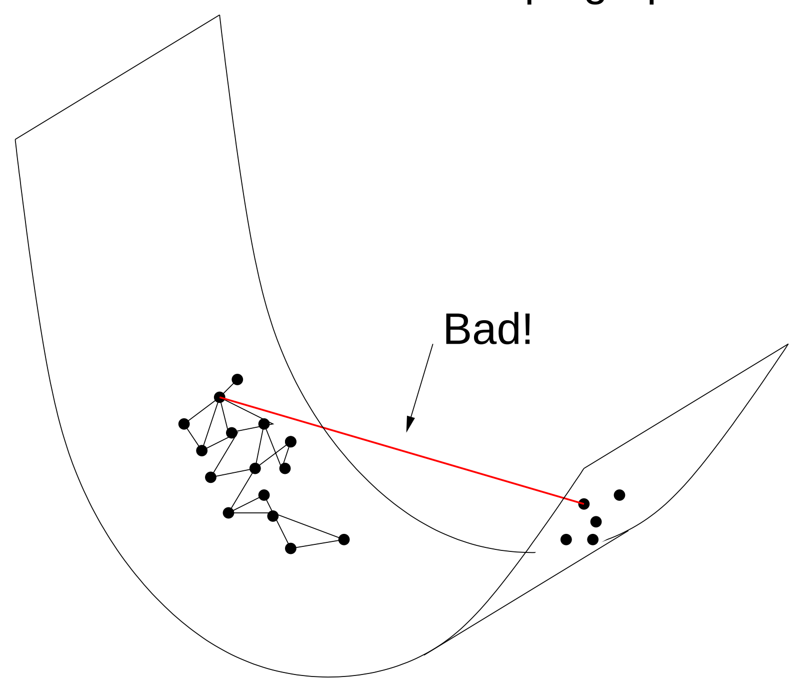
- Rips graph (depends on a real parameter $\varepsilon > 0$): $x_i x_j$ is an edge of $\mathcal{G}$ iff $d(x_i, x_j) \leq \varepsilon$.



3–NN




Rips graph




- Avoid too long edges in $\mathcal{G}$
- $X$ has to sample densely $M$
- The edges of $\mathcal{G}$ are weighted by their length.

# Geodesic distance approximation

The geodesic distance between $x_i$ and $x_j$

$$d_M(x_i, x_j) = \inf\{l(\gamma)|\gamma : [0,1] \to M, \gamma(0) = x_i, \gamma(1) = x_j\}$$

in the manifold $M$ is approximated by the length $d_{\mathcal{G}}(x_i, x_j)$ of the shortest path between $x_i$ and $x_j$ in $\mathcal{G}$ (that can be computed by Dijkstra's algorithm).

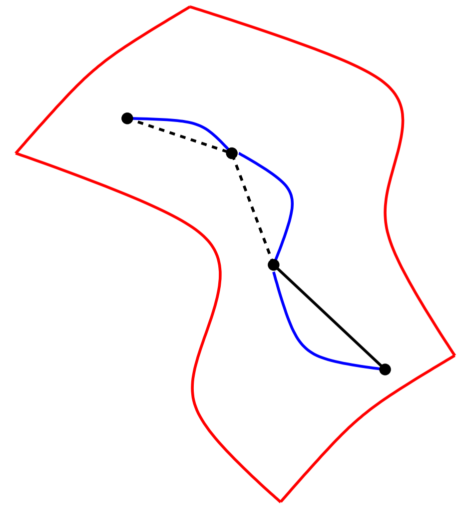
**Theorem [Bernstein & al'00]:** Let $\lambda > 0$. For some small enough $\delta, \varepsilon > 0$ ($\delta < \varepsilon$), if $X$ is a $\delta$-sample of $M$ and if $\mathcal{G}$ is such that $(d(x_i, x_j) < \varepsilon \Leftrightarrow (x_i x_j)\ is\ an\ edge\ of\ \mathcal{G})$ then for all $x_i, x_j$

$$1 - \lambda < \frac{d_{\mathcal{G}}(x_i, x_j)}{d_M(x_i, x_j)} < 1 + \lambda$$

# Geodesic distance approximation

**Sketch of proof:**

Let $d_S(x,x') = \min_P \sum_{j=0}^{p-1} d_M(x_j, x_{j+1})$ where $P = (x_{i_0} = x, x_{i_1}, \cdots x_{i_p} = x') \subset X$.

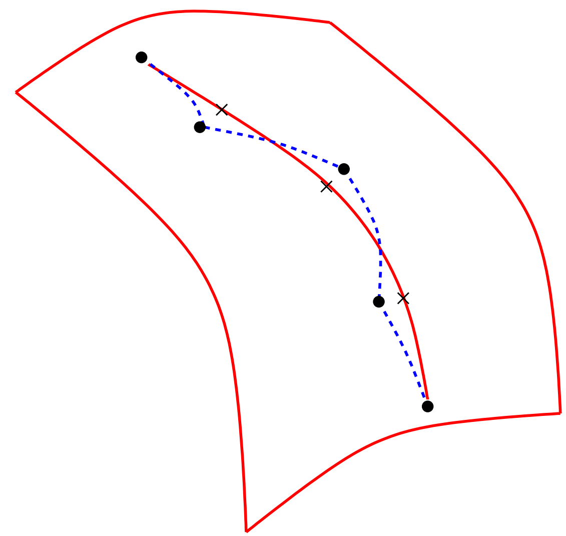


- From a distance function property (Federer):

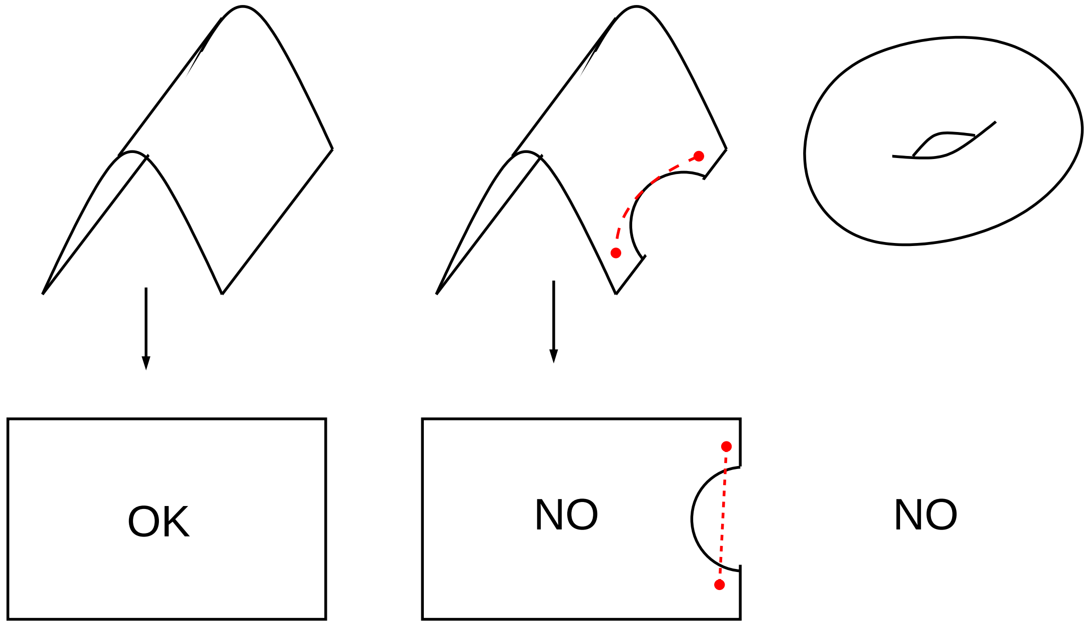
$$\frac{R-\varepsilon}{R} d_S \leq d_{\mathcal{G}} \leq d_S, \quad R = reach(M)$$

- Using that $X$ is a $\delta$-sample of $M$ one "approximately" gets

$$d_M \leq d_S \leq \frac{\varepsilon}{\varepsilon - 2\delta} d_M$$



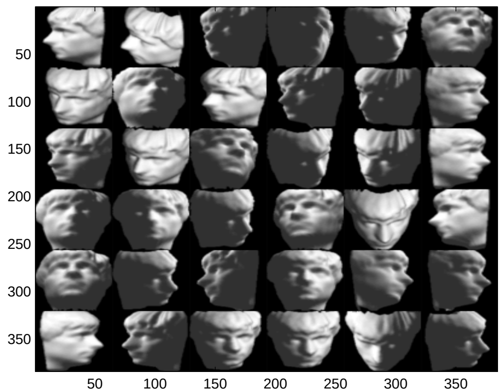
# Theoretical guarantees of ISOMAP

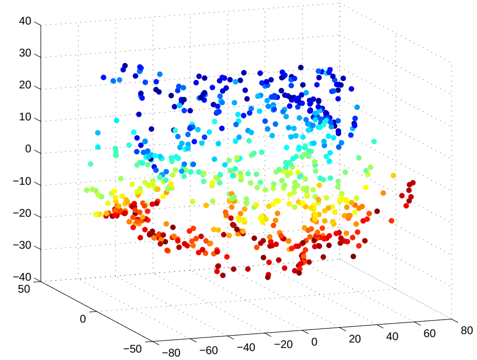



ISOMAP intends to map $X$ into $Y \subset \mathbb{R}^d$ in such a way that the pairewise geodesic distances in $X$ are as close as possible to the pairwise euclidean distances in $Y$

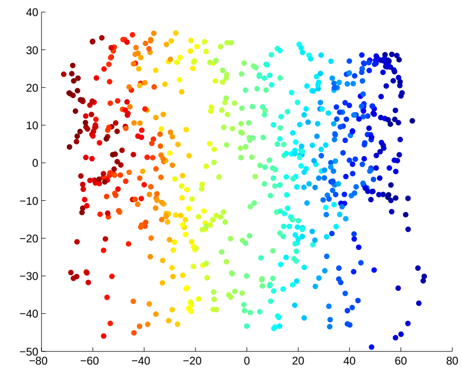
$\Longrightarrow$ $M$ has to be isometric to a convex open subset of $\mathbb{R}^d$, i.e. there exists a convex open $\Omega$ domain in $\mathbb{R}^d$ and an embedding $f : \Omega \to \mathbb{R}^d$ s.t. $f(\Omega) = M$ and for all $y, y' \in \Omega$, $d_M(f(y), f(y')) = \|x - x'\|$.

# ISOMAP: example



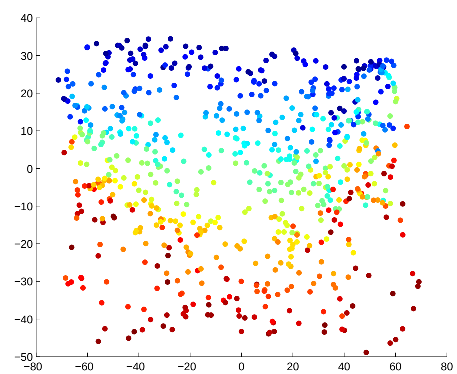

3D-proj: light




2D-proj: pose 1

Dimension: $64 * 64 = 4096$.

$N = 698$

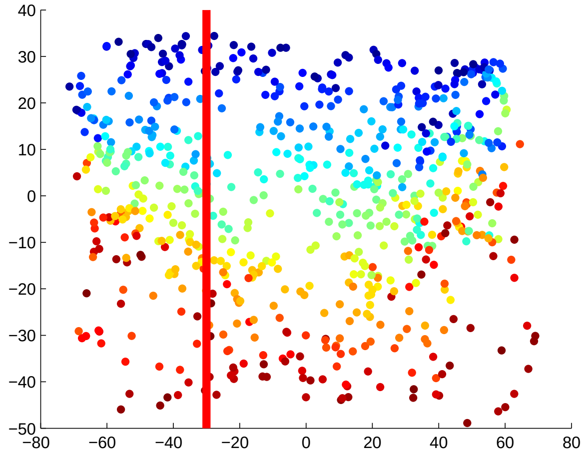



2D-proj: pose 2

3 free parameters:

- left-right pose,
- up-down pose,
- light pose.

$k = 6$ NN



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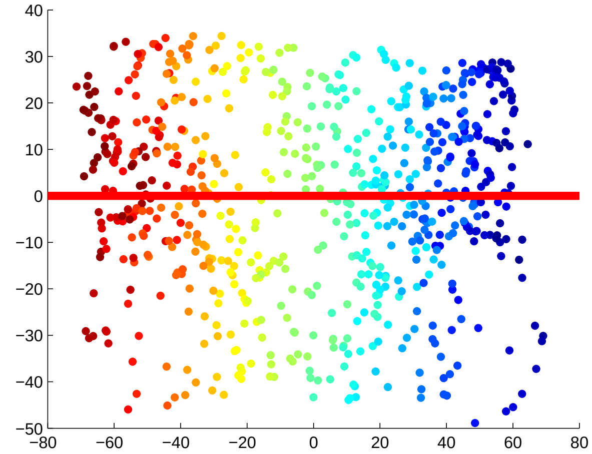

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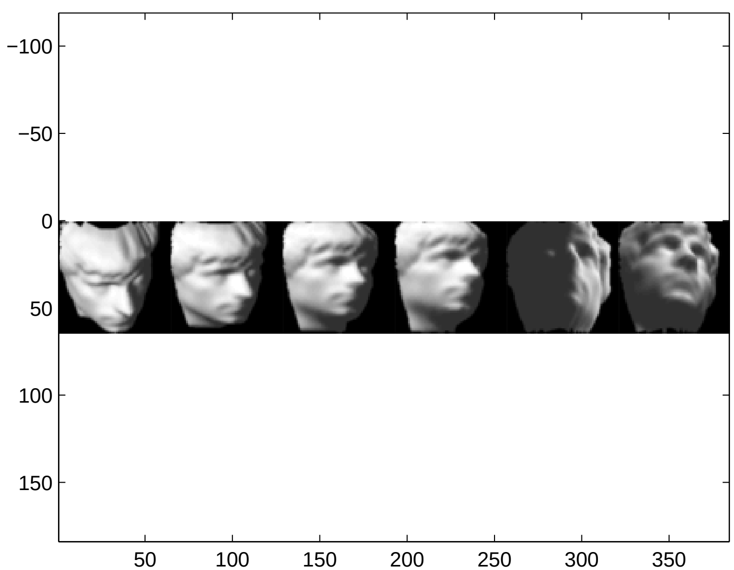

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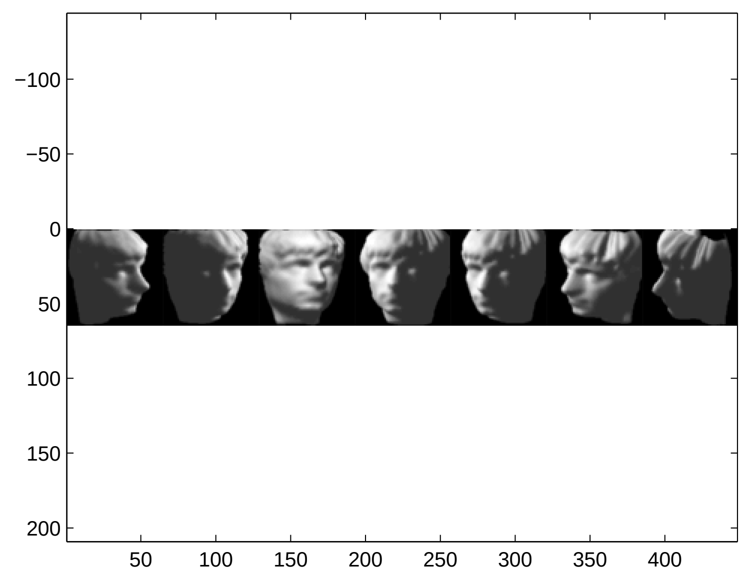

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# Some remarks on ISOMAP

**Advantages:**

- intend to preserve the “intrinsic metric” of the data.
- come with geometric guarantees

**Drawbacks:**

- ISOMAP is a global method: as in MDS, if the size of the data is very large, the computations of the eignevalues/eigenvectors of $G = -0.5JDJ$ is an issue.

  $\Longrightarrow$ Landmark ISOMAP
- Assuming that $M \subset \mathbb{R}^D$ is isometric to a convex open set of $\mathbb{R}^d$ is rather restrictive.

  $\Longrightarrow$ Conformal ISOMAP

# Conformal ISOMAP (de Silva, Tenenbaum)

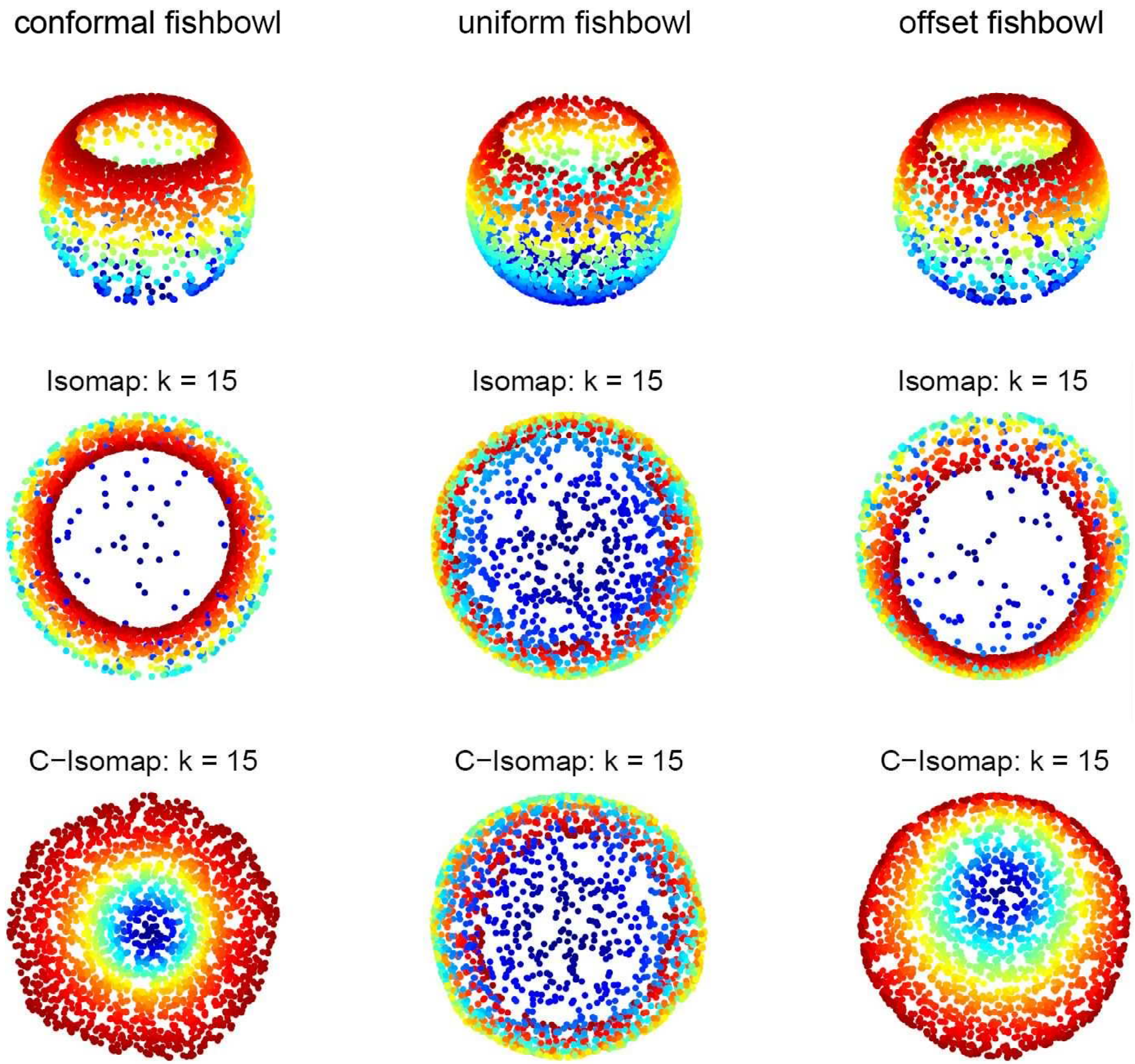
Assume that $M = f(\Omega)$ where $\Omega$ is a domain in $\mathbb{R}^d$ and $f : \Omega \to \mathbb{R}^D$ is a smooth ($\mathcal{C}^2$) conformal embedding: $f$ preserve infinitesimal angles i.e. for any $y \in \Omega$ there exists $s(y) > 0$ s.t. for any $\mathbf{v} \in \mathbb{R}^d$, $\|d_y f(\mathbf{v})\| = s(y)\mathbf{v}$.

- C-ISOMAP is a simple variant of ISOMAP where the weights of the edges $(x_i x_j)$ is replaced by $\frac{d(x_i, x_j)}{\sqrt{M(i)M(j)}}$ where $M(i)$ is the mean distance between $x_i$ and its $k$-nearest neighbors (for some user defined $k$).
- $\sqrt{M(i)M(j)}$ is an approximation of the conformal factor $s(y)$.
- **Theorem [de Silva et al.]:** If $f$ is a smooth conformal embedding of a bounded convex domain $\Omega$ in $\mathbb{R}^d$ and if $X = f(Y)$ where $Y$ is a uniformly sampled of $\Omega$ then $d_\mathcal{G}$ is close to the original distance in $\Omega$: for any $\lambda, \mu > 0$ and for a suitable $k$,

$$1 - \lambda \leq \frac{d_\mathcal{G}}{d_\Omega} \leq 1 + \lambda$$

with probability at least $1 - \mu$ provided that $|X|$ is large enough.

# C-ISOMAP: example



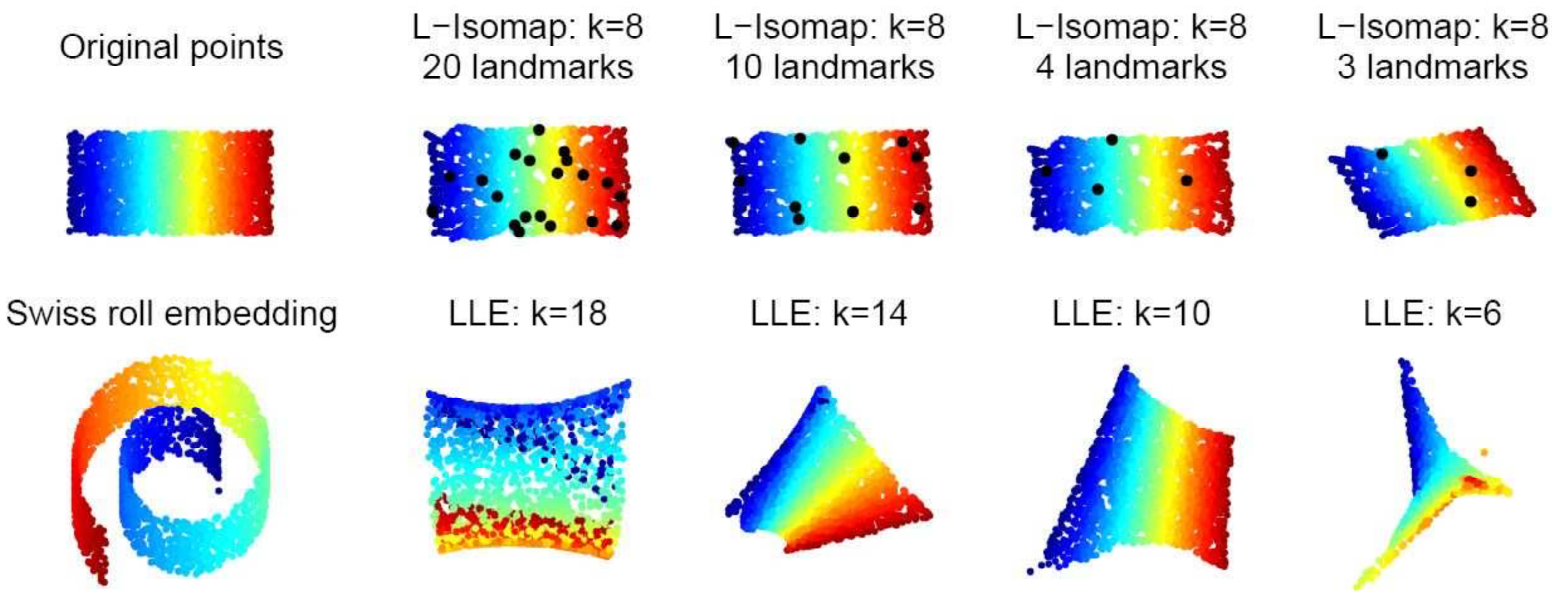

*Results from V. de Silva, J.B. Tenenbaum, NIPS 15, 2003*

# Landmark ISOMAP (de Silva, Tenenbaum)

- Select $n > d$ landmarks among the data points and compute the $n \times N$ matrix $D_{n,N}$ of the squared distances from each data point to the landmarks.
- Replace classical MDS by a Landmark-MDS:
  - Compute the matrix $D_n$ of the squared distances between the landmarks and $G_n = -\frac{1}{2} J D_n J$.
  - The embedding of the landmarks in $\mathbb{R}^d$ is given by (classical) MDS, i.e. by the $n \times d$ matrix $Y_n^T = (\sqrt{\lambda_1}\mathbf{v}_1 \sqrt{\lambda_2}\mathbf{v}_2 \cdots \sqrt{\lambda_d}\mathbf{v}_d)$ where $\lambda_i$ and $\mathbf{v}_i$ are the largest eigenvalues/vectors of $D_n$.
  - Embed the remaining points in the following way: for $x \in X$, let $D_x$ be the vector of the distances between $x$ and the $n$ landmarks and let $\overline{D}_n$ be the vector of the mean of the columns of $D_n$. Then $x$ is sent to

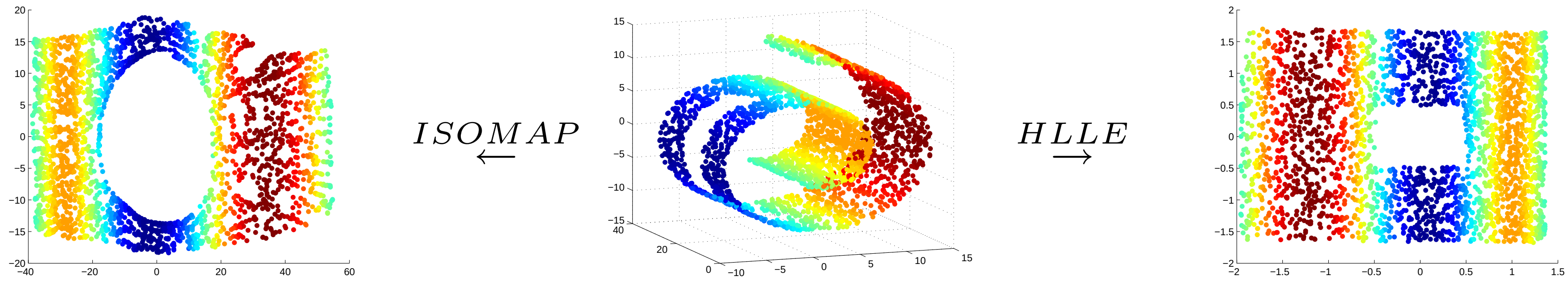
$$y = \frac{1}{2} L^{\#}(\overline{D}_n - D_x) \text{ where } L^{\#} = \begin{pmatrix} \mathbf{v}_1^T / \sqrt{\lambda_1} \\ \mathbf{v}_2^T / \sqrt{\lambda_2} \\ \vdots \\ \mathbf{v}_d^T / \sqrt{\lambda_d} \end{pmatrix}$$

# L-ISOMAP: example




*Results from V. de Silva, J.B. Tenenbaum, NIPS 15, 2003*

# Hessian eigenmaps (D. Donoho, C. Grimes ’03)

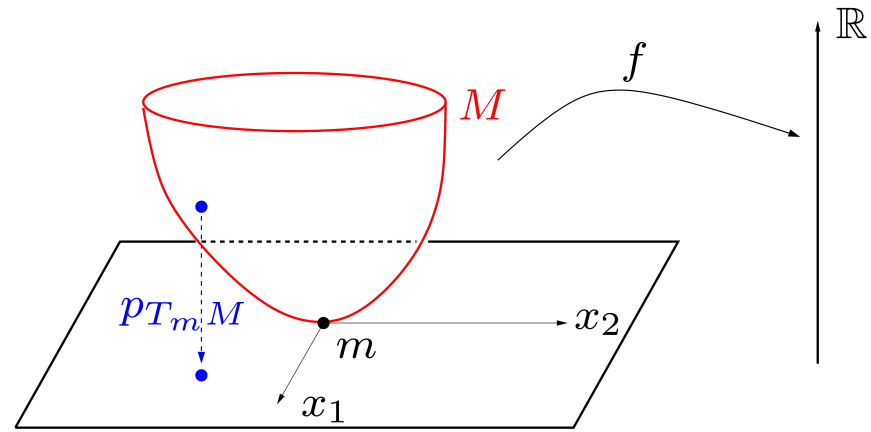



A “proven” method for isometric embeddings of open sets of euclidean spaces:

- $M = \psi(\Omega)$, $\psi : \Omega \subset \mathbb{R}^d \to \mathbb{R}^d$ isometry and $\Omega$ does not need to be convex....
- ... but it involves the estimation of $2^{nd}$ order differential quantities.

# HLLE

$\Omega \subset \mathbb{R}^d$ be an open connected set and let $\psi : \Omega \to M$ be a smooth locally isometric embedding.



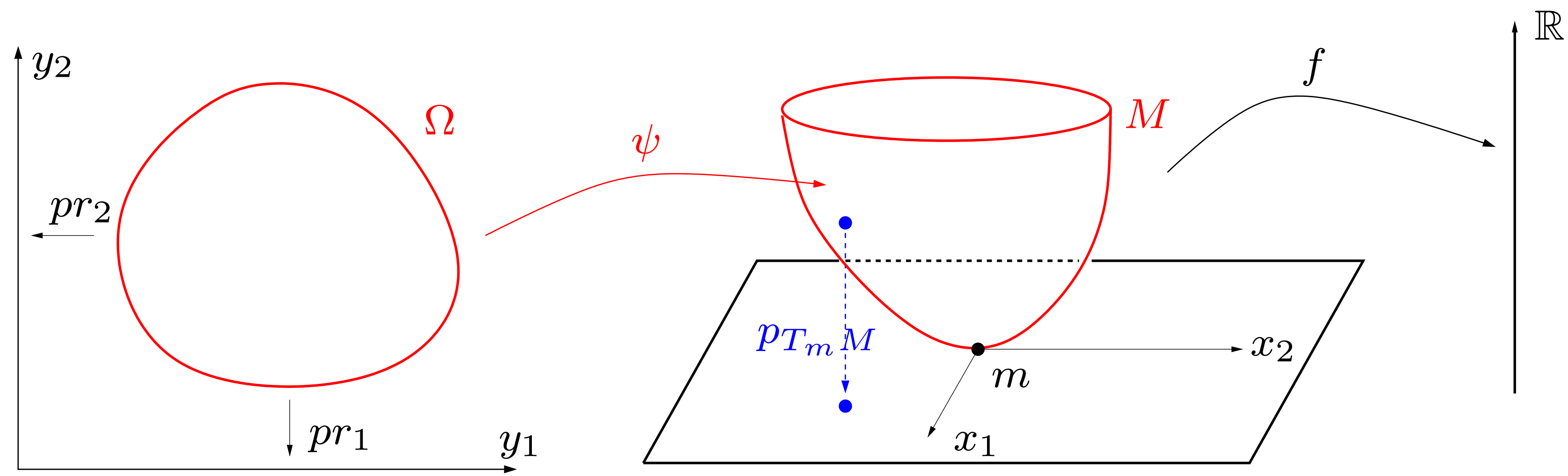

- Let $m \in M$, let $(x_1, \cdots, x_d)$ be an orthonormal coordinate system on $T_m M$. The projection $p_{T_m M}$ of $M$ on $T_m M$ is well- defined on a neighborhood of $m$ in $M$. For any $f \in \mathcal{C}^2(M, \mathbb{R})$, the Hessian of $f$ at $m$ in tangent coordinates is defined by

$$(H_f^{tan}(m))_{ij} = \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} f(p_{T_m M}^{-1}(x))|_{x=0}$$

- Consider the quadratic form on $\mathcal{C}^2(M, \mathbb{R})$ defined by

$$\mathcal{H}(f) = \int_M \|H_f^{tan}(m)\|^2 dm$$

# HLLE

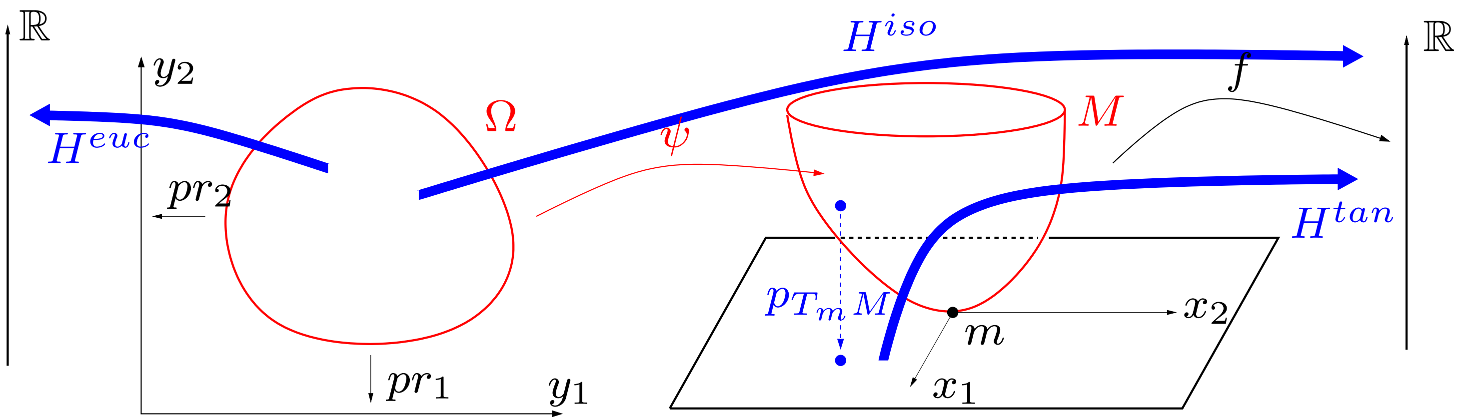



**Theorem [Donoho et al. '03]:** Assume that $M = \psi(\Omega)$ where $\Omega \subset \mathbb{R}^d$ is an open connected set and $\psi$ is a locally isometric embedding of $\Omega$. Then the null-space of the quadratic form

$$\mathcal{H}(f) = \int_M \|H_f^{tan}(m)\|^2 dm$$

is $(d+1)$-dimensional and generated by the constant functions and the $d$ original isometric coordinates $pr_i \circ \psi^{-1}$ where $pr_i : \mathbb{R}^d \to \mathbb{R}$ is the linear projection on the $i^{th}$ coordinate in $\mathbb{R}^d$.

# HLLE




**Sketch of the proof:**

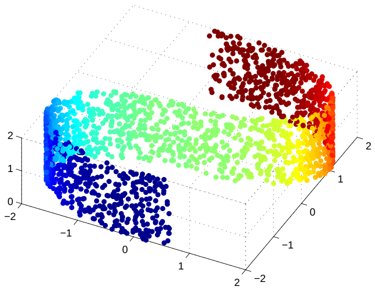
- $H_f^{iso} = H_{f\circ\psi}^{euc} \Rightarrow \mathcal{H}^{iso}(f) = \mathcal{H}^{euc}(f \circ \psi)$ , $\forall f \in \mathcal{C}^2(M, \mathbb{R})$.
- The null-space of $\mathcal{H}^{euc}$ is the $(d+1)$-dimensional space of affine functions on $\mathbb{R}^d$.
- $H_f^{tan}(m) = H_f^{iso}(m)$:
  - let $v \in T_m M$ and let $\gamma_v : [0, \varepsilon) \longrightarrow M$ a unit speed geodesic s.t. $\gamma_v(0) = m$ and $\gamma_v'(0) = v$. Then $(f \circ \gamma_v)''(0) = v^T H_f^{iso}(m) v$.
  - let $\delta_v : [0, \varepsilon) \longrightarrow M$ defined by $\delta_v(t) = p_{T_m M}^{-1}(tv)$. Then $(f \circ \delta_v)''(0) = v^T H_f^{tan}(m) v$.
  - the accelerations of $\gamma_v$ and $\delta_v$ at $0$ are normal to $T_m M$
  $\Rightarrow |\gamma_v(t) - \delta_v(t)| = o(t^2) \Rightarrow (f \circ \gamma_v)''(0) = (f \circ \delta_v)''(0)$.

# HLLE

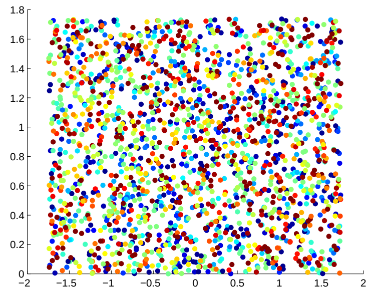
## Algorithm:

1. For each data point $x_i$ identify its $k$ nearest neighbors $\mathcal{N}_i$ (constraint: $\min(k, D) > d$) and for each $i = 1, \cdots, N$ build the recentered matrix $M_i$ with rows $x_j - \overline{x}_i$ where $\overline{x}_i = 1/N \sum_{j \in \mathcal{N}_i} x_j$.
2. Estimation of tangent coordinates: for each $M_i$ compute (using PCA) the $d$-dim. tangent coordinates of the points in $\mathcal{N}_i$
3. Build a tangent Hessian estimator $H^i$ for each $\mathcal{N}_i$.
4. Build the empirical version of the quadratic form $\mathcal{H}$ from $H^i$, $i = 1, \cdots, N$ and find its kernel.

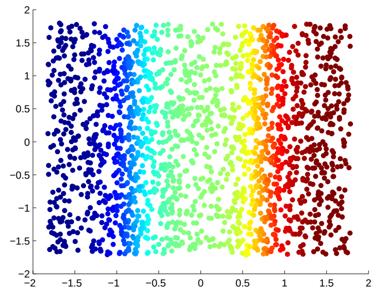
# HLLE: examples



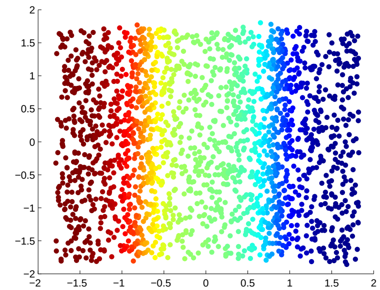
S-shape



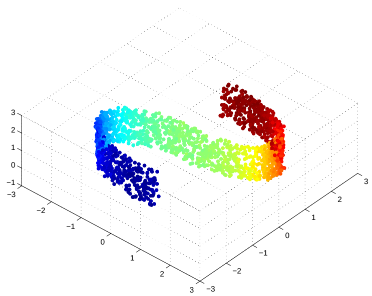
$k = 5NN$



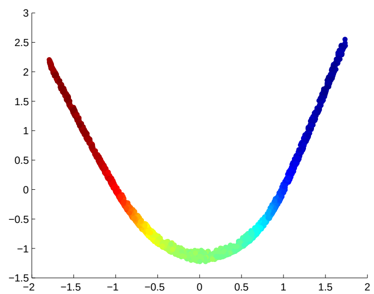
$k = 12NN$



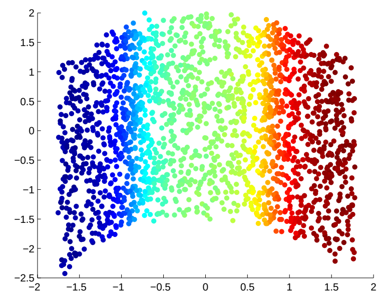
$k = 80NN$



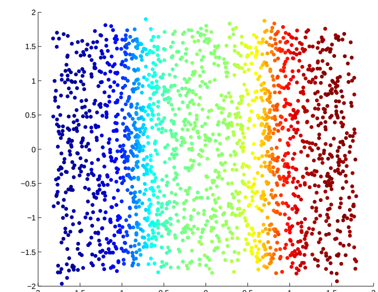
S-shape with small noise



$k = 18NN$

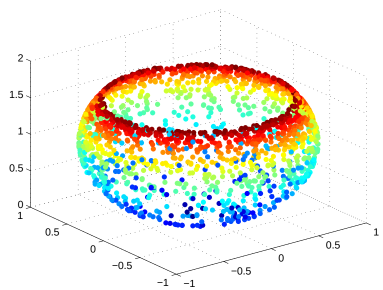


$k = 19NN$

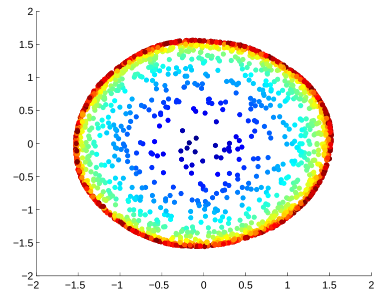


$k = 30NN$

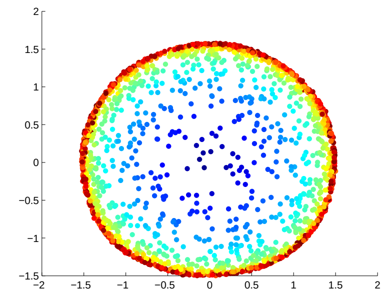
# HLLE: examples



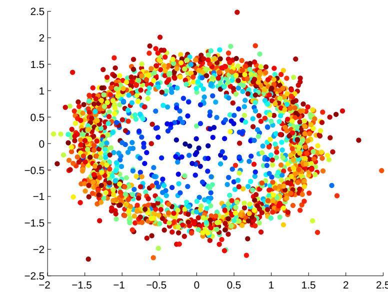
fishbowl



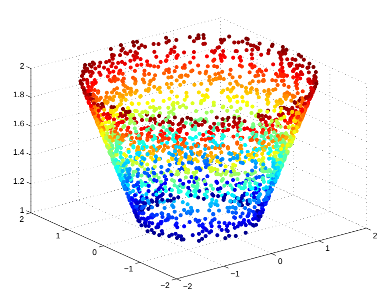
$k = 12NN$



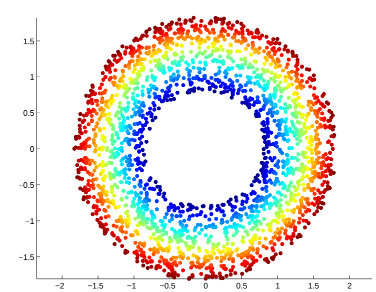
$k = 12NN$



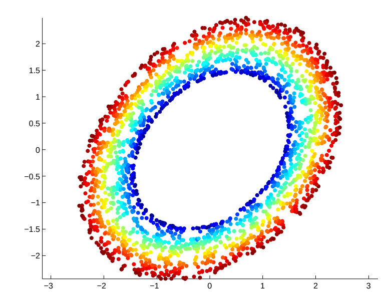
$k = 80NN$



cone

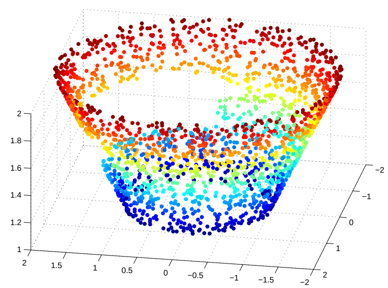


HLLE ($k = 12$)

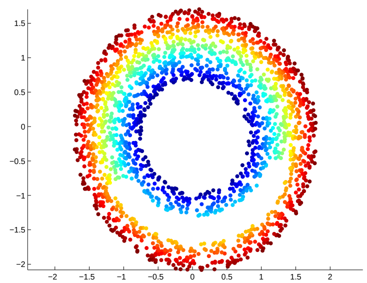


ISOMAP ($k = 12$)

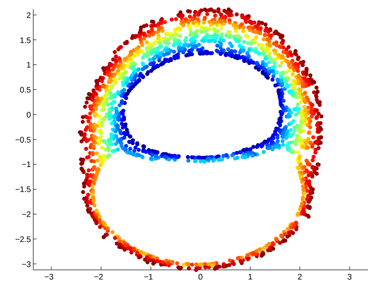
# HLLE: examples



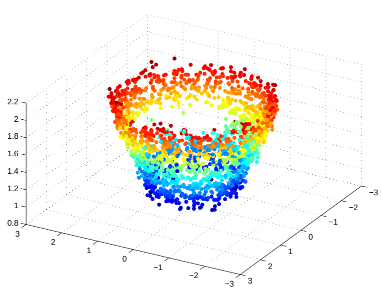
cone



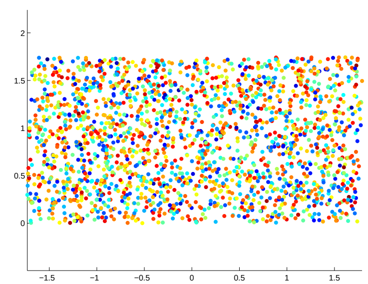
HLLE ($k = 12$)



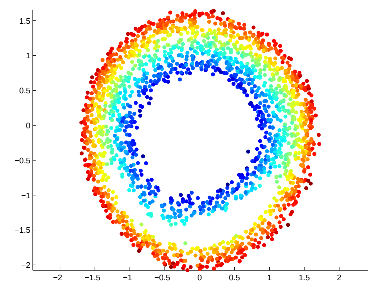
ISOMAP ($k = 12$)



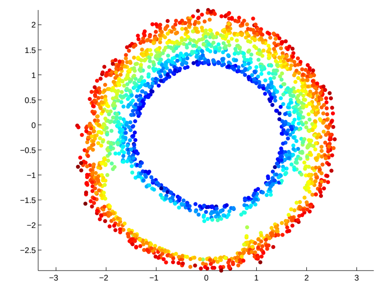
noisy cone



HLLE ($k = 12NN$)

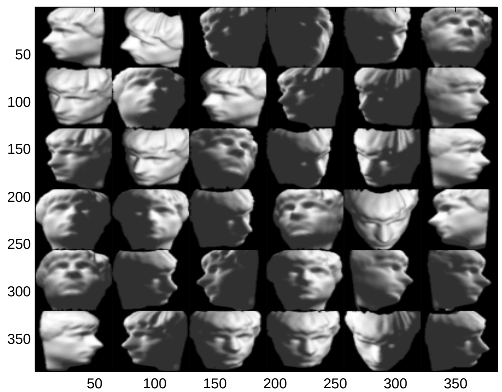


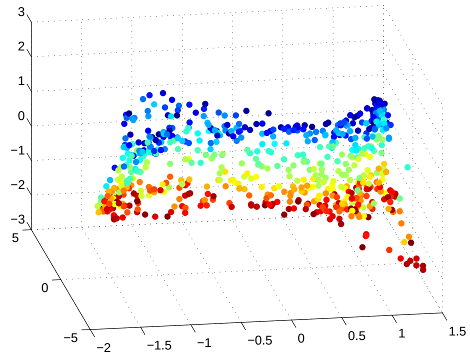
HLLE ($k = 20NN$)



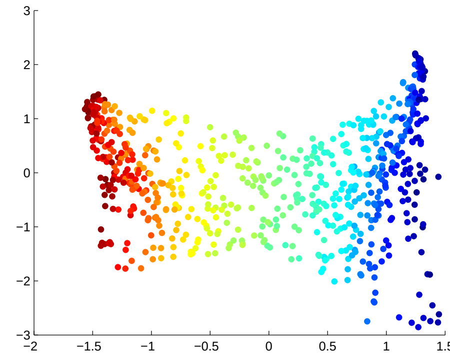
ISOMAP ($k = 20$)

# HLLE: examples



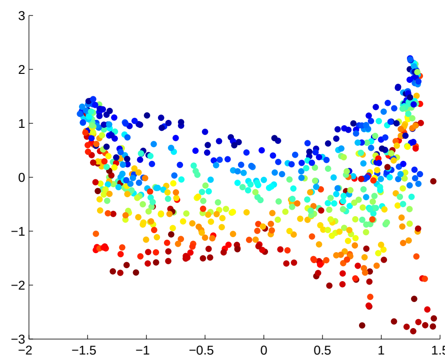

3D-proj: light




2D-proj: pose 1

Dimension: $64 * 64 = 4096$.

$N = 698$



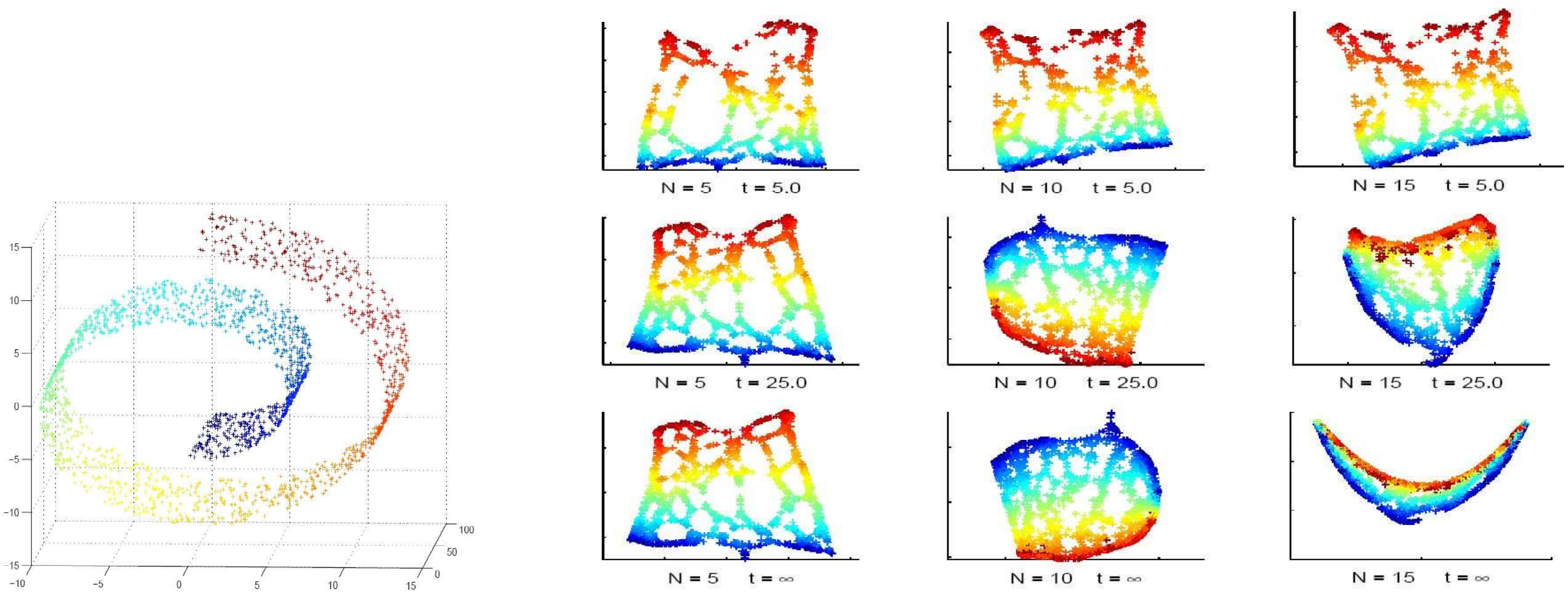

2D-proj: pose 2

3 free parameters:

- left-right pose,
- up-down pose,
- light pose.

$k = 12$ NN

# Laplacian eigenmaps (M. Belkin, P. Niyogi ’02)




(from Belkin et al, Neural Computation, 2003; 15 (6):1373-1396)

- Laplacian eigenmaps intend to embed the data $X$ in a $d$-dimensional in such a way that close/similar points in $X$ remain close in the low dimensional space.
- Analogy with harmonic analysis on the underlying manifold.

# Laplacian eigenmaps

**Overview of the method:**

1. Build a neighborhood graph $\mathcal{G}$ ($k$-NN or Rips).
2. Assign weights $w_{ij}$ to the edges of $\mathcal{G}$ representing the "similarity" between the nodes:
   - Heat kernel: if $(x_i x_j)$ is an edge of $\mathcal{G}$ then

     $$w_{ij} = e^{-\frac{\|x_i - x_j\|^2}{t}}$$

     $w_{ij} = 0$ otherwise.
   - Simple-minded ($t = +\infty$): $w_{ij} = 1$ if $(x_i x_j)$ is an edge of $\mathcal{G}$; $w_{ij} = 0$ otherwise.
3. Compute the eigenvalues and eigenvectors for the generalized eigenvector problem

   $$Lf = \lambda D f$$

   where $D$ is diagonal with $D_{ii} = \sum_j w_{ij}$ and $L = D - W$ is the matrix of the Laplacian operator on $\mathcal{G}$ (see $L$ as an operator acting on the functions defined on the vertices of $\mathcal{G}$).

# Laplacian eigenmaps

## Overview of the method:

3. Compute the eigenvalues and eigenvectors for the generalized eigenvector problem

$$L\mathbf{f} = \lambda D\mathbf{f}$$

where $D$ is diagonal with $D_{ii} = \sum_j w_{ij}$ and $L = D - W$ is the matrix of the Laplacian operator on $\mathcal{G}$ (see $L$ as an operator acting on the functions defined on the vertices of $\mathcal{G}$). Let $\mathbf{f}_0, \cdots, \mathbf{f}_d$ be the solutions aroder according to increasing eigenvalues:

$$\begin{aligned} L\mathbf{f}_0 &= \lambda_0 D\mathbf{f}_0 \\ &\cdots \\ L\mathbf{f}_d &= \lambda_d \mathbf{f}_d \\ 0 &= \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_d \end{aligned}$$

The embedding $y_i \in \mathbb{R}^d$ of $x_i$ is given by $y_i = (\mathbf{f}_1(x_i), \cdots, \mathbf{f}_d(x_i))$ (Note that $\mathbf{f}_0$ corresponding to the eigenvalue $0$ is discarded).

# Laplacian eigenmaps: justification

Assume that one wants to find an embedding $\mathbf{y}^T = (y_1, \cdots y_N)$ of $X$ in $\mathbb{R}$ that minimize

$$E = \sum_{i,j} (y_i - y_j)^2 w_{ij} \quad \text{(with somme additional constraints - see below)}$$

$\longrightarrow$ heavy penalty if close points $x_i$ and $y_i$ are mapped far apart. One has

$$E = \sum_{i,j} (y_i^2 + y_j^2 - 2y_i y_j) w_{ij} = \sum_i y_i^2 D_{ii} + \sum_j y_j^2 D_{jj} - 2 \sum_{i,j} y_i y_j w_{ij} = 2\mathbf{y}^T L \mathbf{y}$$

- $\Rightarrow$ $L$ is positive semidefinite.
- $\Rightarrow$ minimizing $E$ reduces to minimizing $\mathbf{y}^T L \mathbf{y}$ and one has to add a constraint to remove a scaling factor (and avoid obvious solution): $\mathbf{y}^T D \mathbf{y} = 1$ (one uses $D$ rather than $Id$ because it reflects the respective importance of the vertices in $\mathcal{G}$).
- $\Rightarrow$ $\mathbf{y}$ minimizing $E$ is given by the smallest non zero eigenvalue solution to the generalized eigenvalue problem $L\mathbf{y} = \lambda D \mathbf{y}$ (note that the eigenfunction corresponding to the eigenvalue $0$ is the constant function $(1, \cdots, 1)$ mapping all the data points on a single point - corresponding constraint: $\mathbf{y}^T D (1, \cdots, 1)^T = 0$).

# Laplacian eigenmaps: justification

**General case:**

Find $Y = \{y_1, \cdots y_N\} \subset \mathbb{R}^d$ that minimizes

$$E = \sum_{i,j} \|y_i - y_j\|^2 w_{ij} = ?$$

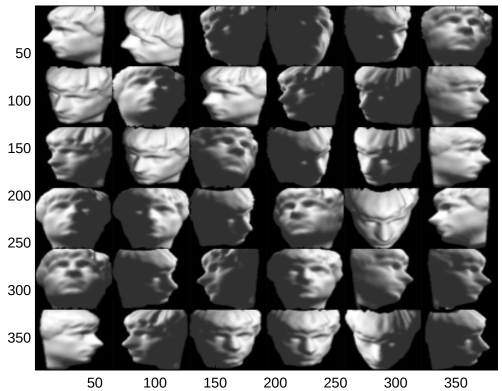
# Laplacian eigenmaps: justification

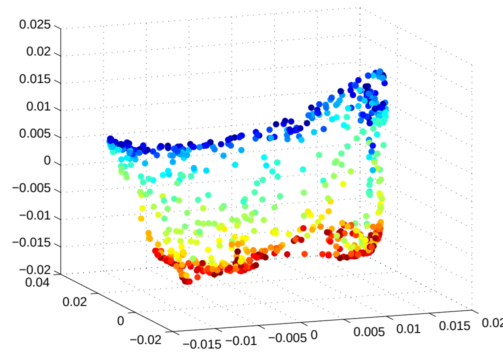
**General case:**

Find $Y = \{y_1, \cdots y_N\} \subset \mathbb{R}^d$ that minimizes

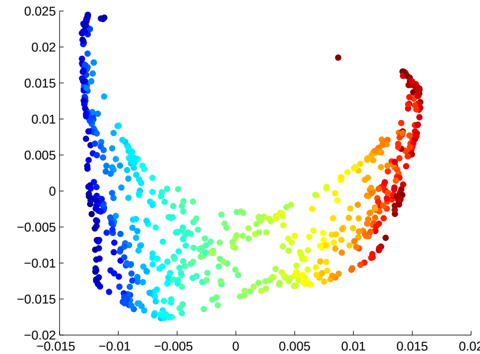
$$E = \sum_{i,j} \|y_i - y_j\|^2 w_{ij} = Tr(Y^T L Y)$$

# Laplacian eigenmaps: example




3D-proj: light




2D-proj: pose 1

Dimension: $64 * 64 = 4096$.

$N = 698$

3 free parameters:

- left-right pose,
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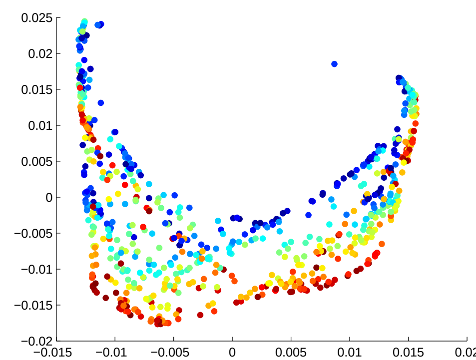
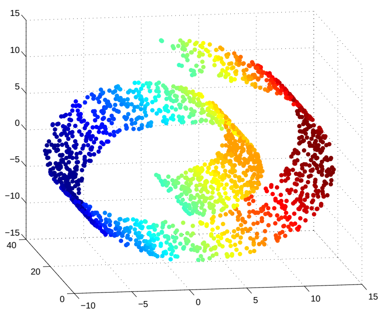


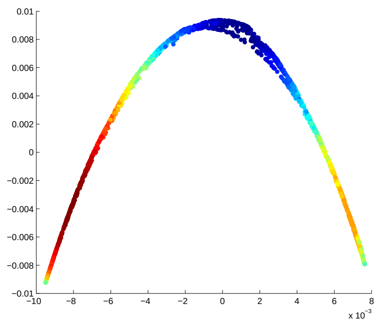

2D-proj: pose 2

$k = 12$ NN, $t = 1$

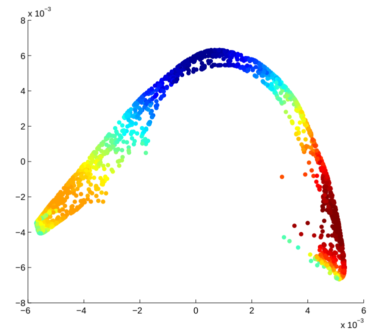
# Laplacian eigenmaps: example



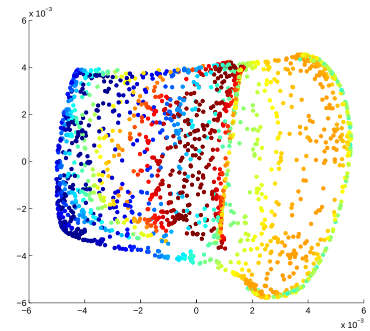
Swiss Roll



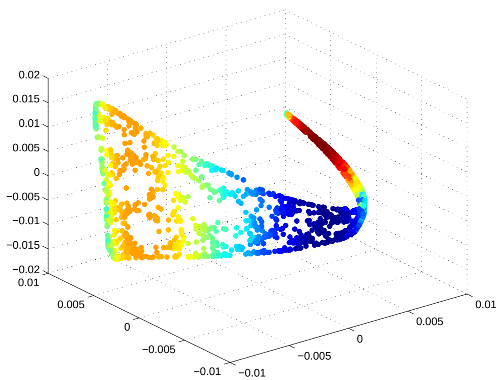
$k = 12$



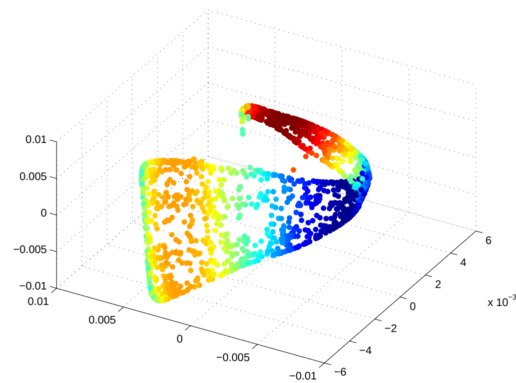
$k = 30$



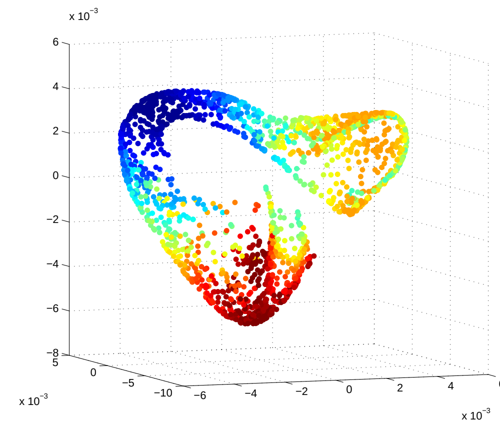
$k = 50$



$k = 12$



$k = 30$



$k = 50$

# Analogy with Laplace-Beltrami operator

**Problem:** Let $M$ be a compact Riemannian $d$-manifold. Find the "best" map $f : M \to \mathbb{R}$ such that the points that are close together on $M$ are mapped close together on $\mathbb{R}$.

Assuming that $f$ is smooth, the way how close points are mapped far away by $f$ is given by $\|\nabla f\|$. So the problem can be stated as find

$$argmin_{\{\|f\|_{L^2(M)}=1\}} \int_M \|\nabla f(m)\|^2 dm$$

Laplace-Beltrami operator on $M$: $\mathcal{L}f := -div\nabla(f)$.

Stokes' formula: for any vector field $\mathbf{X}$ on $M$, $\int_M \langle \mathbf{X}, \nabla f \rangle = -\int_M div(\mathbf{X}) f$

$$\Rightarrow \quad \int_M \|\nabla f(m)\|^2 = \int_M \mathcal{L}(f) f$$

The solution is then given by the eigenfunction $f_1$ corresponding to the first non zero eigenvalue of $\mathcal{L}$.

Belkin, Niyogi'08: the analogy can be turned into a convergence result...

# Choice of the weights

- Heat flow: $f : M \subset \mathbb{R}^D \to \mathbb{R}$ initial heat distribution, $u(x,t)$ heat distribution at time $t$ ($u(x,0) = f(x)$).
- Heat equation: $(\frac{\partial}{\partial t} + \mathcal{L})u = 0$ has solution given by $u(x,t) = \int_M H_t(x,y)f(y)$, $H_t$ being the heat kernel.
- $$\mathcal{L}f(x) = -\mathcal{L}u(x,0) = -\left(\frac{\partial}{\partial t}\int_M H_t(x,y)f(y)\right)_{t=0}$$
- for $x, y$ close and $t$ small,

$$H_t(x,y) \approx \frac{1}{(4\pi t)^{\frac{m}{2}}} e^{-\frac{\|x-y\|^2}{4t}} \quad \text{and} \quad \lim_{t\to 0}\int_M H_t(x,y)f(y) = f(x)$$

- Therefore, for $t$ small,

$$\mathcal{L}f(x) \approx \frac{1}{t}\left(f(x) - \frac{1}{(4\pi t)^{\frac{m}{2}}}\int_M e^{-\frac{\|x-y\|^2}{4t}} f(y)dy\right)$$

# Choice of the weights

- Therefore, for $t$ small,

$$\mathcal{L}f(x) \approx \frac{1}{t}\left(f(x) - \frac{1}{(4\pi t)^{\frac{m}{2}}}\int_M e^{-\frac{\|x-y\|^2}{4t}} f(y)dy\right)$$

- For $x_i \in X$,

$$\mathcal{L}f(x_i) \approx \frac{1}{t}\left(f(x_i) - \frac{1}{N}(4\pi t)^{\frac{m}{2}} \sum_{j,\|x_i-x_j\|<\varepsilon} e^{-\frac{\|x_i-x_j\|^2}{4t}} f(x_j)\right)$$

- note that $\mathcal{L}c^{te} = 0 \Rightarrow (\frac{1}{N}(4\pi t)^{\frac{m}{2}})^{-1} = \sum_{j,\|x_i-x_j\|<\varepsilon} e^{-\frac{\|x_i-x_j\|^2}{4t}}$ and $\frac{1}{t}$ does not affect the eigen decomposition of the discrete laplacian.

$\Rightarrow$ Choice of the weights: $w_{ij} = e^{-\frac{\|x_i-x_j\|^2}{4t}}$ if $\|x_i - x_j\| < \varepsilon$; $w_{ij} = 0$ otherwise.

# Diffusion maps (R. Coifman, S. Lafon, A. Lee, M. Maggioni,... ’05)

**Input:** $X \subset \mathbb{R}^D$ and a weight function $w(x_i, x_j) = w_{ij}$ such that the matrix $W = (w_{ij})$ is symmetric and semi-definite positive.

- Let $d_i = \sum_j w_{ij}$ and let $p_{ij} = p(x_i, x_j) = \frac{w_{ij}}{d_i}$.
  $p_{ij}$ can be seen as the probability for a random walker on $X$ to make a step from $x_i$ to $x_j$ (note that $\sum_j p_{ij} = 1$).
  The iterates $P^t = (p_t(x_i, x_j))$ of $P = (p_{ij})$ can be seen as the the probabilities of going from $x_i$ to $x_j$ in $t$ time steps.
- Diffusion operator:

$$Pf(x_i) = \sum_{j=1}^{N} p_{ij} f(x_j)$$

  It can be seen as an operator acting on the probability distributions $\mu^T = (\mu(x_1), \cdots \mu(x_N))$ on $X$

$$\mu^T P(x_j) = \sum_{i=1}^{N} \mu(x_i) p_{ij}$$

  with a unique stationary distribution $\mu_0(x_i) = \frac{d_i}{\sum_k d_k}$

# Diffusion maps

- The unique stationary distribution $\mu_0(x_i) = \frac{d_i}{\sum_k d_k}$ satisfies

$$\mu_0(x_i)p_{ij} = \mu_0(x_j)p_{ji}$$

- Idea: for a fixed time $t$, define a metric such that two points $x_i$, $x_j$ are close if the conditional probability distributions $p_t(x_i,.)$ and $p_t(x_j,.)$ are close.
- Diffusion distance:

$$D_t^2(x_i,x_j) = \|p_t(x_i,.) - p_t(x_j,.)\|^2_{\frac{1}{\mu_0}} = \sum_k \frac{(p_t(x_i,x_k) - p_t(x_j,x_k))^2}{\mu_0(x_k)}$$

$\rightarrow$ Close connection with the spectral theory of the random walk.

- Left and right eigenvectors of $P$: $1 = |\lambda_0| \geq |\lambda_1| \geq \cdots \geq \lambda_{N-1}$

$$\mu_j^T P = \lambda_j \mu_j^T \quad \text{and} \quad P f_j = \lambda_j f_j$$

with $f_j = \frac{\mu_j}{\mu_0}$.

# Diffusion maps

- Choose normalized $\mu_j, f_j$: $\|\mu_j\|^2_{\frac{1}{\mu_0}} = 1$ and $\|f_j\|^2_{\mu_0} = \sum_k f_j(x_k)^2 \mu_0(x_k) = 1$.
- Biorthogonal decomposition of $P^t$:

$$p_t(x_i, x_j) = \sum_k \lambda_k^t f_k(x_i) \mu_k(x_j)$$

- This implies

$$D_t^2(x_i, x_j) = \sum_{k=1}^{N} \lambda_k^{2t} (f_k(x_i) - f_k(x_j))^2$$

(note that since $f_0 \equiv 1$, it does not enter into the sum).

- The diffusion distance is then approximated by

$$D_t^2(x_i, x_j) \approx \sum_{k=1}^{d} \lambda_k^{2t} (f_k(x_i) - f_k(x_j))^2$$

# Diffusion maps

- The diffusion distance is then approximated by

$$D_t^2(x_i, x_j) \approx \sum_{k=1}^{d} \lambda_k^{2t} (f_k(x_i) - f_k(x_j))^2$$

- Embedding of the data in $\mathbb{R}^d$:

$$x_i \mapsto y_i = (\lambda_1^t f_1(x_i), \cdots \lambda_d^t f_d(x_i))$$

The (approximated) diffusion metric becomes the euclidean metric between the data points in $\mathbb{R}^d$.

# A few references 1/2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  - L. K. Saul, S. T. Roweis, “Think Globally, Fit Locally: Unsupervised Learning of Low Dimensional Manifolds”, Journal of Machine Learning Research 4 (2000), 119-155.
- ISOMAP:
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  - V. de Silva, J. B. Tenenbaum, “Global versus Local Methods in Nonlinear Dimensionality Reduction”, Advances in Neural Information Processing Systems 15, MIT Press, 2003.
- HLLE:
  - D. L. Donoho, C. Grimes, “Heissian Eigenmaps: Locally Linear Embedding Techniques for High-dimensional Data”, Proceedings of the National Academy of Sciences 100, 10, 5591-5596.

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- Laplacian Eigenmaps:
  - M. Belkin, P. Niyogi, “Laplacian Eigenmaps for Dimensionality Reduction for Data Representation”, Neural Computation 15, 6, 1373–1396, 2003.
- Diffusion maps:
  - R. R. Coifman and S. Lafon and A. Lee and M. Maggioni and B. Nadler and F. Warner and S. Zucker, “Geometric Diffusions as a tool for Harmonic Analysis and structure definition of data: Diffusion maps”, Proc. of Nat. Acad. Sci. 102, 7426–7431, 2005.