Topic 2: DIMENSIONALITY REDUCTION

STAT 37710/CAAM 37710/CMSC 35400 Machine Learning
Risi Kondor, The University of Chicago

Dimensionality reduction

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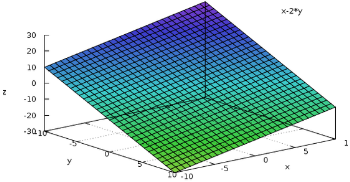
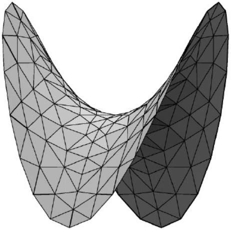
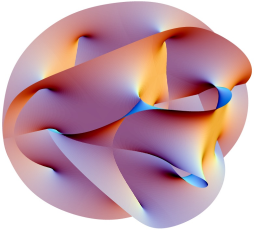
But is the problem intrinsically high dimensional??? Often we can convert high dimensional problems to lower dimensional ones without losing too much information.

Dimensionality reduction







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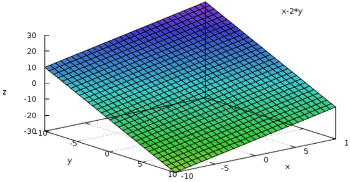

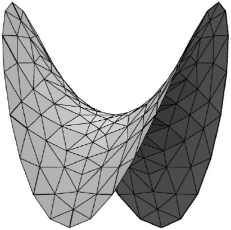

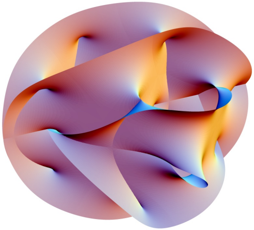

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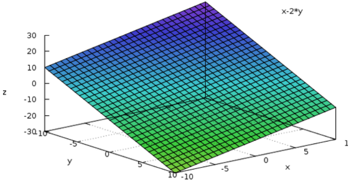

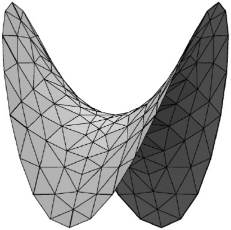

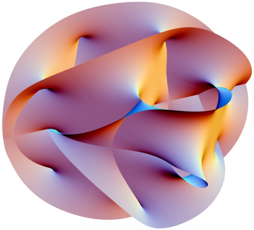

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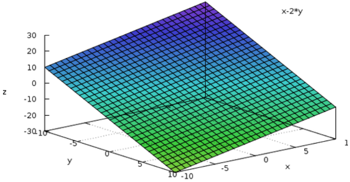

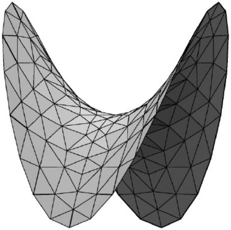

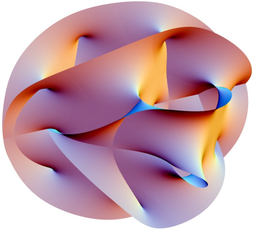

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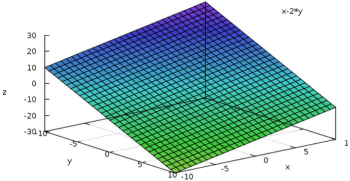

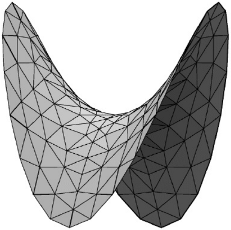

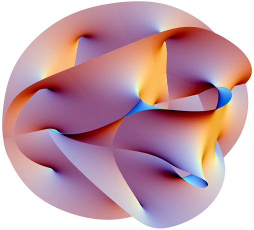

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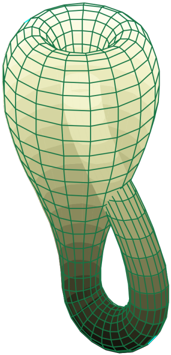
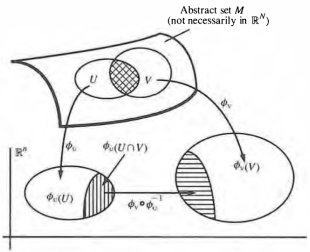
- IDEA: find the manifold and restrict learning algorithm to it.

Differentiable manifolds





In mathematics, a d dimensional **manifold** is a topological space such that each point has a neighborhood that is homeomorphic to $\mathbb{R}^d$. A differentiable manifold has additional structure, and a Riemannian manifold has a metric too $\rightarrow$ geodesics.

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- **Computational efficiency:** learning algorithms work faster in low dimensions.
- **Better performance:** the projection might eliminate noise.
- **Interpretability:** the vectors spanning the subspace might have interesting interpretations.

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  - etc.

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Note: If the eigenvalues are not distinct, then the eigenvectors are not unique. However, there is always some choice of eigenvectors which forms an orthonormal basis.

Fact 2 (Rayleigh quotient)

Let $\mathbf{v}_1, \ldots, \mathbf{v}_d$ be the normalized eigenvectors of a symmetric matrix $A \in \mathbb{R}^{d \times d}$ and let $\lambda_1 < \lambda_2 < \ldots < \lambda_d$ be the corresponding eigenvalues. Then

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Similarly,

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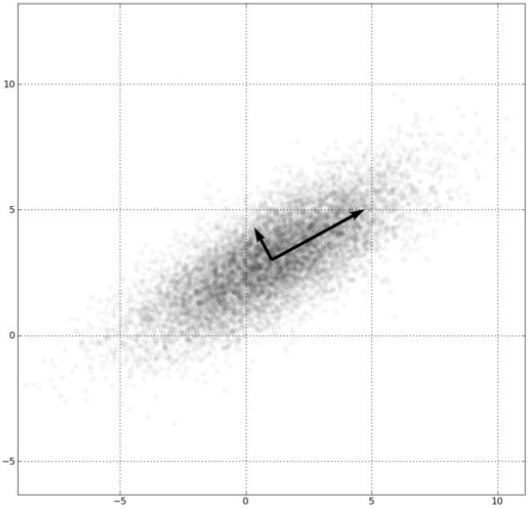
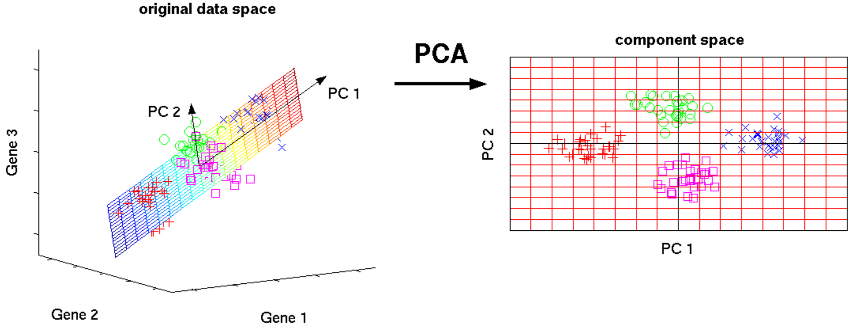
Principal Component Analysis

The principal directions in data

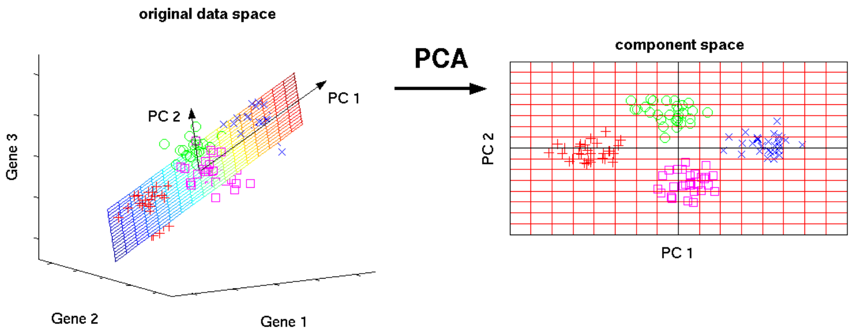


Finding the principal subspace



How can we find the most relevant subspace for the data?

Finding the principal subspace



How can we find the most relevant subspace for the data? By finding a basis for it. The individual basis vectors are called the **principal components**.

The first principal component

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This vector is called the first **principal component** of the data.

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Since $\|\mathbf{v}\| = 1$, (1) is equivalent to the Rayleigh quotient optimization problem

$$\boldsymbol{p}_1 = \operatorname*{arg\,max}_{\mathbf{v}\in\mathbb{R}^d\setminus\{0\}} \frac{\mathbf{v}^\top \widehat{\Sigma}\,\mathbf{v}}{\|\mathbf{v}\|},$$

so $\boldsymbol{p}_1$ is indeed the eigenvector $\mathbf{v}_d$ of A with largest eigenvalue.

Further principal components

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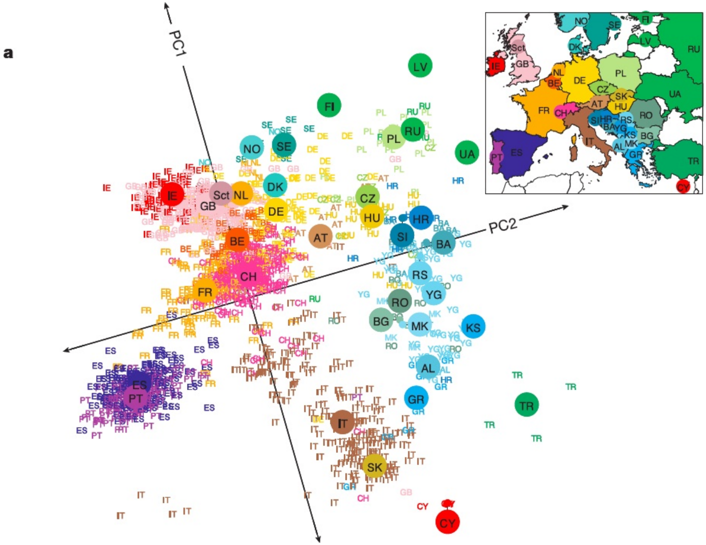
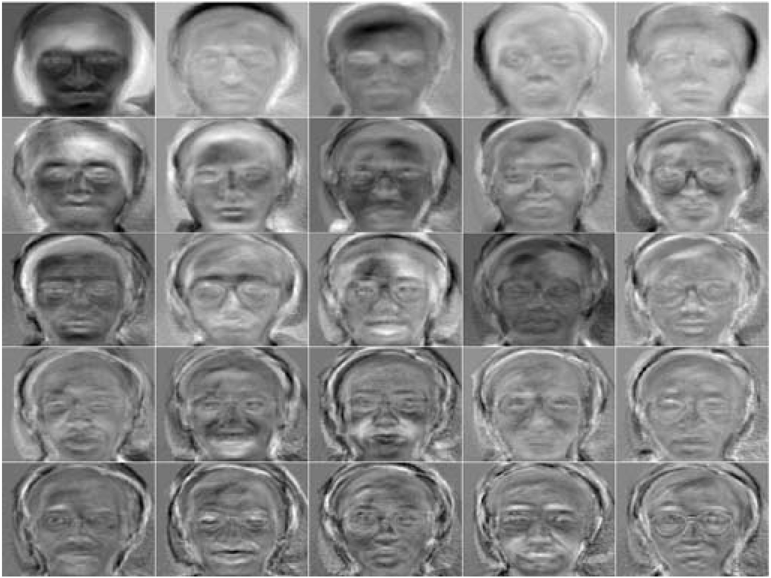
DNA data



[Matthew Stephens, John Novembre]

Eigenfaces

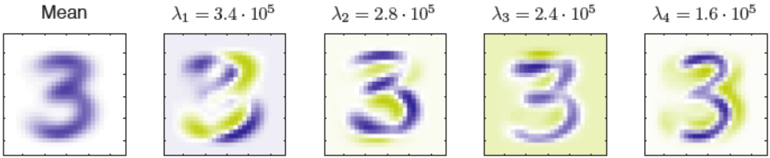


[Christopher de Coro]

Reconstruction from eigenfaces

[Christopher de Coro]

Example: digits



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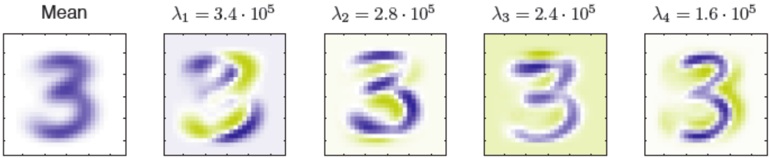

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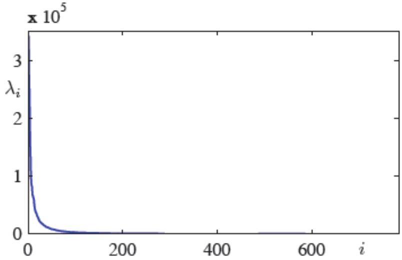
- Sometimes there is a sharp drop somewhere, called the **spectral gap** $\rightarrow$ natural place to put cut-off



[Source: Peter Orbanz]

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Advantages:

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NONLINEAR DIMENSIONALITY REDUCTION

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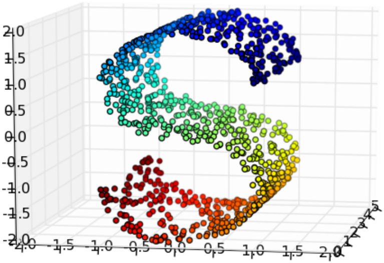
- But what if the data lies on a nonlinear **manifold**? Data which at first looks very high dimensional often really has low dimensional structure.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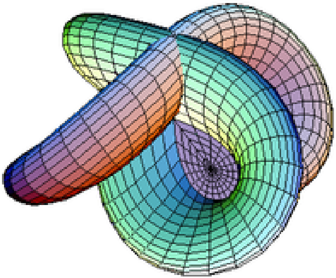
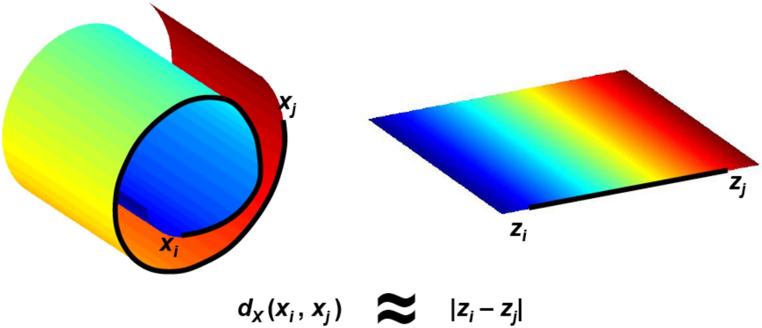
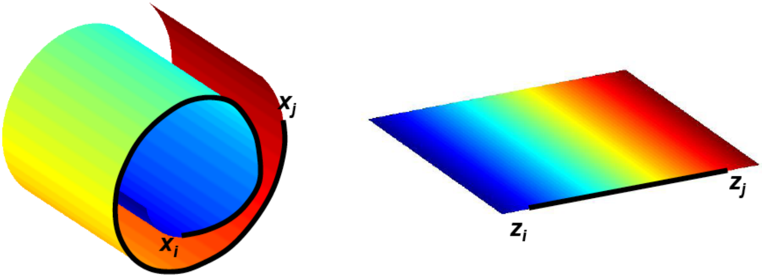


General principle



Find a map $\phi\colon \mathbb{R}^d \to \mathbb{R}^p$ that maps the manifold to a lower dimensional Euclidean space in a way that preserves local distances as much as possible (some methods can only map individual data points not the whole of $\mathbb{R}^d$).

General principle



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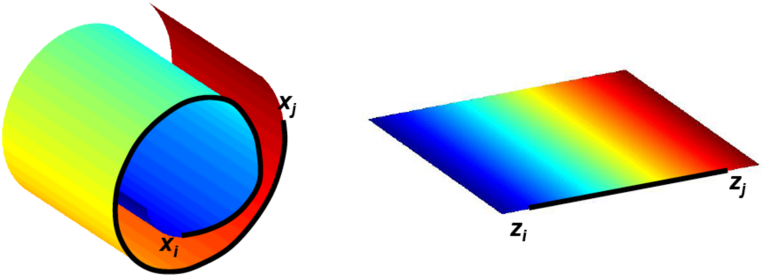

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Question: Can this always be done? Depends on the topology.

Methods

- Multidimensional Scaling

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Multidimensional scaling (MDS)

Classical MDS

- **Input:** n data points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$.

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- **Output:** n corresponding lower dimensional points $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^p$ (with $p \ll d$) that minimize the so-called *strain*

$$\mathcal{E}_{\text{CMDS}} = \|D - D^*\|^2_{\textsf{Frob}} = \sum_{i,j} (D_{i,j} - D^*_{i,j})^2,$$

where $D_{i,j} = \|\mathbf{x}_i - \mathbf{x}_j\|^2$ and $D^*_{i,j} = \|\mathbf{y}_i - \mathbf{y}_j\|^2$.

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The **Gram matrix** of $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ is the $n \times n$ positive semidefinite matrix

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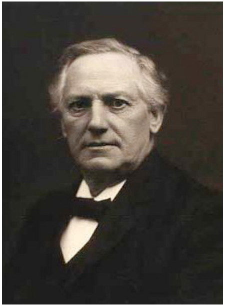

Jørgen Pedersen Gram
1850–1916

Exercise: Prove that if $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$, then $\mathrm{rank}(G) \leq d$.

Classical MDS

Proposition 1. The CMDS problem can equivalently be written as minimizing

$$\mathcal{E} = \| G - G^* \|^2_{\text{Frob}},$$

where G is the centered Gram matrix of $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ and G^* is the Gram matrix of $\{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$.

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Classical MDS

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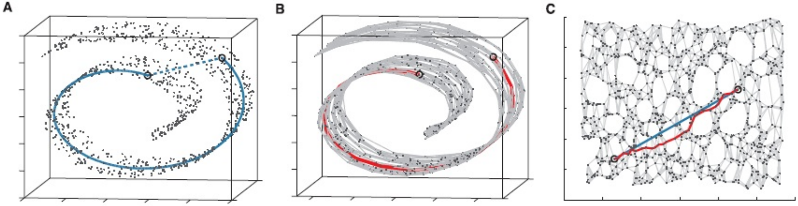
Isomap

Tenenbaum, de Silva & Langford, 2000

Isomap



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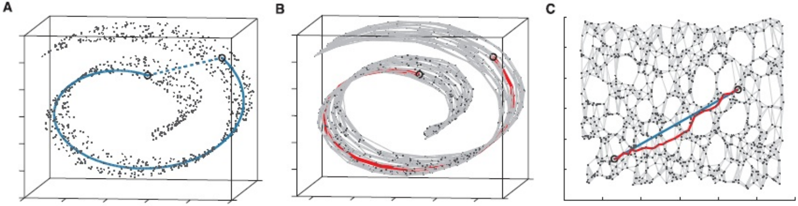

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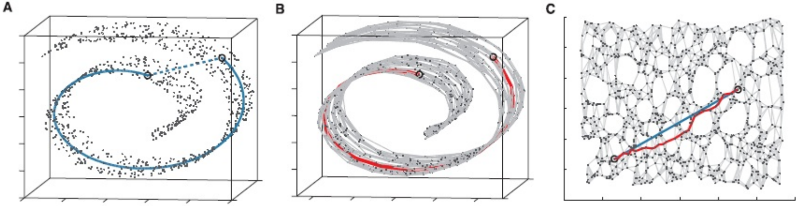

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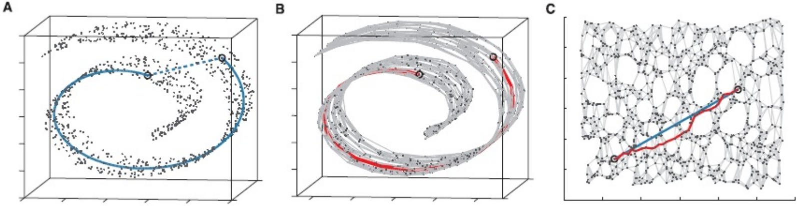

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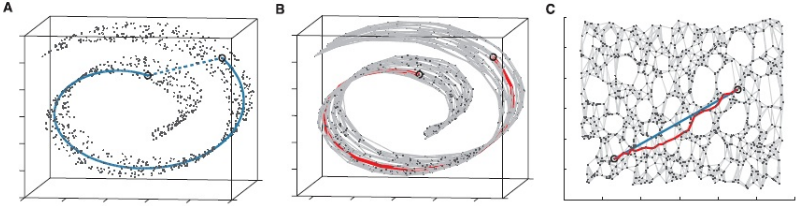

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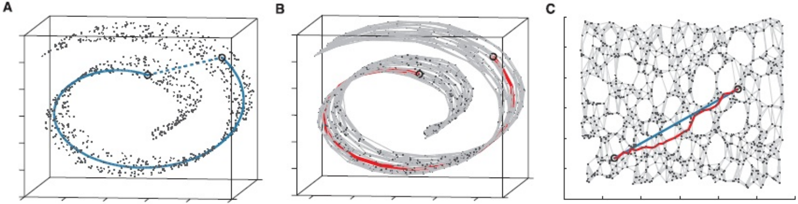

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3. The optimal embedding preserves these distances as much as possible.

Shortest path distances

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The shortest path distance in $\mathcal{G}$ from i to j is

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Floyd–Warshall algorithm

```
INPUT: matrix A with A_{i,j} = δ_{i,j} as on previous slide;
for k = 1 to n {
  for i = 1 to n {
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      if (A_{i,j} > A_{i,k} + A_{k,j}) then A_{i,j} ← A_{i,k} + A_{k,j} ;
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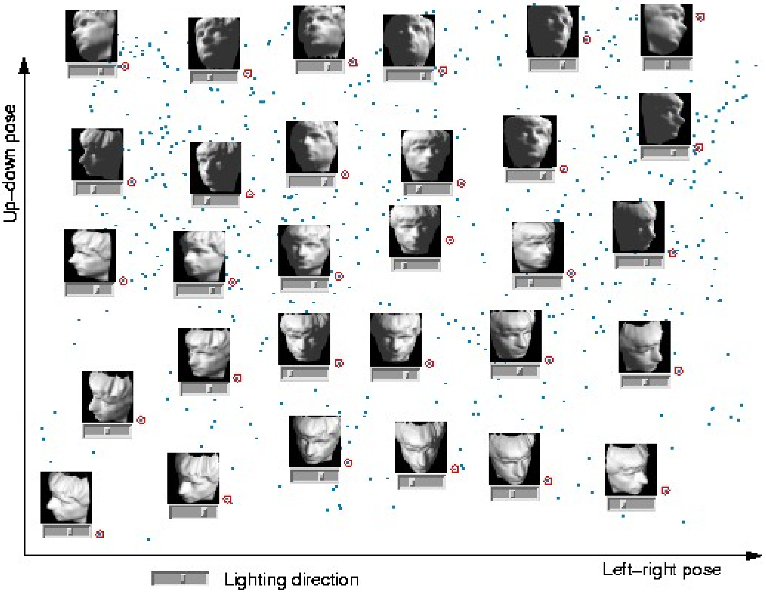
Overall complexity: $O(n^3)$.

Isomap example



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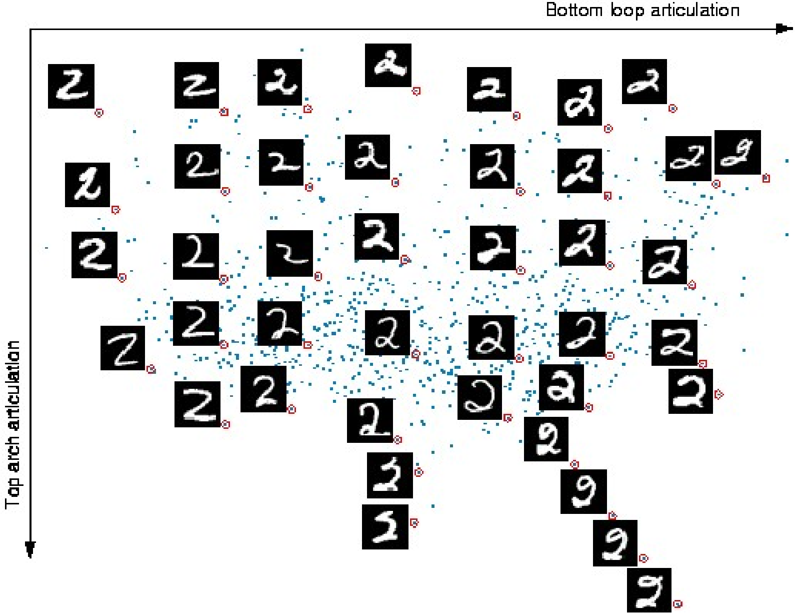

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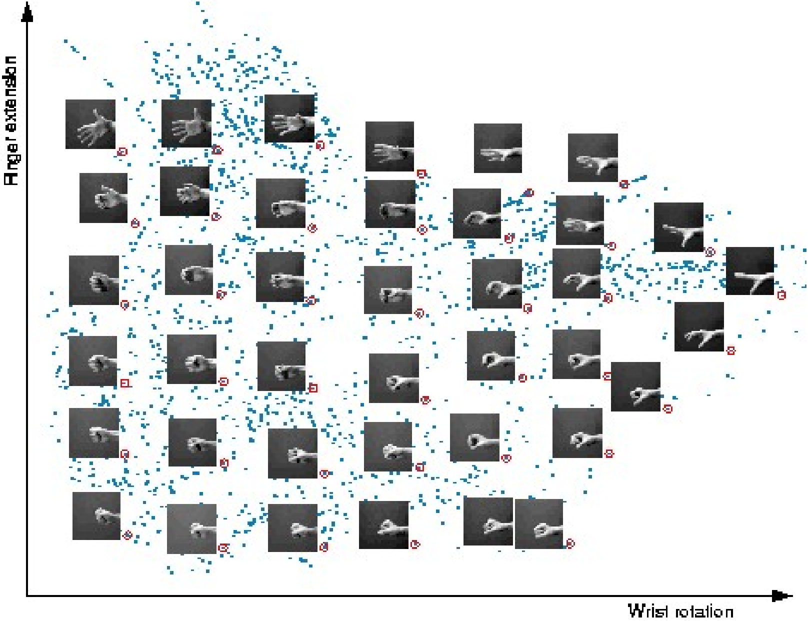

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- Not obvious how to set k.

Locally Linear Embedding (LLE)

Roweis & Saul, 2000

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IDEA: Each point should be approximately reconstructable as a linear combination of its neighbors (locally linear property of manifolds):

$$\mathbf{x}_i \approx \sum_{j \in \mathrm{knn}(i)} w_{i,j} \mathbf{x}_j,$$

where $(w_{i,j})_{i,j}$ is a matrix of weights. Also have constraints $\sum_j w_{i,j} = 1$.

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Now find an embedding that preserves these weights, i.e., n vectors $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^p$, such that

$$\mathbf{y}_i \approx \sum_j w_{i,j} \mathbf{y}_j$$

for the same matrix of weights.

Phase 1: find the weights

Do this separately for each i. Formulate it as minimizing

$$\Phi = \left\| \mathbf{x}_i - \sum_{j \in \mathrm{knn}(i)} w_{i,j} \mathbf{x}_j \right\|^2 \qquad \text{s.t.} \qquad \sum_j w_{i,j} = 1.$$

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where $K^{(i)}$ is the local Gram matrix, $K^{(i)}_{j,j'} = (\mathbf{x}_i - \mathbf{x}_j)^\top (\mathbf{x}_i - \mathbf{x}_j)$, and $\mathbf{w} = (w_j)_{j \in \mathrm{knn}(i)}$.

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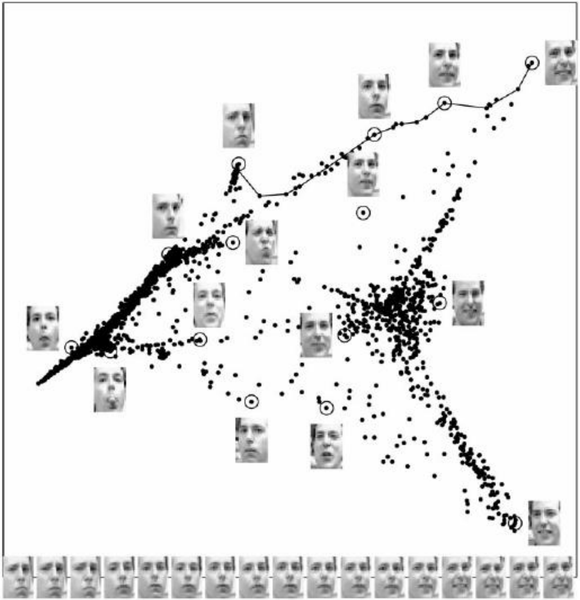
Phase 2: find the $\boldsymbol{y}_i$'s

Now minimize (w.r.t. $\mathbf{y}_1, \ldots, \mathbf{y}_n$)

$$\Psi = \sum_i \| \mathbf{y}_i - \sum_j w_{i,j} \mathbf{y}_j \|^2 \qquad s.t. \qquad \sum_i \mathbf{y}_i = 0 \qquad \frac{1}{n} \sum_i \mathbf{y}_i \mathbf{y}_i^\top = I.$$

Solution.

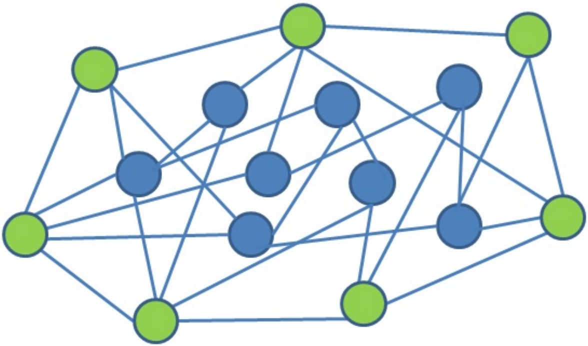
$$\Psi = \sum_{i,j} \mathbf{y}_i^\top M \mathbf{y}_j \ldots$$



Laplacian Eigenmaps

Belkin and Niyogi, 2002

Spectral Graph Theory



Spectral graph theory is about relating functions on graphs (i.e., $f : V \to \mathbb{R}$ where V is the vertex set of the graph) to the structure of the graph.

Unweighted graphs

Let $\mathcal{G}$ be an unweighted, undirected graph with vertex set $V = \{1, 2, \ldots, n\}$ and edge set $E \subseteq V \times V$.

- The **adjacency matrix** of $\mathcal{G}$ is the matrix $A \in \{0,1\}^{n \times n}$ with

$$A = \begin{cases} 1 & \text{if } i \sim j \\ 0 & \text{otherwise,} \end{cases}$$

  where $i \sim j$ means that vertices i and j are adjacent.

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- The **Laplacian matrix** of $\mathcal{G}$ is

$$L = D - A.$$

Laplacian as a quadratic form

The Laplacian can be written as

$$L = \sum_{i\sim j} E_{i,j} \quad \text{where} \quad [E_{i,j}]_{p,q} = \begin{cases} 1 & \text{if } p=q=i \text{ or } p=q=j \\ -1 & \text{if } (p,q)=(i,j) \text{ or } (p,q)=(j,i) \\ 0 & \text{otherwise.} \end{cases}$$

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Exercise: Prove that L is a psd matrix.

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Let $\mathcal{G}$ be a weighted, undirected graph with edge weights $(w_{i,j})_{i,j}$. Note that $w_{i,j=w_{j,i}}$, and if $i \not\sim j$, then $w_{i,j} = 0$.

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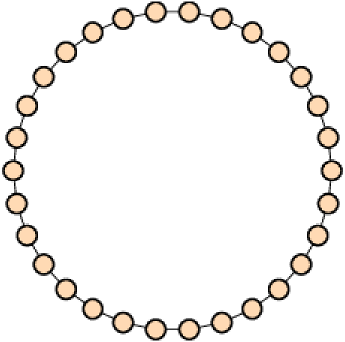
The normalized Laplacian

When the degree distribution is uneven, it is often much better to work with the **normalized Laplacian**

$$\tilde{L} = D^{-1/2} L D^{-1/2} = I - D^{-1/2} A D^{-1/2}.$$

Example: cycle graph



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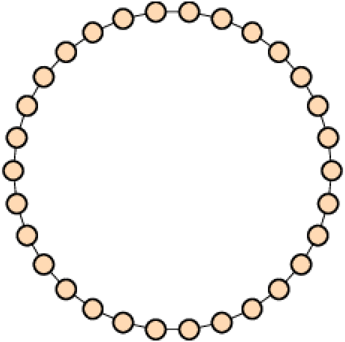
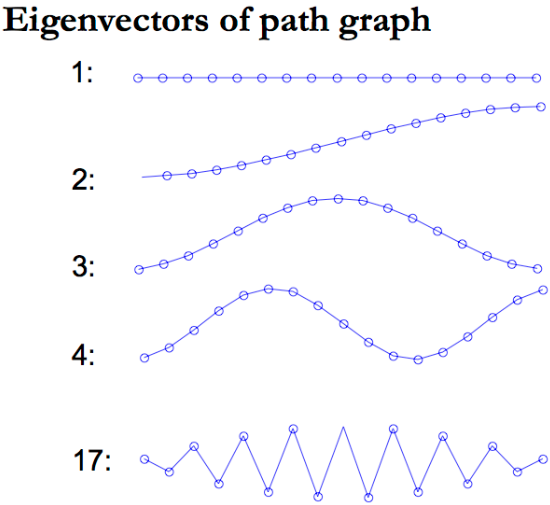


$$f_k(v_i) = \sin(2\pi ki/n) \qquad k = 1, 2, \ldots \lfloor n/2 \rfloor$$
$$g_k(v_i) = \cos(2\pi ki/n) \qquad k = 0, 1, 2, \ldots, \lfloor (n-1)/2 \rfloor,$$

Example: path graph



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- By the above, $\lambda_1 = 0$ and $v_1 = \frac{1}{\sqrt{n}}\mathbf{1}$ for any graph.
- The second eigenvector v_2, is called the **Fiedler vector**, and is particularly informative about how to cluster the graph.

Cheeger's inequality

Let $S \subset V$, $= V \setminus S$, and $E(S, \overline{S}) = \sum_{i \in S} \sum_{j \in \overline{s}} w_{i,j}$.

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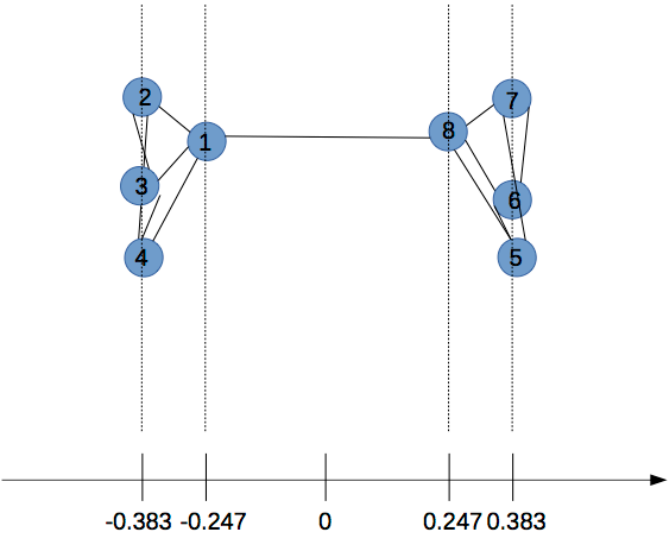
- **Cheeger's inequality** states that

$$\frac{\phi_{\mathcal{G}}^2}{2d_{\text{max}}} \leq \lambda_2 \leq \phi_{\mathcal{G}},$$

where d_{max} is the maximum degree of any vertex in $\mathcal{G}$.

Example



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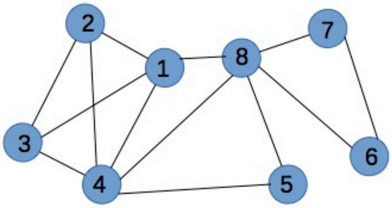

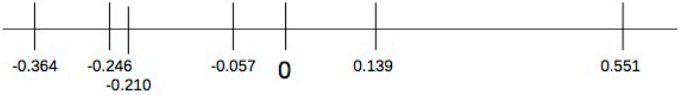

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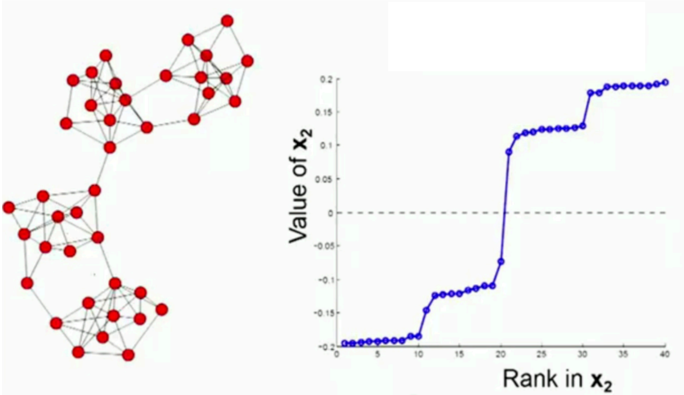

The first few eigenvectors can be used for clustering $\rightarrow$ spectral graph partitioning

The Laplace–Beltrami operator

The graph Laplacian is the discrete analog of the Laplace-Beltrami operator.

- The Laplacian operator on $\mathbb{R}^d$ is

$$\Delta = \nabla^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \ldots + \frac{\partial^2}{\partial x_d^2}.$$

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- More generally, the Laplace–Beltrami operator on a d dimensional Riemannian manifold with metric tensor g is

$$\Delta = \frac{1}{\sqrt{\det g}} \sum_{i,j=1}^{d} \partial_i \sqrt{\det g} g^{i,j} \, \partial_j.$$

The graph Laplacian can be regarded as a discretization of these operators.

Discretization of Laplacian

- In $\mathbb{R}$, the (finite difference) discretization of $\nabla = \frac{\partial}{\partial x}$ is derived from

$$(\nabla f)(x) = \left(\frac{\partial}{\partial x} f\right)(x) = \frac{f(x+h/2) - f(x-h/2)}{h}.$$

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The heat equation

The flow of heat in a homogenous medium is governed by the equation

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$$f(\mathbf{x}, t) = e^{\kappa t \Delta} f(\mathbf{x}, 0) \qquad \text{where} \qquad e^T := I + T + \frac{1}{2}T^2 + \frac{1}{6}T^3 + \ldots.$$

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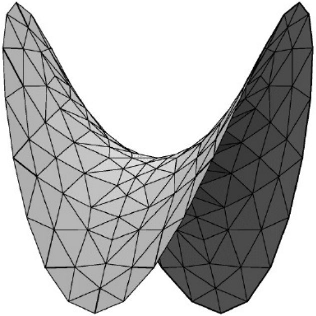
The long time behavior of the system is determined by the low $|\lambda_i|$ modes!!!

Laplacian Eigenmaps [Belkin&Niyogi]



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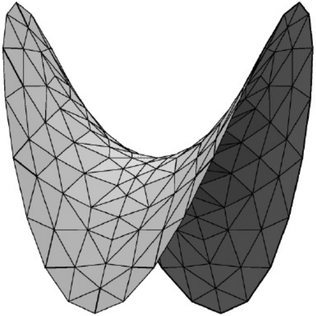

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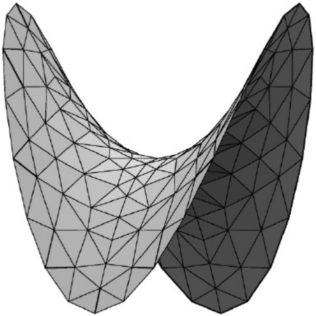

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- Intuition: these are the smoothest functions on the graph, and they give global coordinates

Laplacian Eigenmaps: detail

Formulate the problem as minimizing the strain

$$\mathcal{E} = \sum_{i,j} w_{i,j} \left\| \mathbf{y}_i - \mathbf{y}_j \right\|^2 = 2\mathrm{tr}(Y^\top L Y).$$

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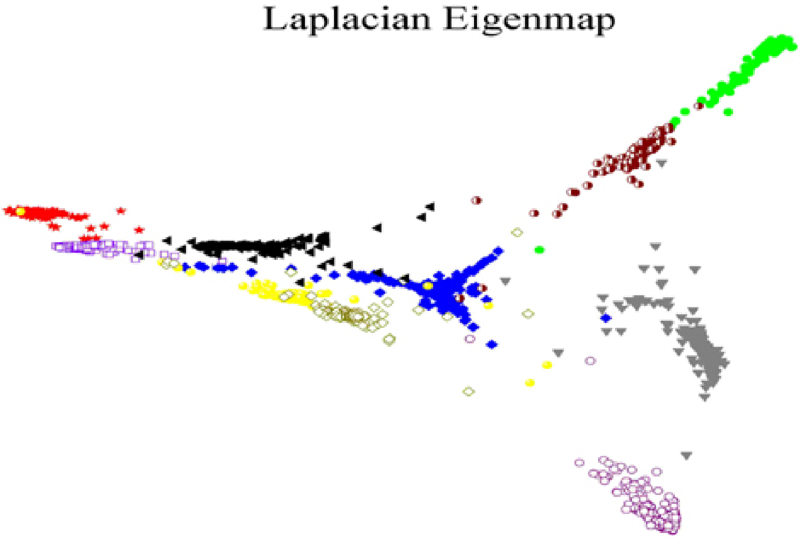
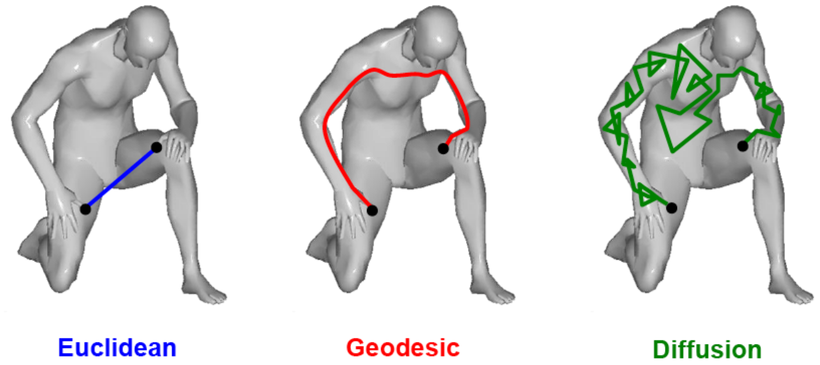
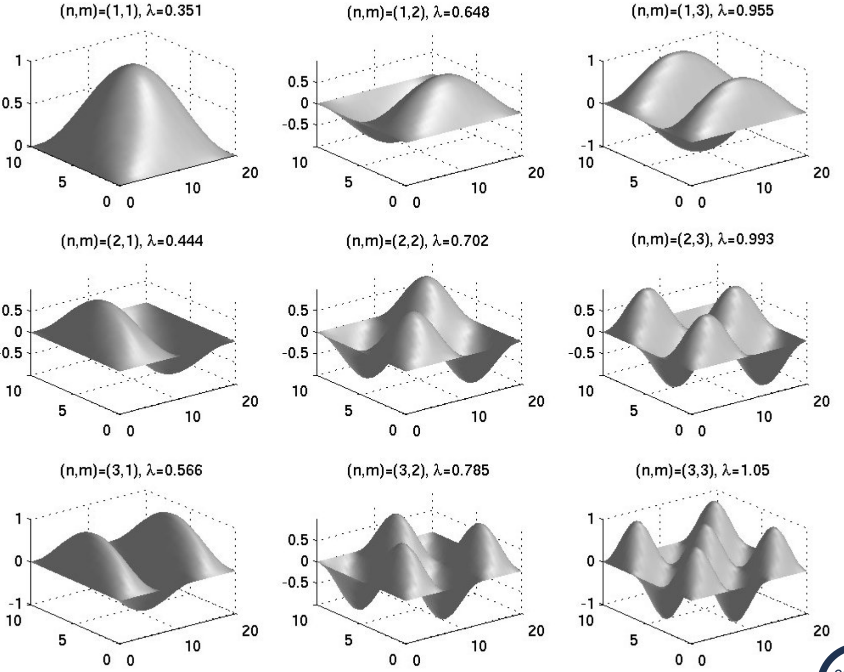
Adding the additional constraint $Y^\top D Y = I$, after some algebra, this leads to the generalized eigenvalue problem $LY = DY$.

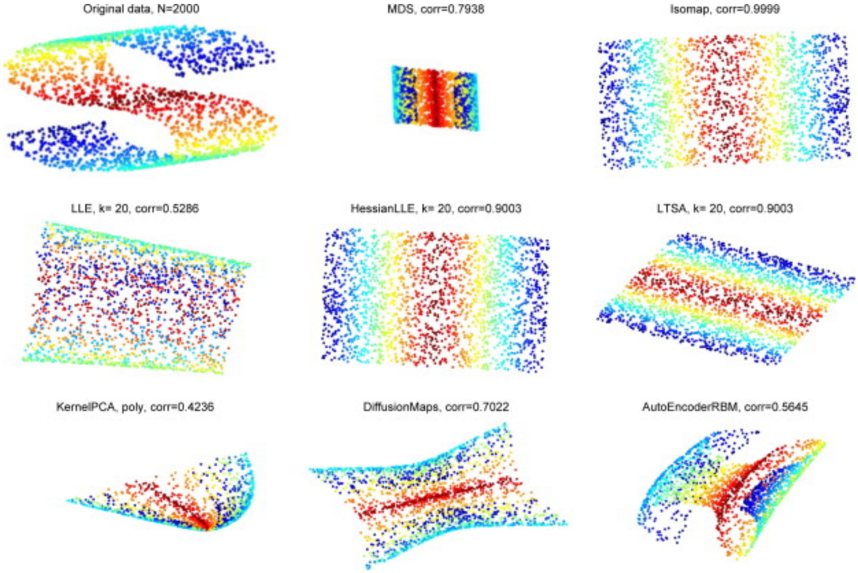

Laplacian Eigenmap

Three different metrics



Laplacian eigenmaps corresponds to PCA w.r.t. the diffusion metric on the manifold, because the diffusion (heat) kernel is exactly $e^{-\beta L}$ [K and Lafferty, 2001].


(n,m)=(1,1), λ=0.351
(n,m)=(1,2), λ=0.648
(n,m)=(1,3), λ=0.955
(n,m)=(2,1), λ=0.444
(n,m)=(2,2), λ=0.702
(n,m)=(2,3), λ=0.993
(n,m)=(3,1), λ=0.566
(n,m)=(3,2), λ=0.785
(n,m)=(3,3), λ=1.05
1
0.5
0
-0.5
-1
10
5
0
20


Original data, N=2000
MDS, corr=0.7938
Isomap, corr=0.9999
LLE, k= 20, corr=0.5286
HessianLLE, k= 20, corr=0.9003
LTSA, k= 20, corr=0.9003
KernelPCA, poly, corr=0.4236
DiffusionMaps, corr=0.7022
AutoEncoderRBM, corr=0.5645