UNSUPERVISED LEARNING 2011

LECTURE : MANIFOLD LEARNING

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Some slides are due to L.Saul, V. C. Raykar, N. Verma

Topics

- PCA
- MDS

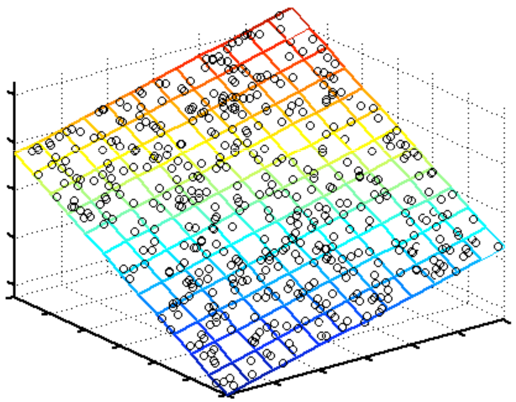
Done!

- IsoMap
- LLE
- EigenMaps

Dimensionality Reduction

- Data representation

  Inputs are real-valued vectors in a high dimensional space.



- Linear structure

  Does the data live in a low dimensional subspace?

- **Nonlinear structure**

  Does the data live on a low dimensional submanifold?

Notations

- Inputs (**high dimensional**)

  $\boldsymbol{x_1, x_2, \ldots, x_n}$ points in R^D

- Outputs **(low dimensional)**

  $\boldsymbol{y_1, y_2, \ldots, y_n}$ points in R^d ($d \ll D$)

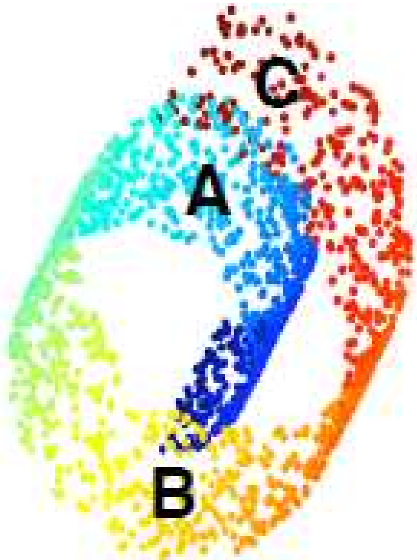
- Goals

  Nearby points remain nearby.

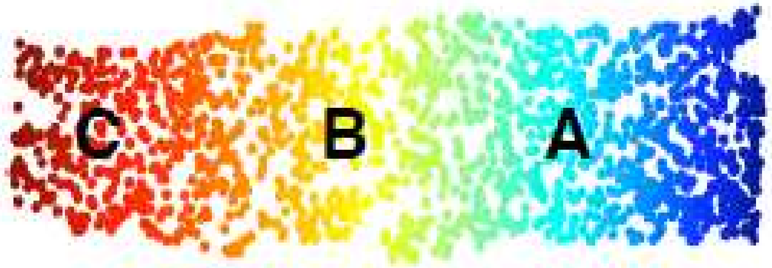
  Distant points remain distant.

Non-metric MDS for manifolds?

Rank ordering of Euclidean distances is NOT preserved in “manifold learning”.

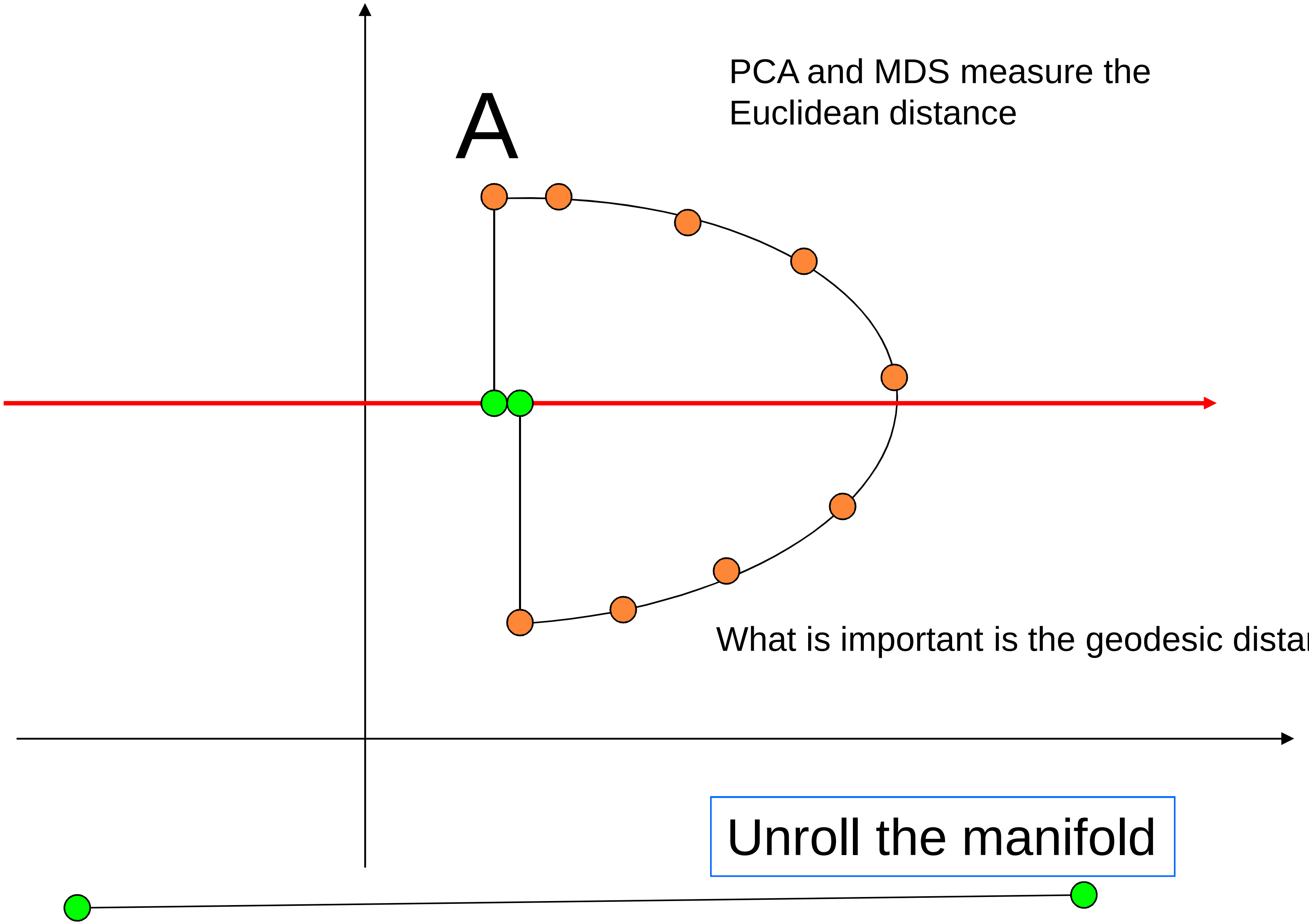


$$d(A,C) < d(A,B)$$



$$d(A,C) > d(A,B)$$

Nonlinear Manifolds

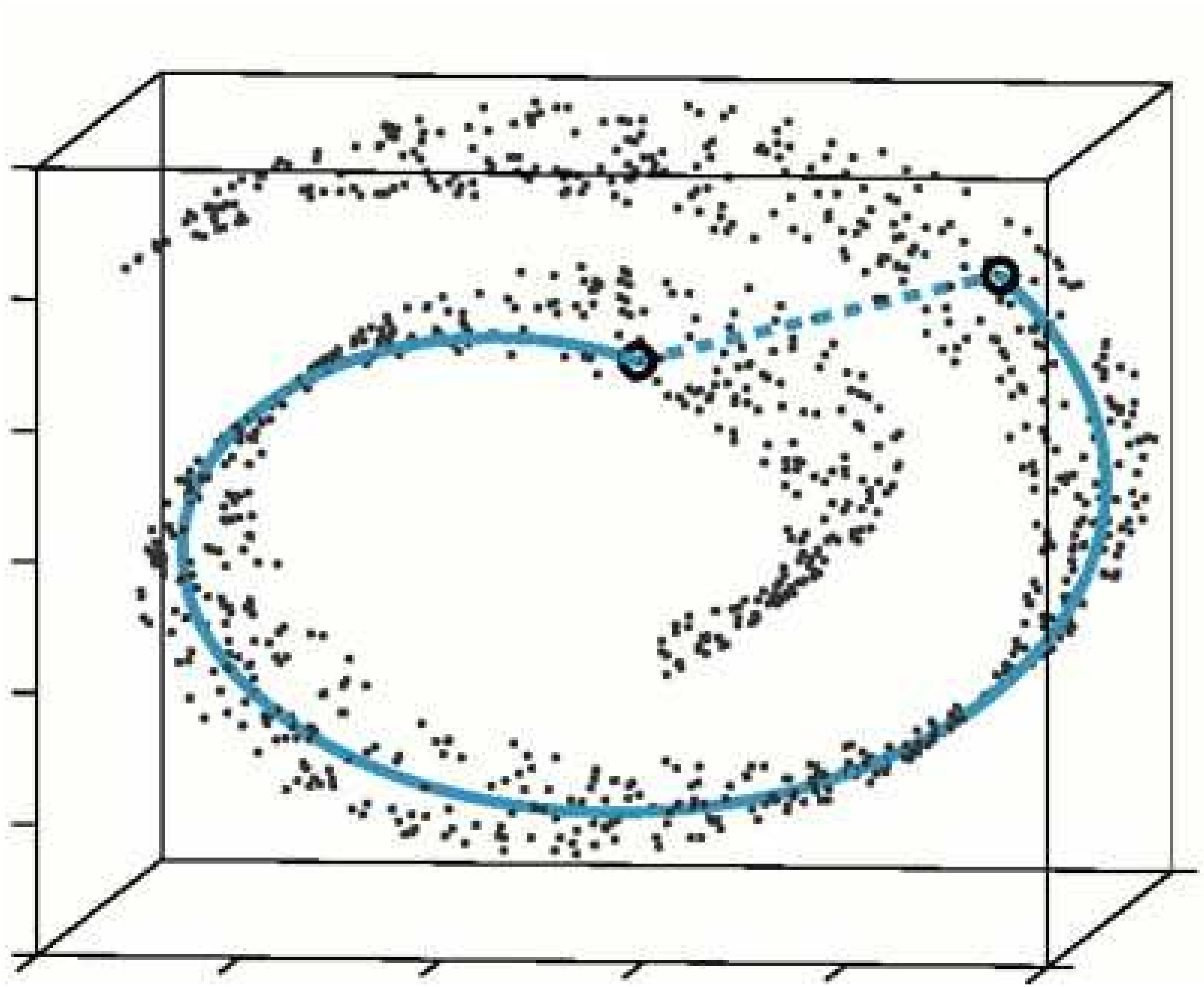


PCA and MDS measure the Euclidean distance

What is important is the geodesic distance

Unroll the manifold

To preserve structure preserve the geodesic distance and not the euclidean distance.



Graph-Based Methods

- Tenenbaum et.al's Isomap Algorithm
  - Global approach.

    Preserves global pairwise distances.

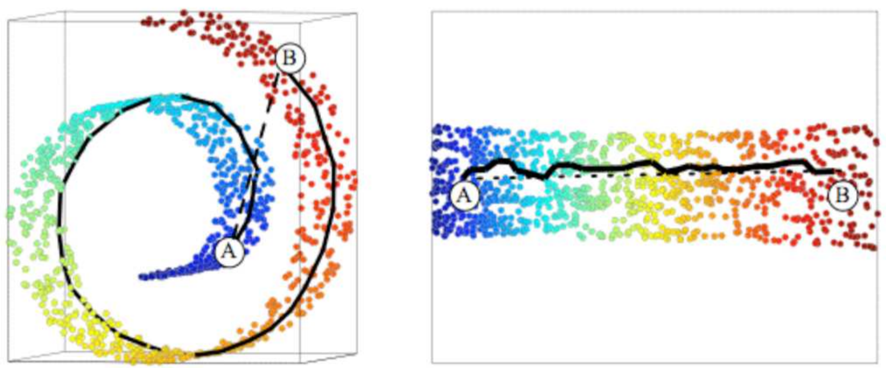
- Roweis and Saul's Locally Linear Embedding Algorithm
  - Local approach

    Nearby points should map nearby

- Belkin and Niyogi Laplacian Eigenmaps Algorithm
  - Local approach
  - minimizes approximately the same value as LLE

Isomap - Key Idea:

- Use **geodesic** instead of Euclidean distances in MDS.
  - For neighboring points Euclidean distance is a good approximation to the geodesic distance.
  - For distant points estimate the distance by a series of short hops between neighboring points. Find shortest paths in a graph with edges connecting neighboring data points.



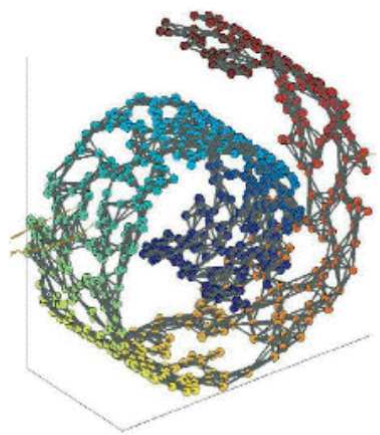
Step 1. Build adjacency graph.

- Adjacency graph

  Vertices represent inputs. Undirected edges connect neighbours.

- Neighbourhood selection

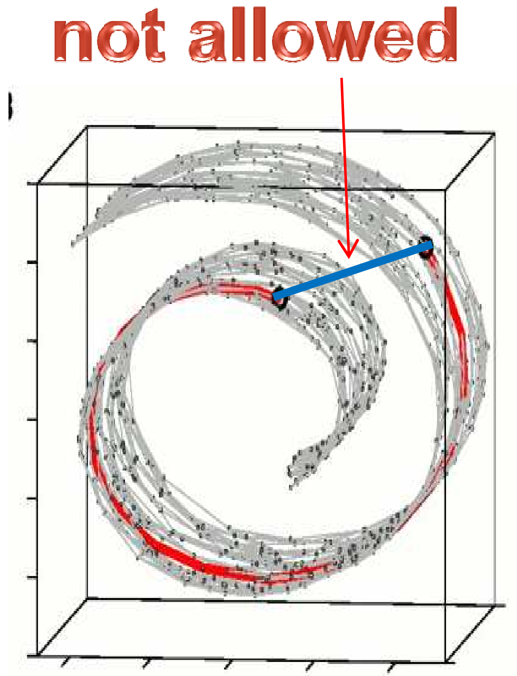
  Many options: k-nearest neighbours, inputs within radius r, prior knowledge.



Graph is discretized approximation of submanifold.

Building the graph

- Computation
  - kNN scales naively as $O(n^2 D)$
  - Faster methods exploit data structures.
- Assumptions
  1. Graph is connected.
  2. Neighbourhoods on graph reflect neighbourhoods on manifold.



Step 2. Estimate geodesics

- Dynamic programming
  - Weight edges by local distances.
  - Compute shortest paths through graph.
- Geodesic distances
  - Estimate by lengths of shortest paths: denser sampling = better estimates.
- Computation
  - Djikstra’s algorithm for shortest paths $O(n^2 \log n + n^2 k)$.

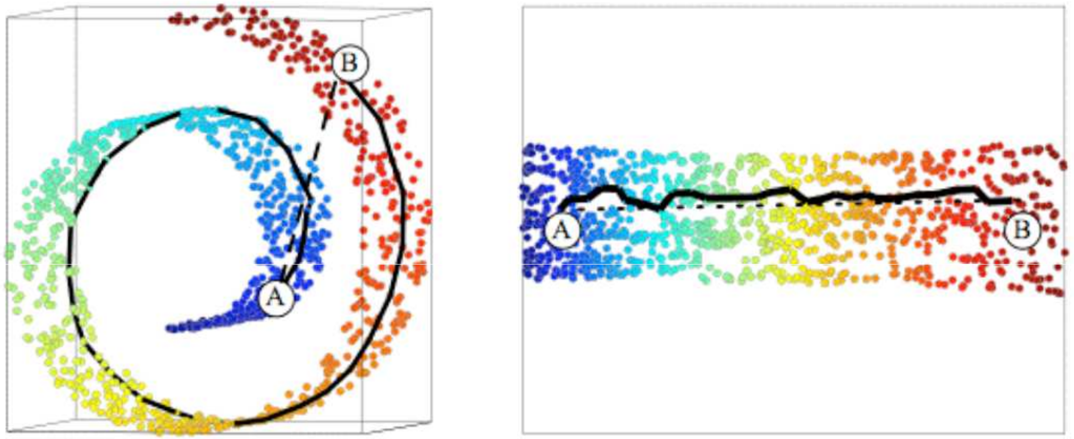
Step 3. Metric MDS

- Embedding
  - Top d eigenvectors of Gram matrix yield embedding.
- Dimensionality
  - Number of significant eigenvalues yield estimate of dimensionality.
- Computation
  - Top d eigenvectors can be computed in $O(n^2d)$.

Summary

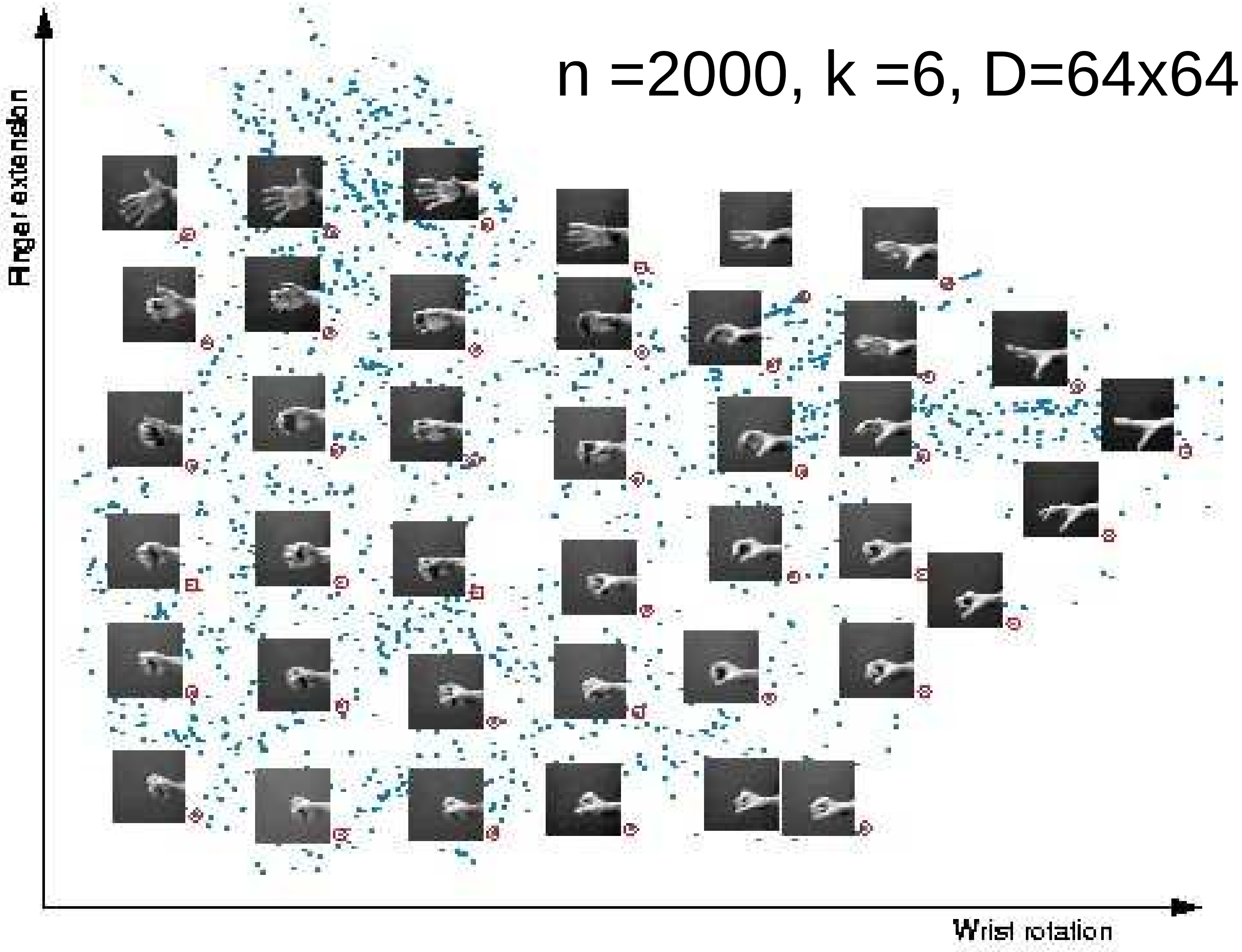
- Algorithm
  1. k nearest neighbours
  2. shortest paths through graph
  3. MDS on geodesic distances

Swiss Roll

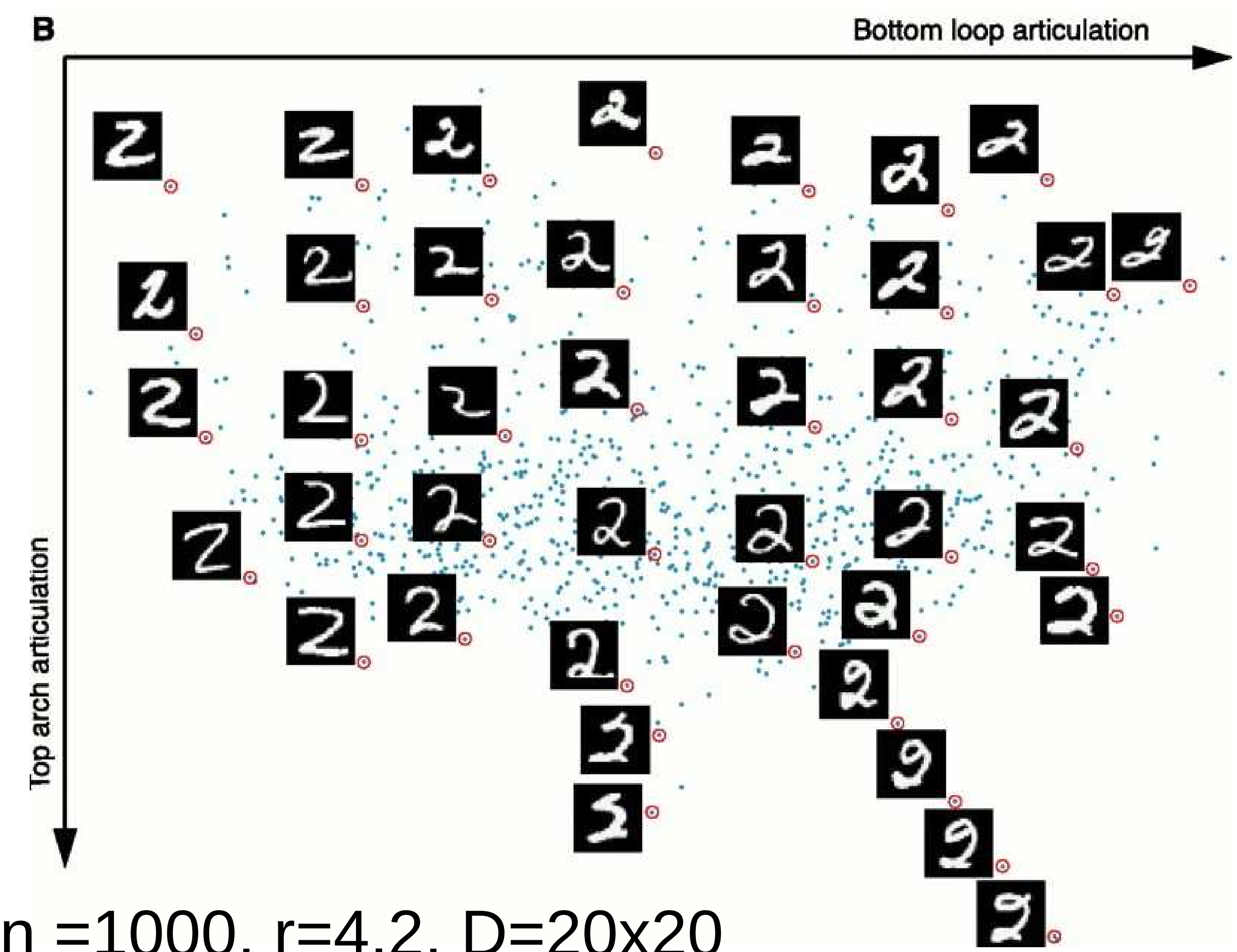


n (points) =1024
k (neighbors) =12

Isomap: Two-dimensional embedding of hand images (from Josh. Tenenbaum, Vin de Silva, John Langford 2000)



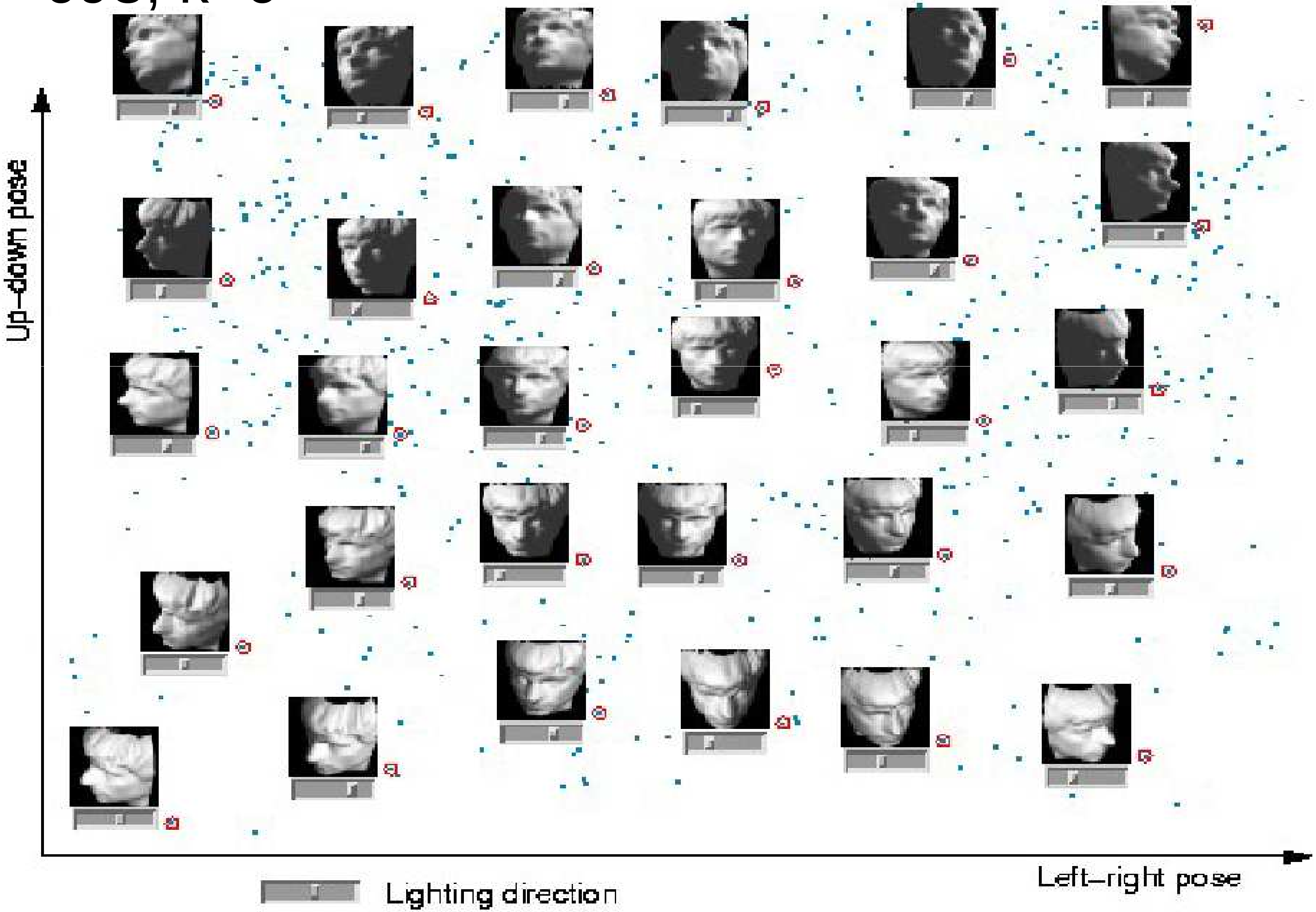
Isomap: two-dimensional embedding of hand-written '2' (from Josh. Tenenbaum, Vin de Silva, John Langford 2000)



n =1000, r=4.2, D=20x20

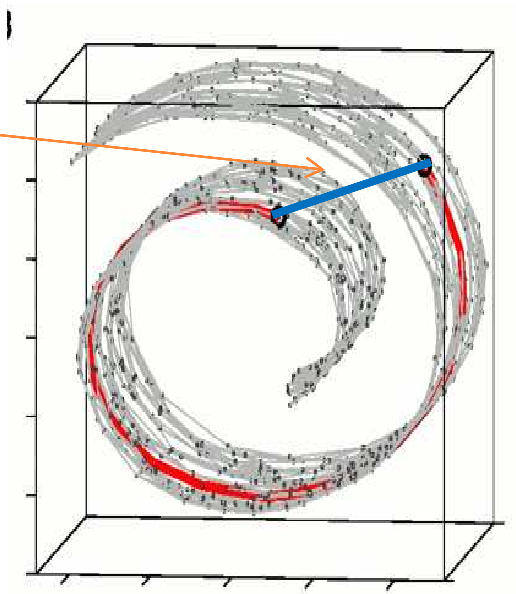
Isomap: three-dimensional embedding of faces (from Josh. Tenenbaum, Vin de Silva, John Langford 2000)

n =698, k=6



Properties of Isomap

- Strengths :
  - Preserves the global data structure
  - Performs global optimization
  - Non-parametric (Only heuristic is neighbourhood size)
- Weaknesses :
  - Sensitive to "shortcuts"
  - Very slow



Spectral Methods

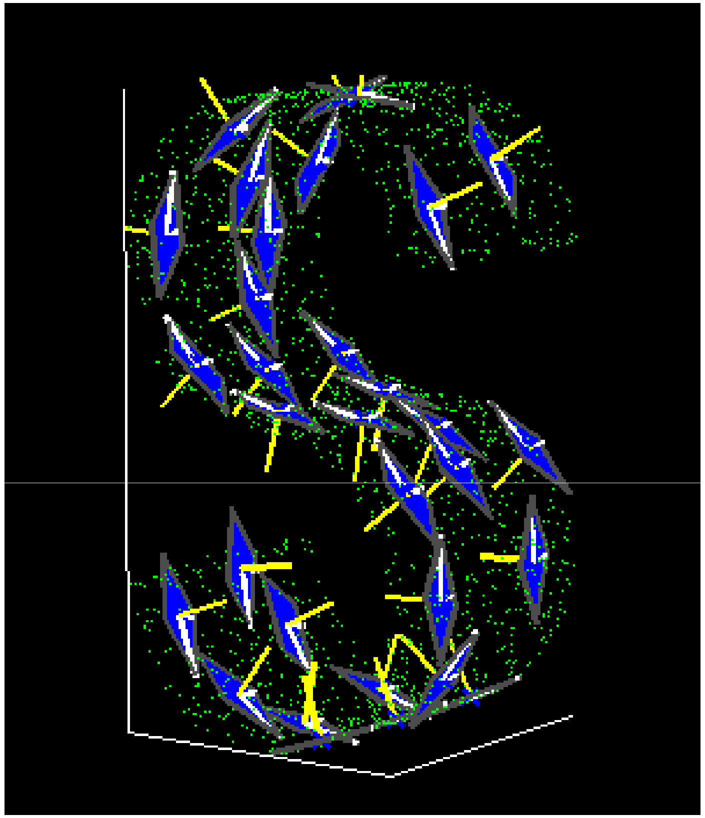
- Common framework
  1. Derive sparse graph from *kNN.*
  2. Derive matrix from graph weights.
  3. Derive embedding from eigenvectors.

- Varied solutions

  Algorithms differ in step 2. Types of optimization: shortest paths, least squares fits, semidefinite programming.

Locally Linear Embedding (LLE)

- Assume that data lies on a manifold: each sample and its neighbors lie on approximately linear subspace
- Idea:
  1. Approximate data by a set of linear patches
  2. Glue these patches together on a low dimensional subspace s.t. neighborhood relationships between patches are preserved.

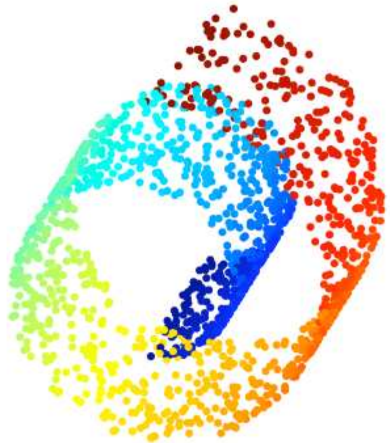


Algorithm: http://cs.nyu.edu/~roweis/lle/algorithm.html

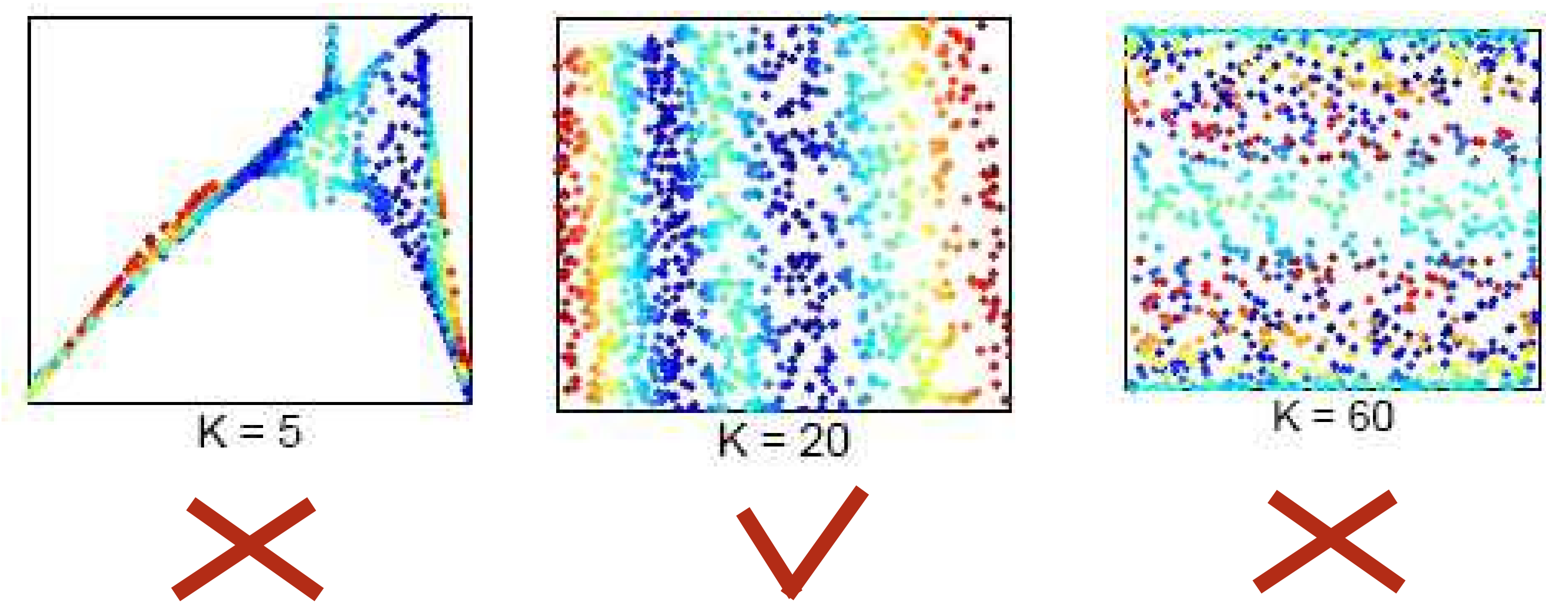
LLE at glance

- Steps
  1. Nearest neighbour search.
  2. Least squares fits.
  3. Sparse eigenvalue problem.
- Properties
  - Obtains highly nonlinear embeddings.
  - Not prone to local minima.
  - Sparse graphs yield sparse problems.

Step 1. Nearest neighbours search

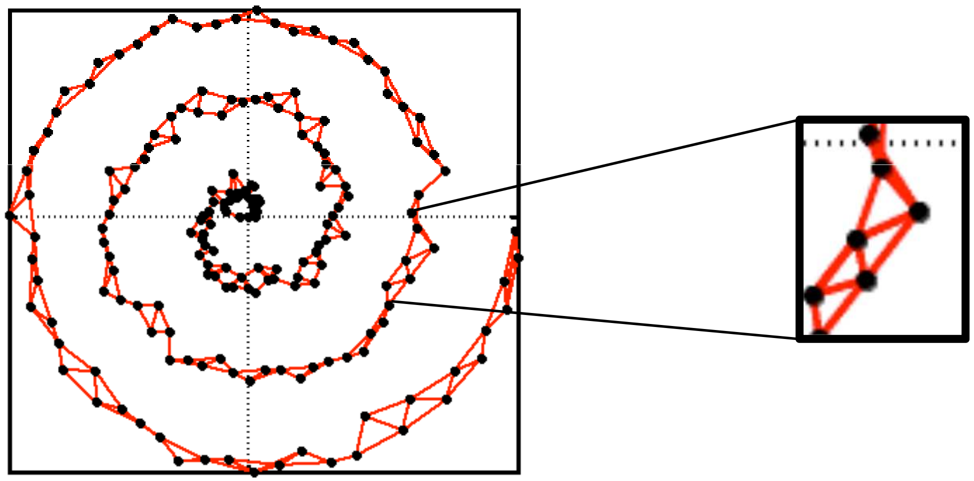


Effect of Neighbourhood Size



Step 2. Compute weights

- Characterize local geometry of each neighbourhood by weights Wij.



- Compute weights by reconstructing each input (linearly) from neighbours.

Linear reconstructions

- Local linearity
  - Assume neighbours lie on locally linear patches of a low dimensional manifold.
- Minimize reconstruction error
  - Each point can be written as a linear combination of its neighbors.
  - The weights chosen to minimize the reconstruction error:

$$\min_{W} \sum_{i} \left| x_i - \sum_{j} W_{ij} x_j \right|^2$$

Least squares fits (Computing W_{ij})

- Local reconstructions
  - Choose weights to minimize: $\Phi(W) = \sum_i \left| x_i - \sum_j W_{ij} x_j \right|^2$
- Constraints
  - Set $W_{ij} = 0$ if x_j is not a neighbor of x_i
  - Weights must sum to one: $\sum_j W_{ij} = 1$

invariance to translation

- Local invariance
  - Optimal weights W_{ij} are invariant to rotation, translation, and scaling.

Step 3. Finding the Embedding

- Low dimensional representation

  Map inputs to outputs: $x_i \in R^D \rightarrow y_i \in R^d$

- Minimize reconstruction errors

  Optimize outputs for fixed weights:

$$\Psi(y) = \sum_i \left| y_i - \sum_j W_{ij} y_j \right|^2$$

- Constraints:
  - Center outputs on origin $\sum_i y_i = 0$
  - Impose unit covariance matrix $\frac{1}{N} \sum_i y_i y_i = I_d$

Minimization

- Quadratic form:

$$\Psi(y) = \sum_{ij} M_{ij} \left(y_i \cdot y_j \right)$$

$$M_{ij} = \delta_{ij} - W_{ij} - W_{ji} + \sum_k W_{ki} W_{kj},$$

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

It can be shown that

$$M = (I - W)^T (I - W)$$

Sparse eigenvalue problem

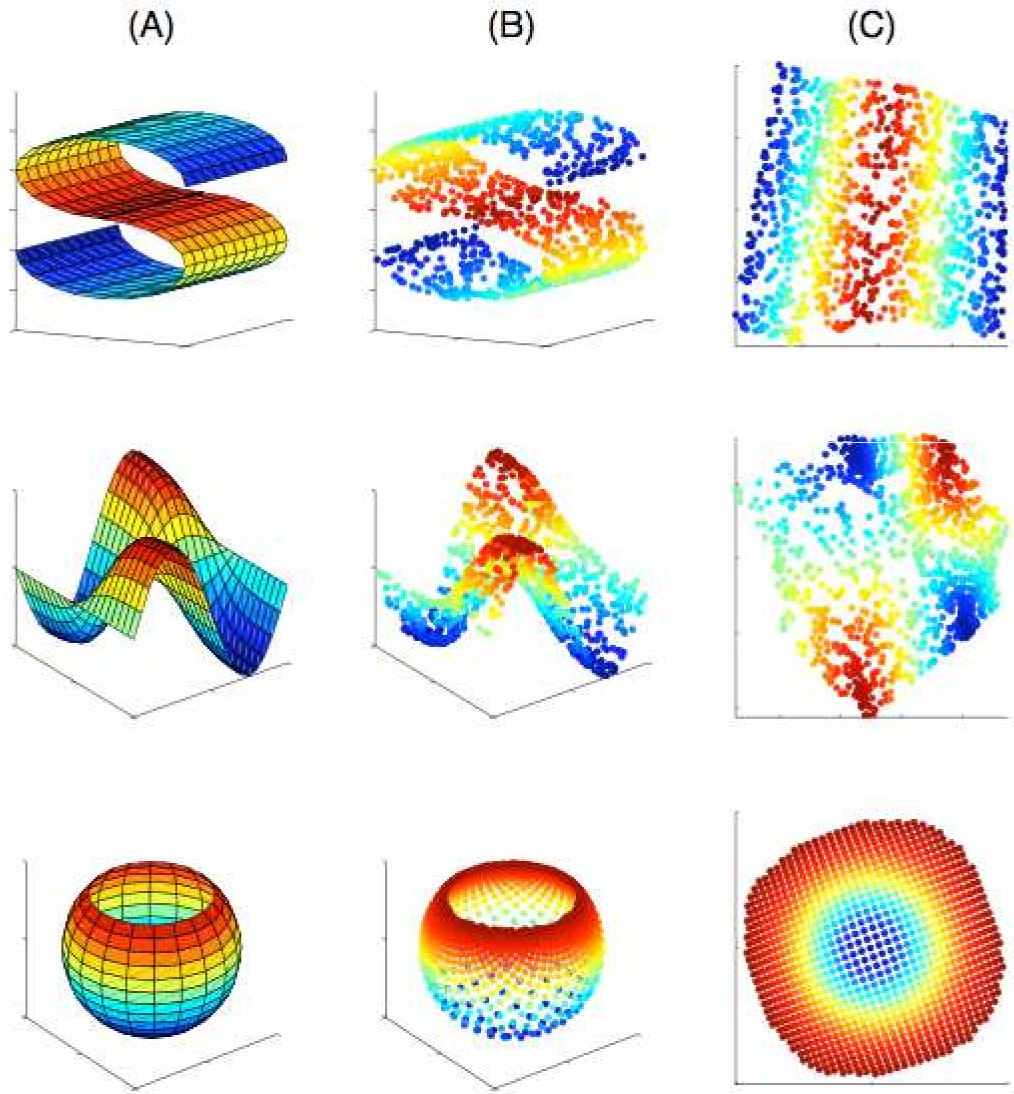
- Optimal embedding

  given by bottom d+1 eigenvectors, corresponding to the d+1 smallest eigenvalues (Rayleigh-Ritz theorem).

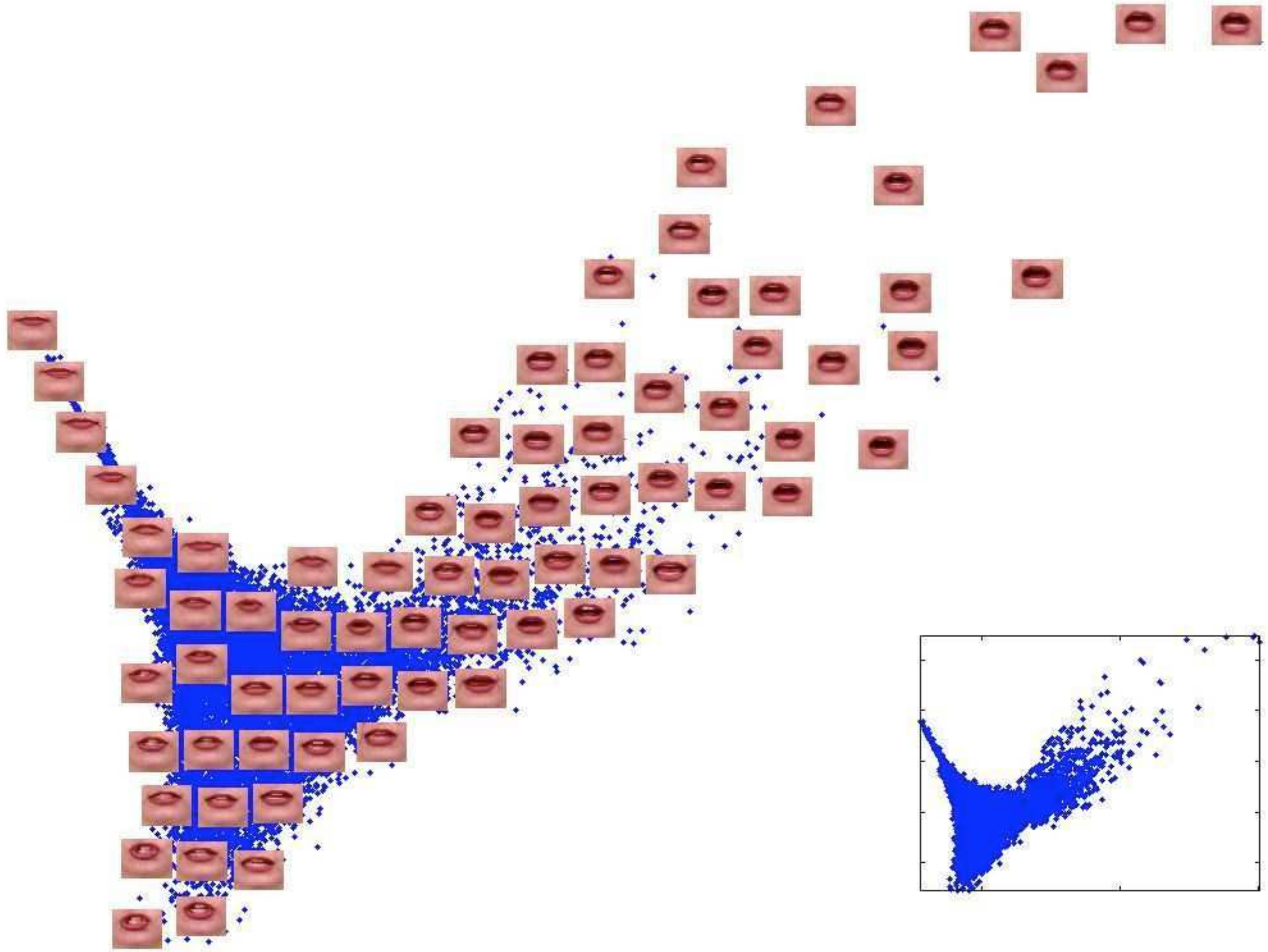
- Solution
  - Discard bottom eigenvector [1 1 … 1] (with eigenvalue zero).
  - Other eigenvectors satisfy constraints.

Surfaces

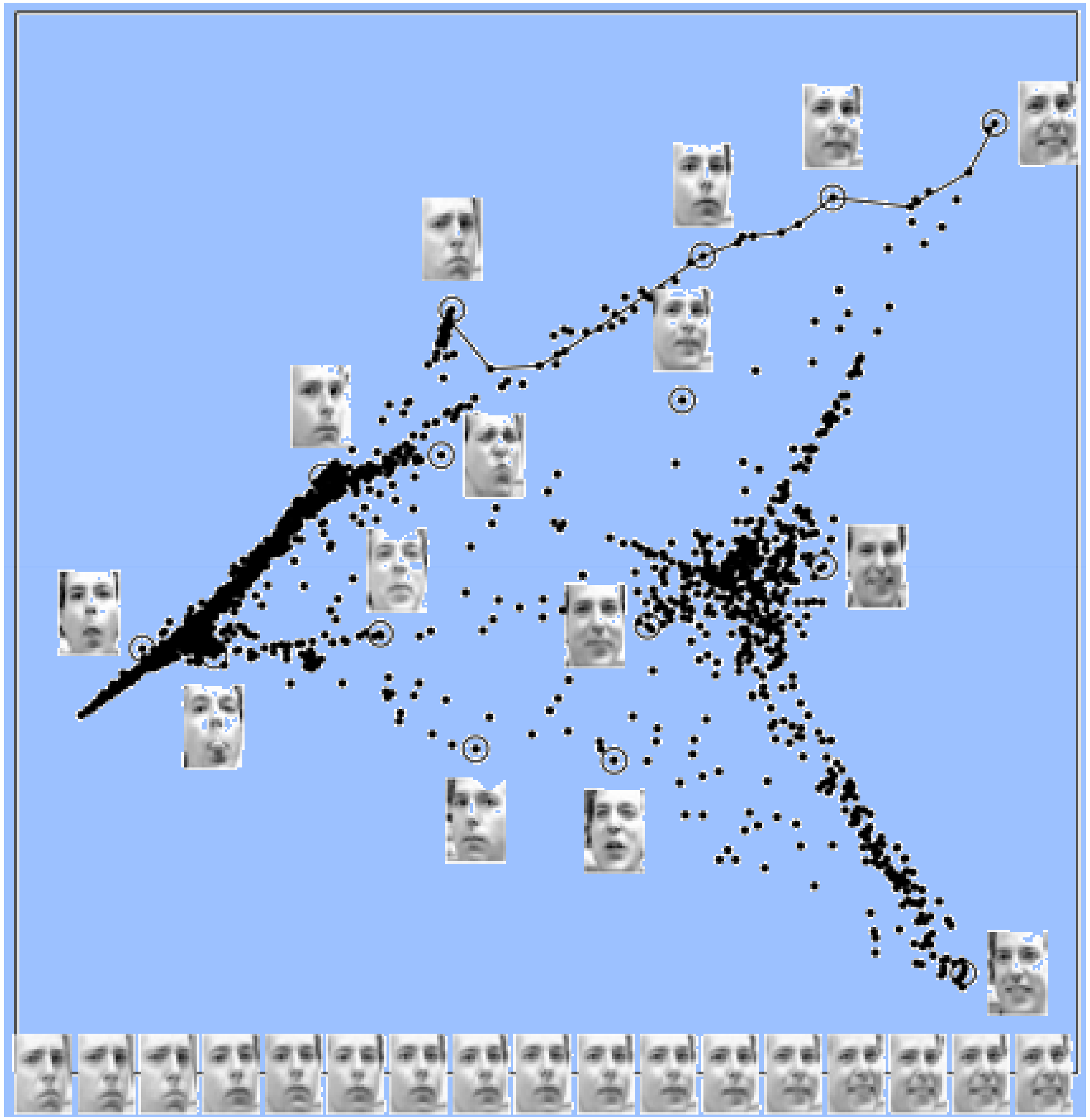
N=1000
inputs
k=8
nearest
neighbors



Lips
N=15960 images
K=24 neighbors
D=65664 pixels
d=2 (shown)



Pose and expression
N=1965 images
k=12 nearest neighbors
D=560 pixels
d=2 (shown)



Properties of LLE

- Strengths:
  - Fast
  - No local minima
  - Non-iterative
  - Non-parametric (only heuristic is neighbourhood size).
- Weaknesses:
  - Sensitive to “shortcuts”
  - No estimate of dimensionality

LLE versus Isomap

- Many similarities
  - Graph-based, spectral method
  - No local minima
- Essential differences
  - Does not estimate dimensionality ☹
  - No theoretical guarantees ☹
  - Constructs sparse vs. dense matrix ☺
  - Preserves weights vs. distances
  - Much faster ☺

Laplacian Eigenmaps

- Map nearby inputs to nearby outputs, where nearness is encoded by graph.

- Summary of the Algorithm
  1. Identify k-nearest neighbours (as in LLE)
  2. Assign weights to neighbours
  3. Sparse eigenvalue problem

Step 2. Construct the graph

- Vertices represent inputs.
- Undirected edges connect neighbours.
- Assign weights to neighbours:
  - Simple: $W_{ij} = 1$

    or
  - Heat kernel $W_{ij} = \exp\left(-\beta \left\| x_i - x_j \right\|^2\right)$

Step 3. Graph Laplacian

- Compute outputs by minimizing:

$$\Psi(y) = \sum_{ij} W_{ij} \left\| y_i - y_j \right\|^2$$ under appropriate constraints

$$\Psi(y) = \sum_{ij} W_{ij} \left(y_i^2 + y_j^2 - 2 y_i y_j \right)$$ W_{ij} is symmetric

$$= \sum_i y_i^2 D_{ii} + \sum_j y_j^2 D_{jj} - 2 \sum_{ij} y_i y_j W_{ij} = 2 y^t L y$$

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

Graph Laplacian $L = D - W$

Step 3. Generalized eigenvalue problem

- Minimize $y^t L y$
  constrained by $y^t D y = 1$

- Optimal embedding: $(Le = \lambda De)$
  given by bottom d+1 eigenvectors (corresponding to the d+1 smallest eigenvalues).

- Solution:
  Discard bottom eigenvector [1 1 … 1] (with eigenvalue zero). Other eigenvectors satisfy constraints.

Analysis on Manifolds

- Consider Riemannian manifold $\Omega \in \Re^D$
  - a real differentiable manifold in which tangent space is equipped with dot product.
- Laplace Beltrami operator
  - Ω has a 'natural' operator Δ on differentiable functions.
  - Δ is a second order differential operator defined as a "divergence of the gradient"

$$\Delta = \sum_i \frac{\partial^2}{\partial x_i^2}$$

Spectral desomposition of Δ

- Assume $\mathscr{L}^2(\Omega)$ is space of all square integrable functions on Ω
- Δ is a self-adjoint positive semi-definate operator and its eigenfunctions form the basis.
- Thus all f in $\mathscr{L}^2(\Omega)$ can be written as

$$f(x) = \sum_i \alpha_i e_i(x)$$

(provided Ω is compact)

Smoothness functional

- Defined as

$$S(f) = \int_{\Omega} |\nabla f|^2 d\omega = \int f \Delta f \; d\omega = \langle \Delta f, f \rangle_{L^2(\Omega)}$$

  - value close to zero implies *f* being smooth.

- Since

$$S(e_i) = \langle \Delta e_i, e_i \rangle = \lambda_i$$

we have

$$S(f) = \langle \Delta f, f \rangle = \left\langle \sum_i \alpha_i \Delta e_i, \sum_i \alpha_i e_i \right\rangle = \sum_i \lambda_i \alpha_i$$

choosing the lowest p eigenfunctions provides a maximally smooth approximation to the manifold.

Spectral graph theory

- Weighted graph is discretized representation of manifold.
- Laplacian measures smoothness of functions over manifold and graph.

Manifold: $$\int_{\Omega} |\nabla f|^2 \, d\omega = \int f \Delta f \, d\omega$$

Graph: $$\sum_{ij} W_{ij} \left(f_i - f_j \right)^2 = f^t L f$$

Interpreting Laplacian Eigenmaps

- Eigenvectors

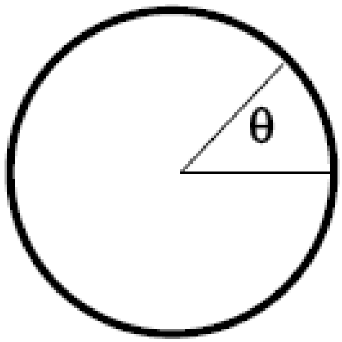
  functions from nodes to $\mathbb{R}$ in a way that "close by" points are assigned "close by" values.

- Eigenvalues

  measure how close are the values of neighbouring points – smoothness.

Example: S1 (the circle)

- Continuous
  - Eigenfunctions of Laplacian are basis for periodic functions on circle, ordered by smoothness.
  - Eigenvalues measure smoothness.

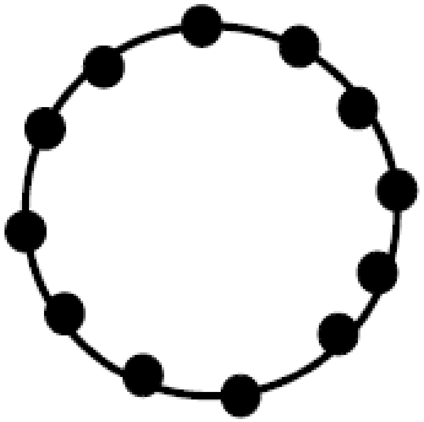


$$-\frac{\partial^2 f_m}{\partial^2 \theta} = \lambda_m f_m(\theta)$$

$$f_m(\theta) = \begin{Bmatrix} \sin(m\theta) \\ \cos(m\theta) \end{Bmatrix} \text{ with } \lambda_m = m^2$$

Example: S1 (the circle)

- Discrete (n equally spaced points)
  - Eigenvectors of graph Laplacian are discrete sines and cosines.
  - Eigenvalues measure smoothness.



Graph embedding from Laplacian eigenmaps:

$$\vec{y}_k = \left(\cos\left(2\pi k/n\right), \sin\left(2\pi k/n\right)\right)$$

Laplacian vs LLE

- More similar than different
  - Graph-based, spectral method
  - Sparse eigenvalue problem
  - Similar results in practice
- Essential differences
  - Preserves locality vs local linearity
  - Uses graph Laplacian