Nonlinear Dimensionality Reduction (a.k.a. Manifold Learning)

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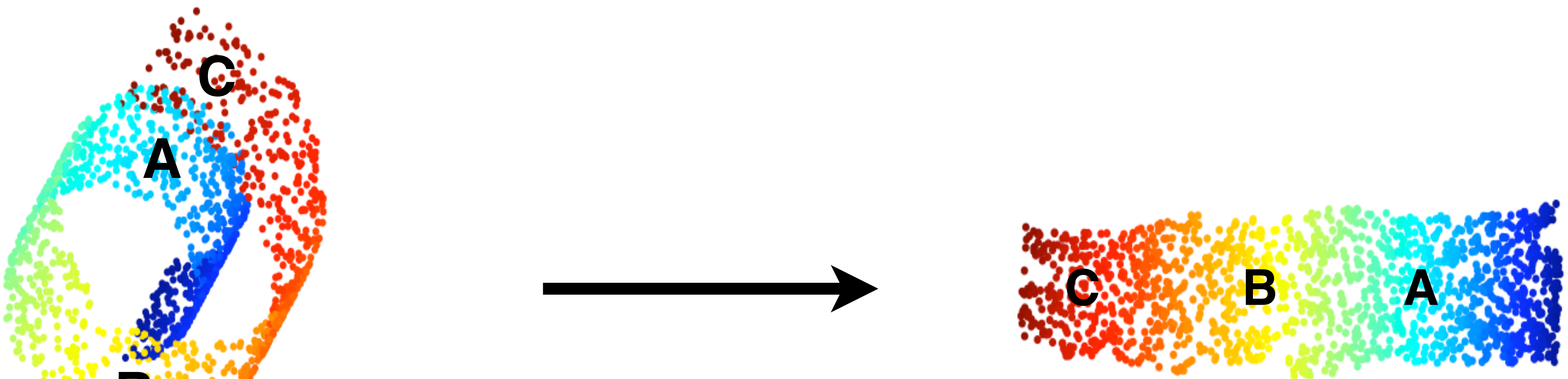
What is "nonlinear dimensionality reduction?"



High-dimensional data

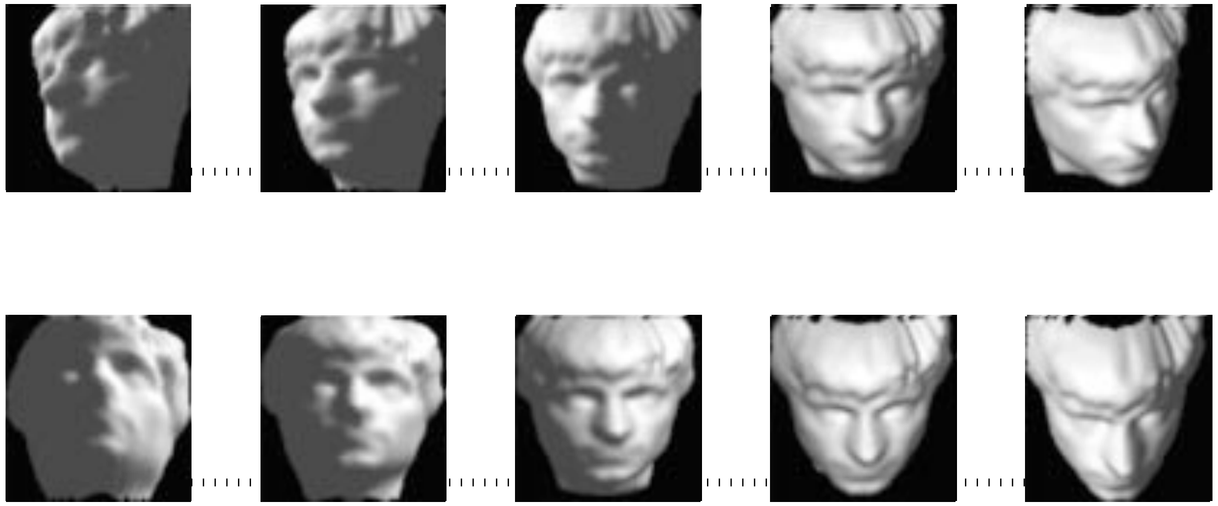
NDR
(Manifold Learning)

Low-dimensional
embedding

- We often suspect that high-dim may actually lie on or near a low-dim manifold (often much lower!)
- It would be useful if we could reparametrize the data in terms of this manifold, yielding a low-dim *embedding*
- **BUT -** we typically don't know the form of this manifold

Why might this be useful?

- The variation observed in high-dimensional signals often has much lower-dimensional explanation



64x64 pixel images parametrized by just 3 variables (pose and lighting direction)

- Discovering these modes of variation helps us understand the underlying structure of the data and the process that generated it
  - Visualization of high-dimensional data
  - Machine learning and pattern recognition

Okay, so how do we learn the embedding?

- Given high-dim data sampled from an unknown low-dim manifold, how can we automatically recover a good embedding?

A Global Geometric Framework for Nonlinear Dimensionality Reduction

Tenenbaum, de Silva and Langford
Science (Vol. 290, Dec 2000, 2319-2323)

Nonlinear Dimensionality Reduction by Locally Linear Embedding

Roweis and Saul
Science (Vol. 290, Dec 2000, 2323-2327)

Outline

- Linear subspace embedding
  - Principal Components Analysis (PCA)
  - Metric Multidimensional Scaling (MDS)

- Non-linear manifold learning
  - Isomap (Tenenbaum et al.)
  - Locally Linear Embedding (Roweis et al.)

- Some examples

An excellent tutorial ...

Spectral Methods for Dimensionality Reduction

Prof. Lawrence Saul

Dept of Computer & Information Science
University of Pennsylvania

NIPS*05 Tutorial, December 5, 2005

Penn
University of Pennsylvania

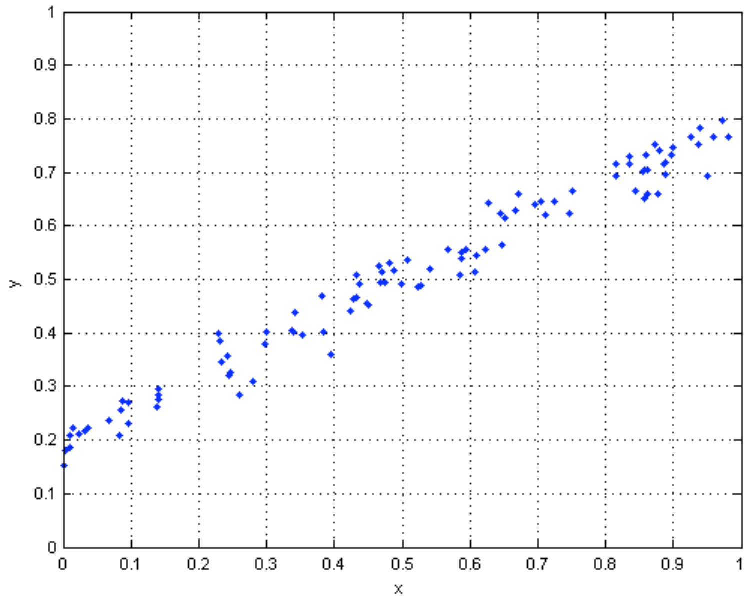
Neural Information Processing Systems Conference

... from which I have borrowed liberally! Thanks Lawrence!

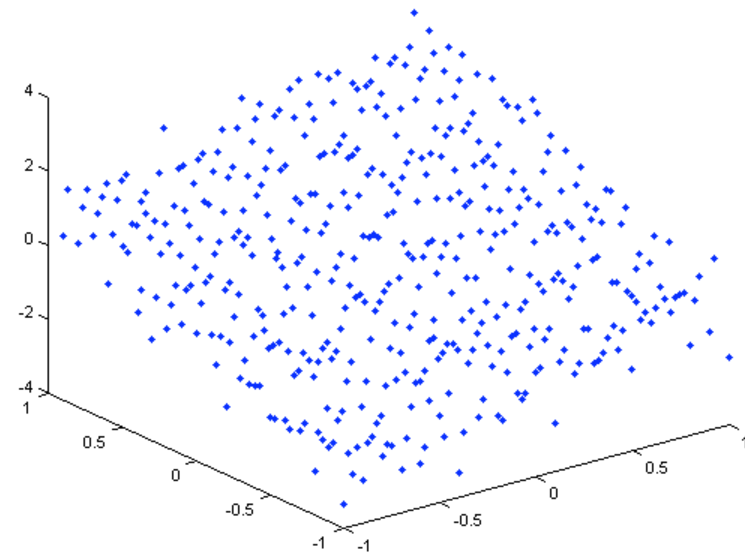
Background - Linear Subspace Embedding

Linear subspaces

- We may often assume that our high-dim data lies on/near a linear subspace



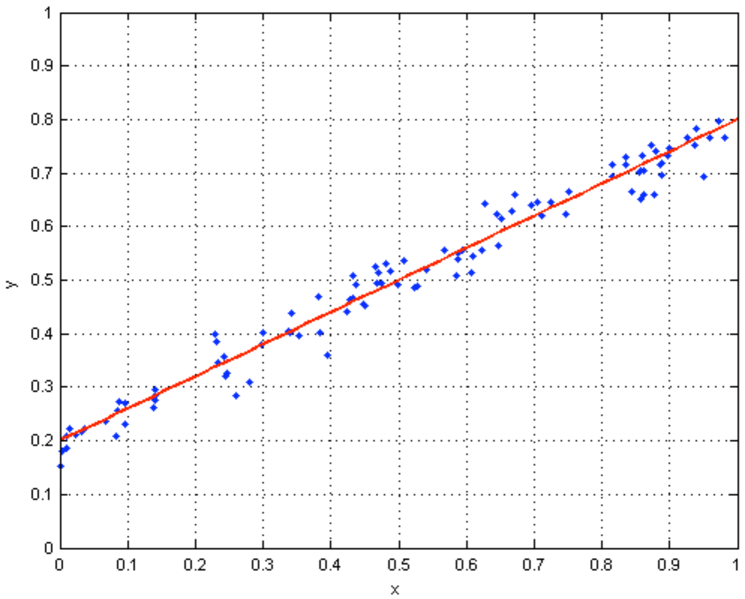
$D_{high}=2$
$D_{low}=1$



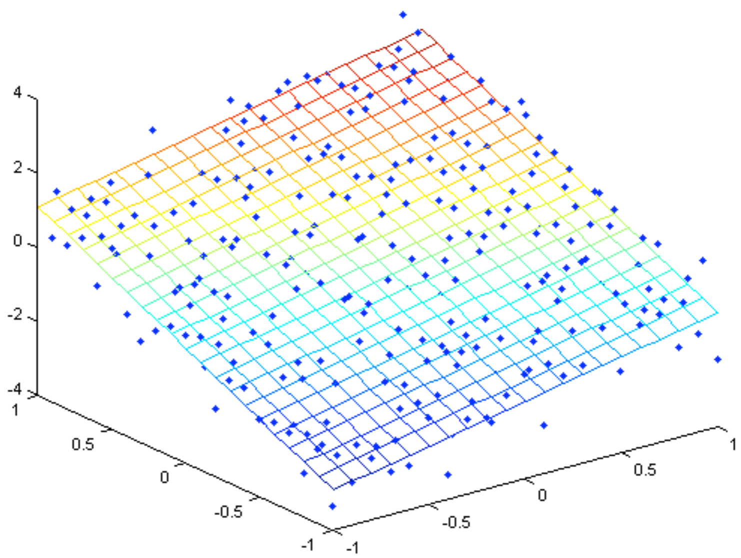
$D_{high}=3$
$D_{low}=2$

Linear subspaces

- We may often assume that our high-dim data lies on/near a linear subspace



$D_{high}=2$
$D_{low}=1$



$D_{high}=3$
$D_{low}=2$

- In this case, well-known, stable tools exist for determining the parameters of this subspace
  - Principal Components Analysis
  - Metric Multidimensional Scaling
- Among the most widely-used algorithms in engineering!

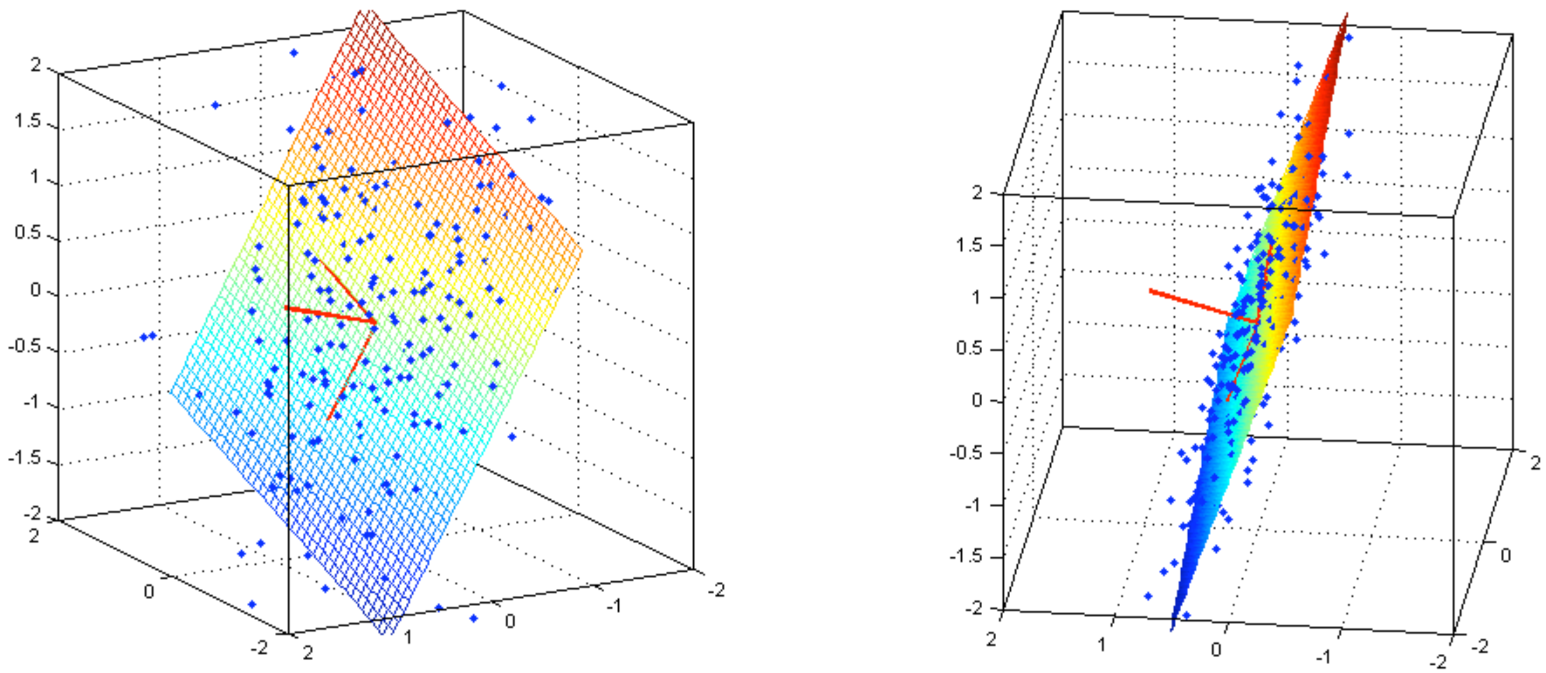
Notation

- We have a quantity **N** of **D**-dimensional data points **x**
- We seek to map **x** to a set of **d**-dimensional points **y**
- **N** is large and **d** << **D**

Principal Components Analysis (PCA)

- Project data onto an **orthonormal basis,** chosen so as to **maximize the variance** of the projected data

$$\vec{y}_i = P\vec{x}_i$$



- Choose subspace as the d-dimensional hyper-plane spanned by directions of maximum variance

Principal Components Analysis (PCA)

- First, we center the data to have zero empirical mean

$$\sum_i \vec{x}_i = \vec{0}$$

- Then we determine an orthonormal linear projection

$$\vec{y}_i = P\vec{x}_i$$

- ... so as to maximize the projected variance

$$\mathrm{var}(\vec{y}) = \frac{1}{n}\sum_i \| P\vec{x}_i \|^2$$

Principal Components Analysis (PCA)

- Projected variance is given by

$$\mathrm{var}(\vec{y}) = \mathrm{Tr}(PCP^{\mathrm{T}}) \;\text{ with }\; C = n^{-1}\sum \vec{x}_i \vec{x}_i^T$$

- where C is the DxD data covariance matrix, with eigen-value decomposition

$$C = \sum_{\alpha=1}^{D} \lambda_\alpha \vec{e}_\alpha \vec{e}_\alpha^{\mathrm{T}} \;\text{ with }\; \lambda_1 \geq \cdots \geq \lambda_D \geq 0$$

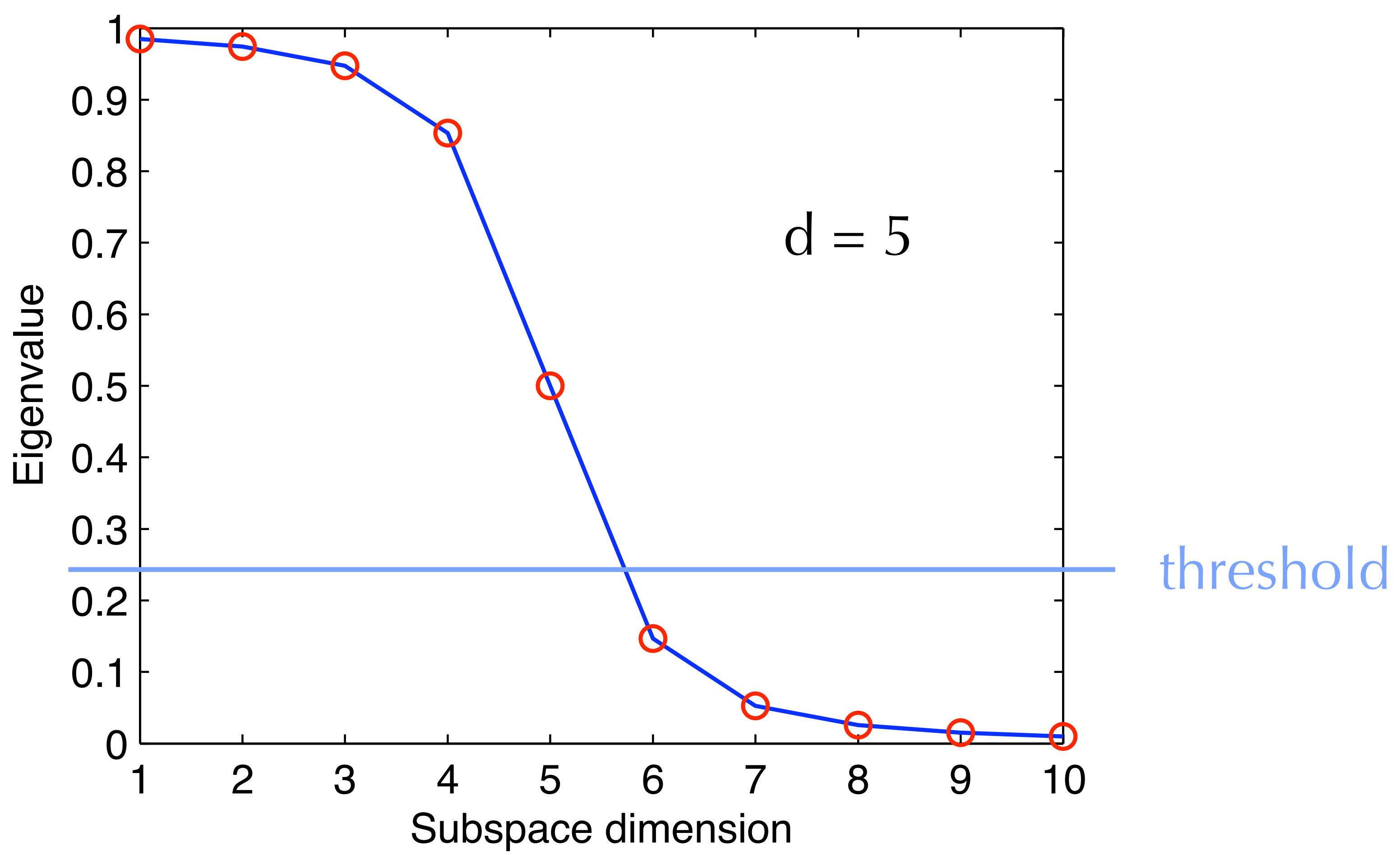
- The projected variance is maximized when

$$P = \sum_{\alpha=1}^{d} \vec{e}_\alpha \vec{e}_\alpha^{\mathrm{T}}$$

- i.e. projecting into the sub-space spanned by the eigenvectors corresponding to the largest eigenvalues

Principal Components Analysis (PCA)

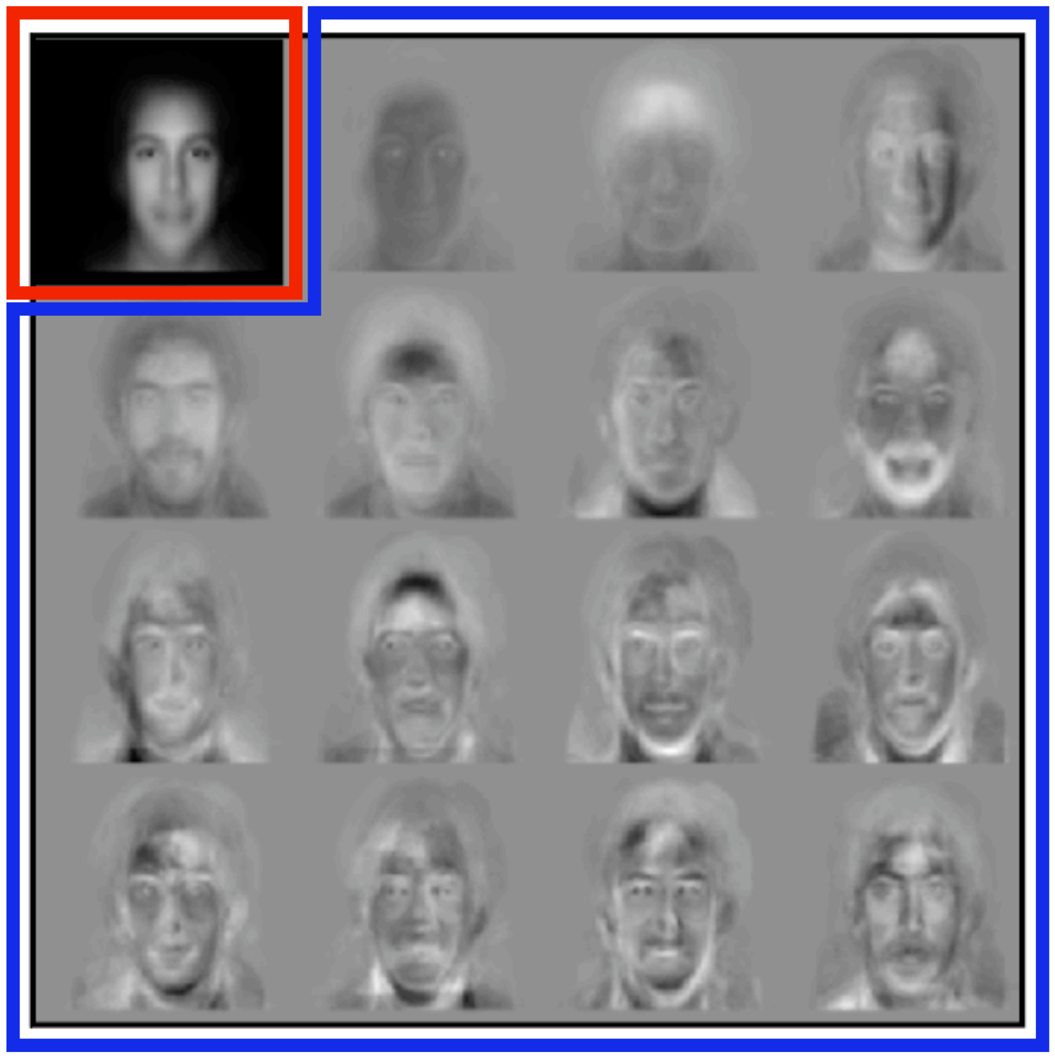
- The intrinsic dimensionality of the subspace may be estimated as the number of significantly large eigenvalues



PCA Example : Eigenfaces

- Sirovich and Kirby (JOSA '87) pioneered application of PCA to model the variation observed in face images
- High-dim (e.g. 128x128 pixel) face images may be modeled by just 50-100 principal components

"Mean" face



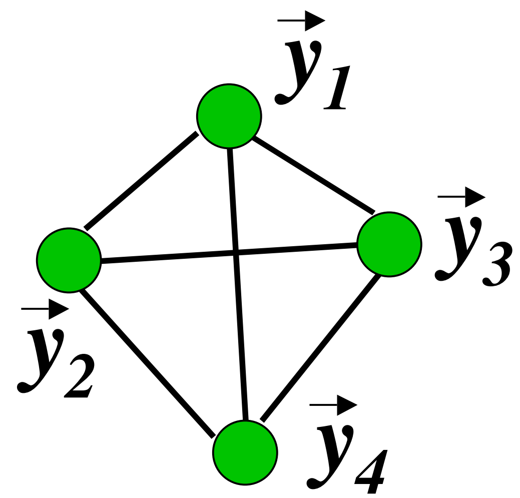
PCA applied to 7562 face images

Top 15 most significant principal components

Multidimensional Scaling (MDS)

- An alternative approach to PCA based on preserving pairwise distances

$$\begin{bmatrix} 0 & \Delta_{12} & \Delta_{13} & \Delta_{14} \\ \Delta_{12} & 0 & \Delta_{23} & \Delta_{24} \\ \Delta_{13} & \Delta_{23} & 0 & \Delta_{34} \\ \Delta_{14} & \Delta_{24} & \Delta_{34} & 0 \end{bmatrix}$$



Given $n(n-1)/2$ pairwise distances $d_{ij} = \|X_i - X_j\|$, find a low-dimensional embedding $X \to y$ such that $\|y_i - y_j\| \approx d_{ij}$.

Multidimensional Scaling (MDS)

- Given centered mean-zero data X, we can express the dot products G_{ij} = <X_i,X_j> in terms of pairwise distances d_{ij}

$$G_{ij} = \frac{1}{2}\left[\frac{1}{n}\sum_k (d_{ik}^2 + d_{kj}^2) - d_{ij}^2 - \frac{1}{n^2}\sum_{kl} d_{kl}^2\right]$$

(n.b. useful lemma!)

- We then seek new vectors y_i so as to minimize the error function

$$err(y) = \sum_{ij} \left(G_{ij} - y_i^\top y_j\right)^2$$

- Matrix **G**, consisting of all possible dot products <i,j> is known as a *Gram* matrix

Multidimensional Scaling (MDS)

- We aim to approximate **G**

$$err(y) = \sum_{ij} \left(G_{ij} - y_i^\top y_j \right)^2$$

- Again using the eigen-decomposition of the Gram matrix

$$G = \sum_{\alpha=1}^{n} \lambda_\alpha \vec{v}_\alpha \vec{v}_\alpha^{\mathrm{T}} \quad \text{with} \quad \lambda_1 \geq \cdots \geq \lambda_n \geq 0$$

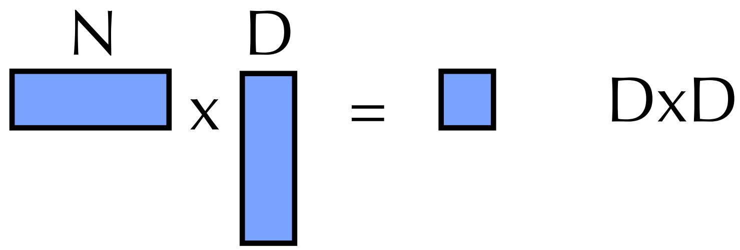
- We immediately see that the optimal approximation of **G** is given by an outer-product of the most significant eigenvectors

$$y_{\alpha i} = \sqrt{\lambda_\alpha} v_{\alpha i} \quad \text{for } \alpha = 1,2,\ldots,\mathrm{d}$$

PCA vs. MDS

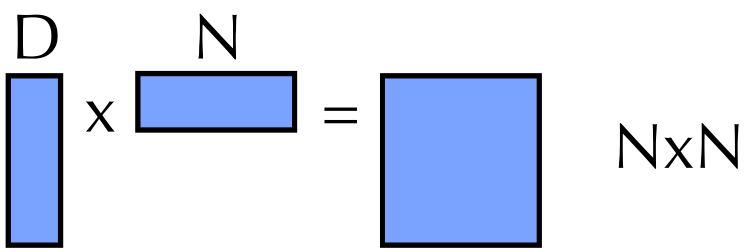
- The methods are in some sense "dual" to each other
  - In PCA, we compute the DxD covariance matrix

$$C_{ij} = \frac{1}{n}\sum_k x_{ik}x_{jk}$$



  - In MDS, we compute the NxN Gram matrix

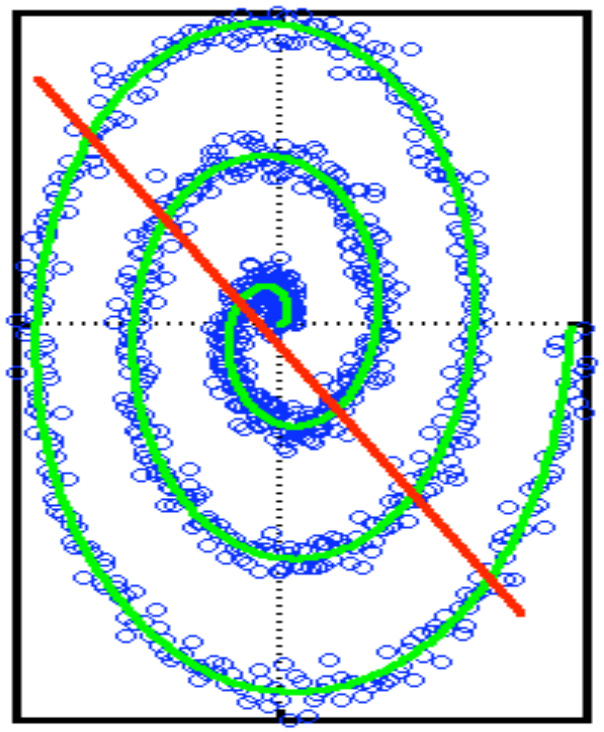
$$G_{ij} = \vec{x_i} \circ \vec{x_j}$$



- For Euclidean distances d_{ij} in MDS, the two methods yield the same embedding results (up to an arbitrary rotation)

PCA vs. MDS

- Both PCA and MDS have similar strengths
  - polynomial time algorithms (non-iterative)
  - no local optima
  - no parameters to set
  - can estimate subspace dimension
  - very well understood!



- BUT - Limited to linear projections

- **How can we generalize to arbitrary manifolds?**

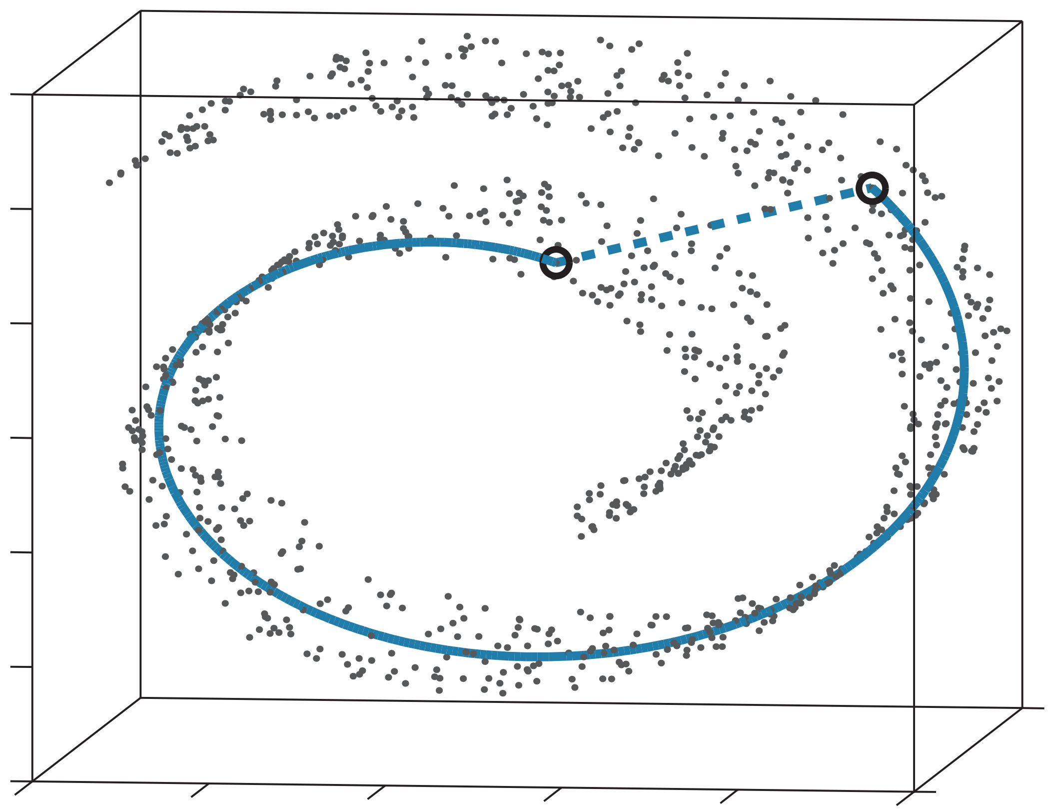
Nonlinear Dimensionality Reduction

Method 1: Isometric Feature Mapping (IsoMap)

Isometric Feature Mapping (IsoMap)

Tenenbaum et al. (Science, Dec '00)

- Recall that MDS seeks an embedding that preserves pairwise distances between data points
- **BUT -** Geodesic distances measured on the manifold may be longer than the corresponding Euclidean straight-line distance d_{ij}



IsoMap

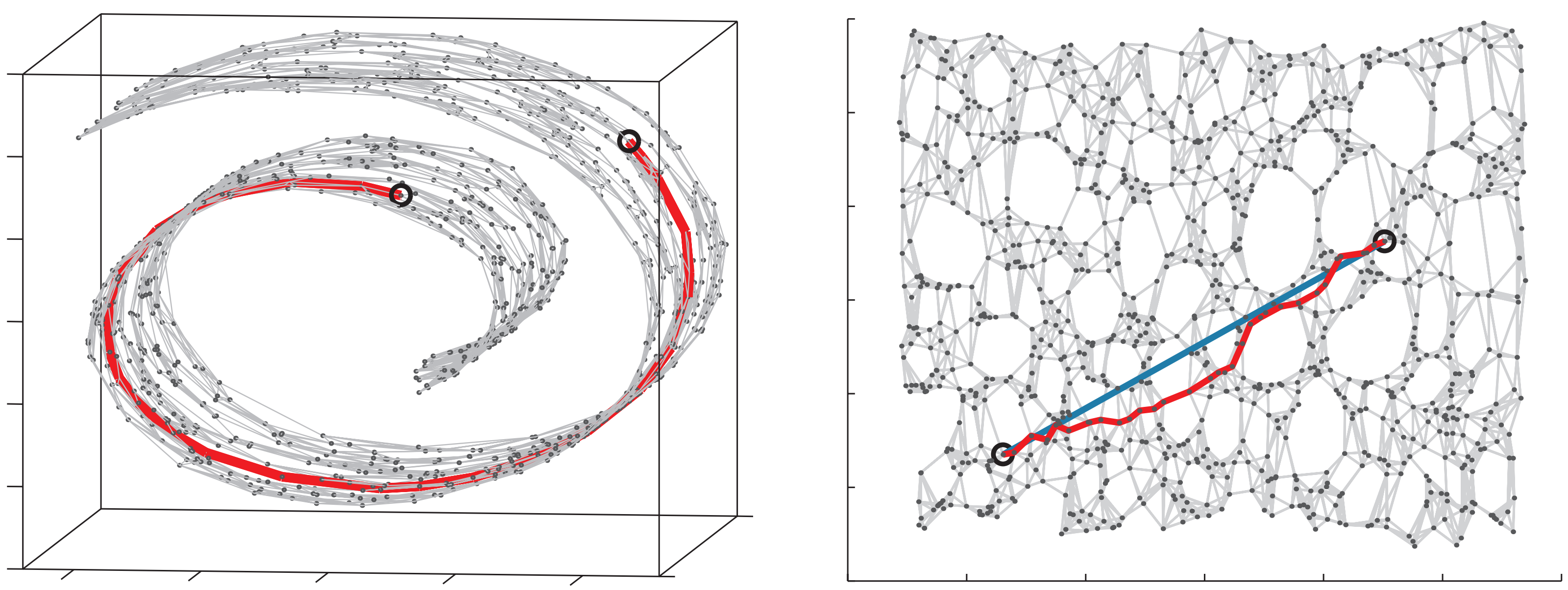
- **Idea : Use geodesic rather than Euclidean distances in MDS**

- **But -** How can we compute geodesics without knowing the manifold?

IsoMap

- **Idea : Use geodesic rather than Euclidean distances in MDS**

- **But -** How can we compute geodesics without knowing the manifold?



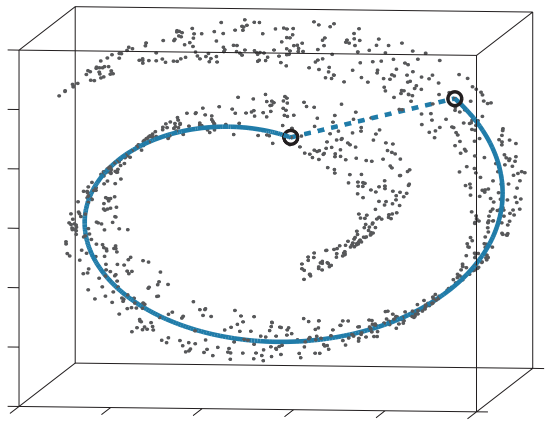
- **Answer :** Build an adjacency graph and approximate geodesic distances by shortest-paths through the graph

IsoMap

- **Step 1 - Build the adjacency graph over high-dim points X**

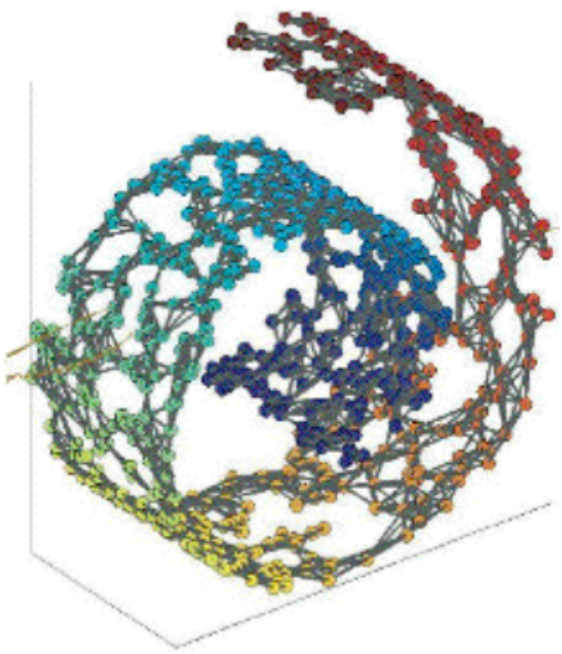
- Neighborhood selection
  - Choice 1: k-nearest neighbors
  - Choice 2: neighbors within a fixed radius (epsilon-ball)

- Assume graph is fully connected
  - no isolated islands of points
- Assume graph neighborhoods reflect manifold neighborhoods
  - no “short-cuts” between distant points on manifold
  - sensitive to choice of neighborhood size



IsoMap

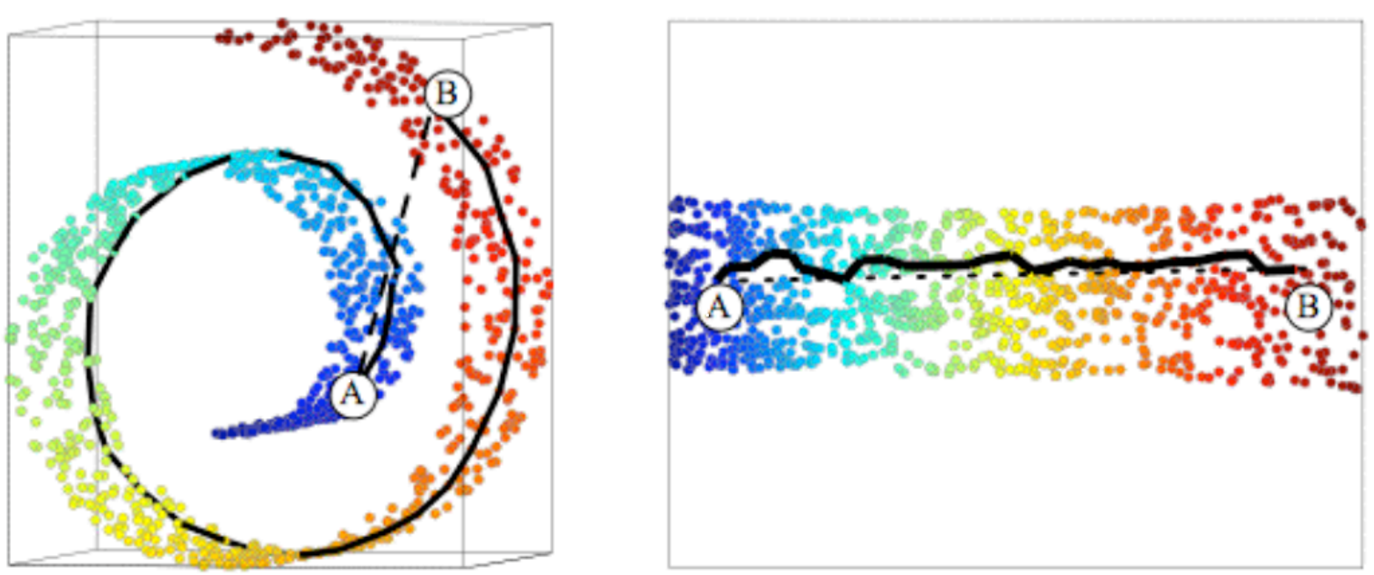
- **Step 2 - Compute approximate geodesics**
- Weight graph edges by inter-point distances
- Apply Dijkstra's all-pairs shortest-paths algorithm $\mathbf{O(N^2 lgN+N^2k)}$



IsoMap

- **Step 3 : Apply MDS to geodesic distances**

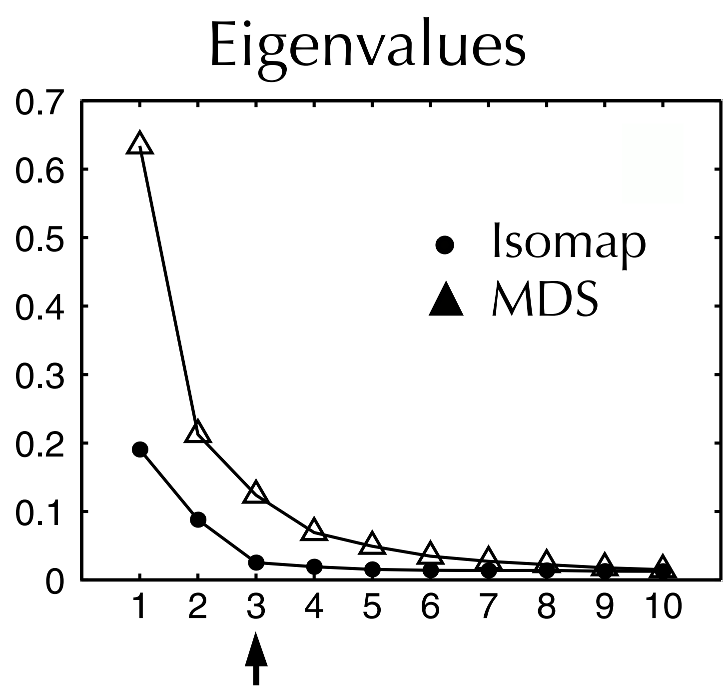
- Top **d** eigenvectors of Gram matrix give the embedded, **d**-dimensional points
- Dimensionality of manifold may be estimated by number of significant eigenvalues, just as in PCA/MDS

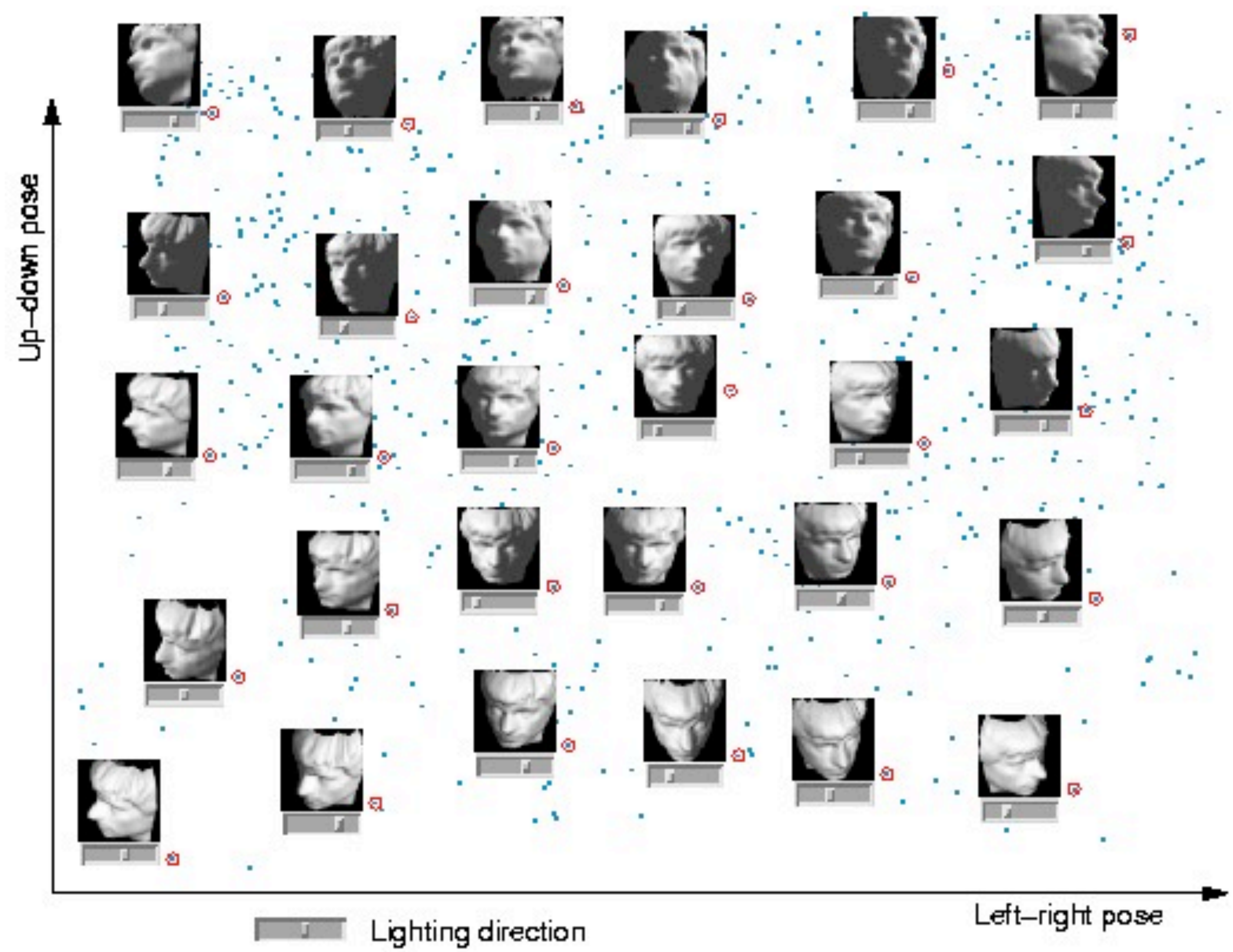


N = 1024 points
k = 12 nearest neighbours

IsoMap examples

- Faces - varying pose and illumination
- 3 true degrees of freedom (dof) in total
  - 64x64 pixel images
  - N = 698
  - k = 6



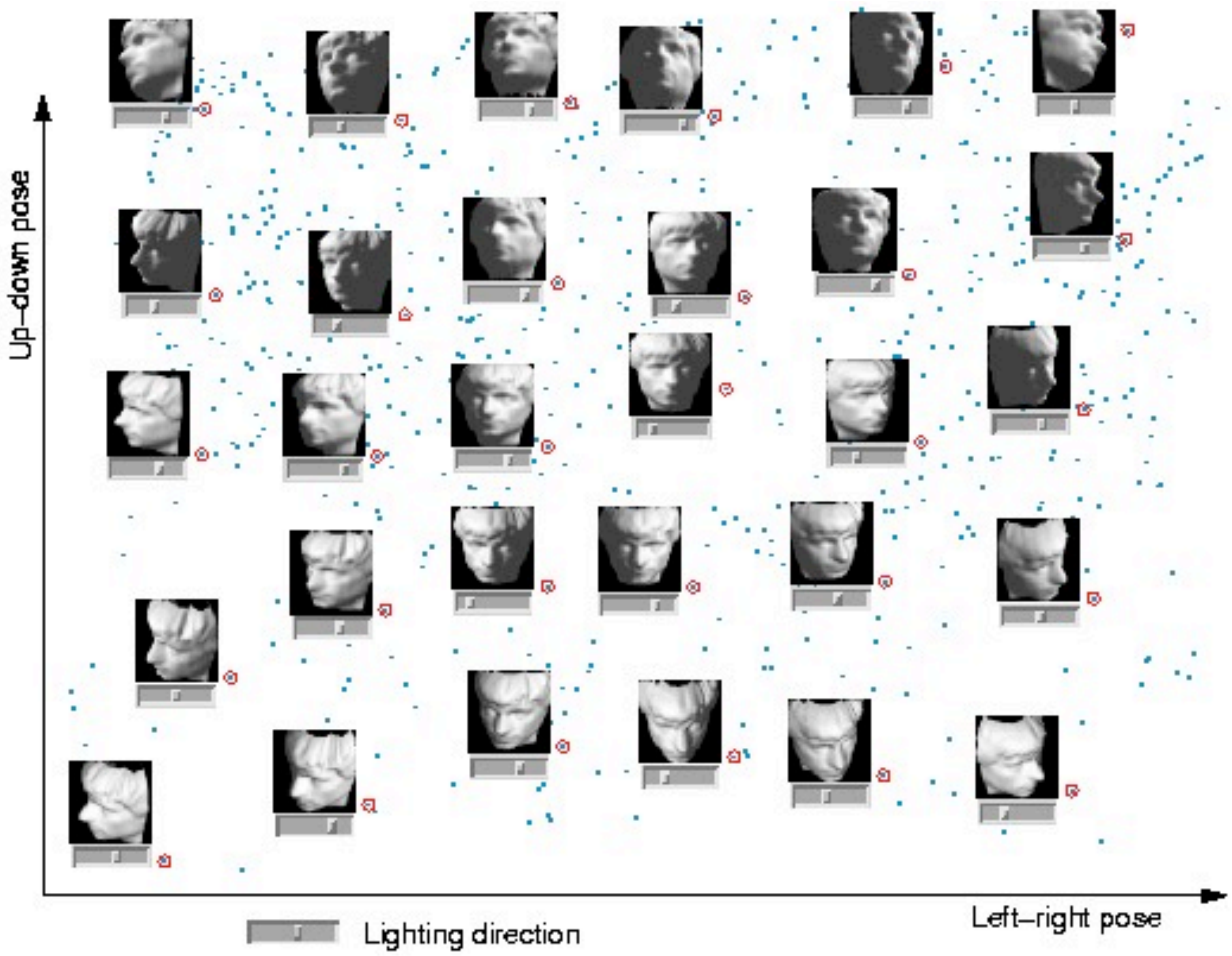


IsoMap examples

- Faces - varying pose and illumination
- 3 true degrees of freedom (dof) in total

IsoMap recovers the low-dimensional structure in the data

Coordinates in the embedding correspond to meaningful modes of variation in the image

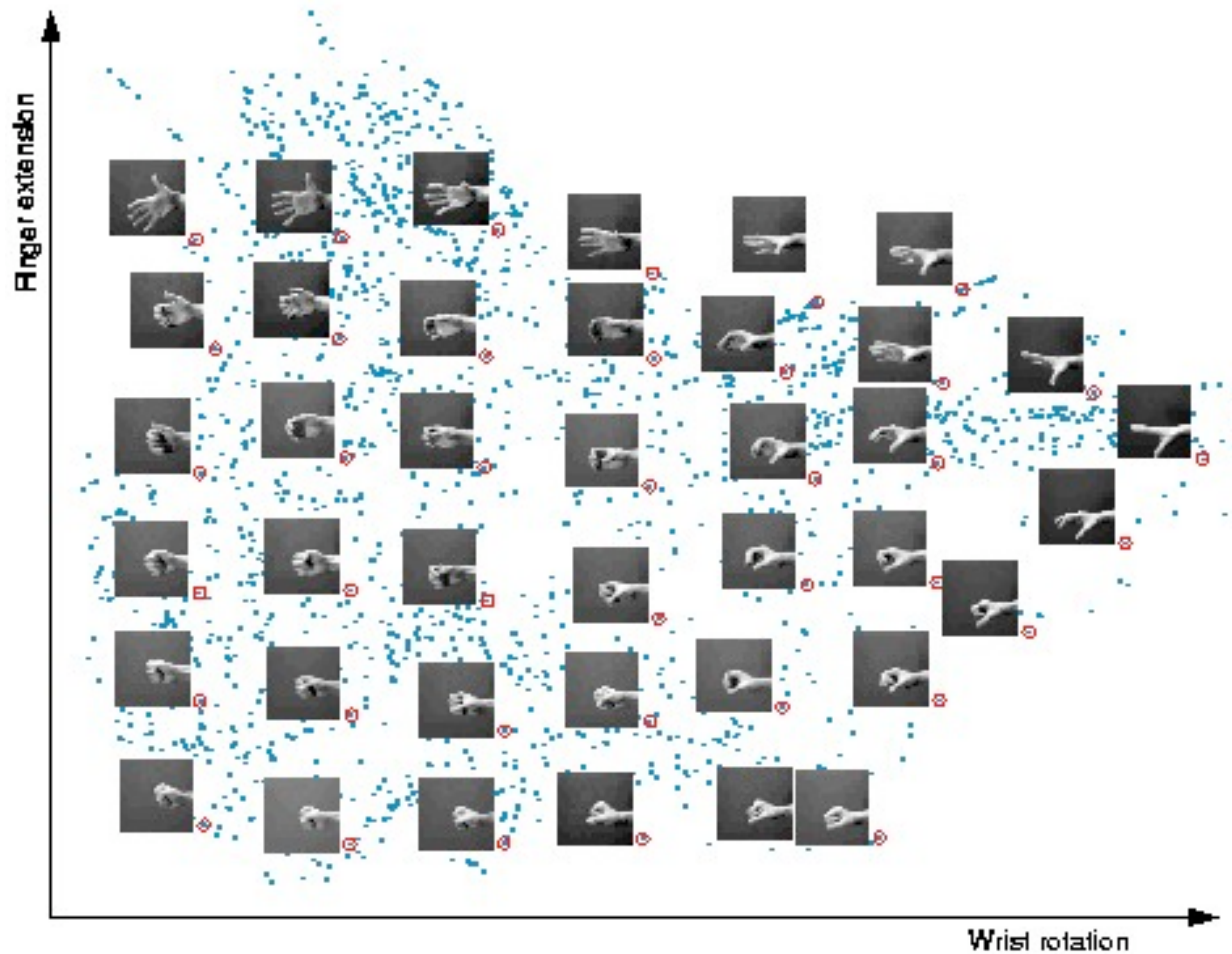


IsoMap examples

- Hand images - varying wrist rotation and finger extension

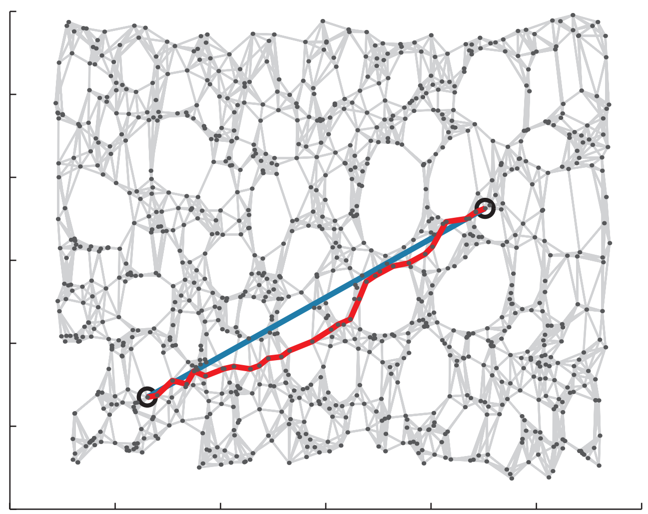
  - 64x64 pixel images
  - N = 2000
  - k = 6

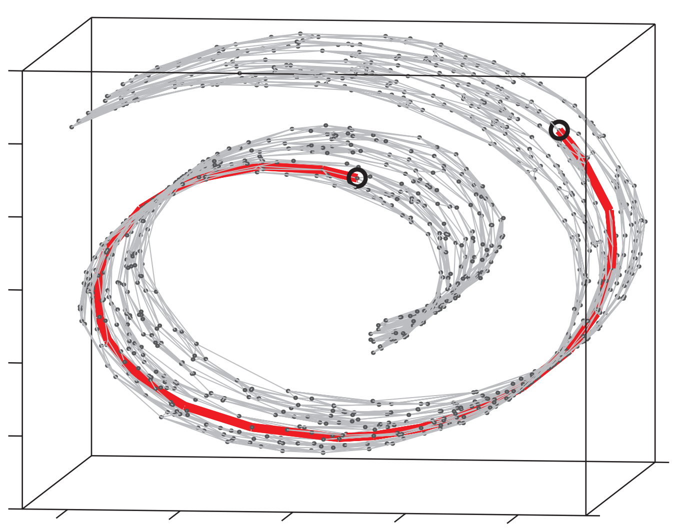
Trajectories in the embedding correspond to meaningful variations in the image

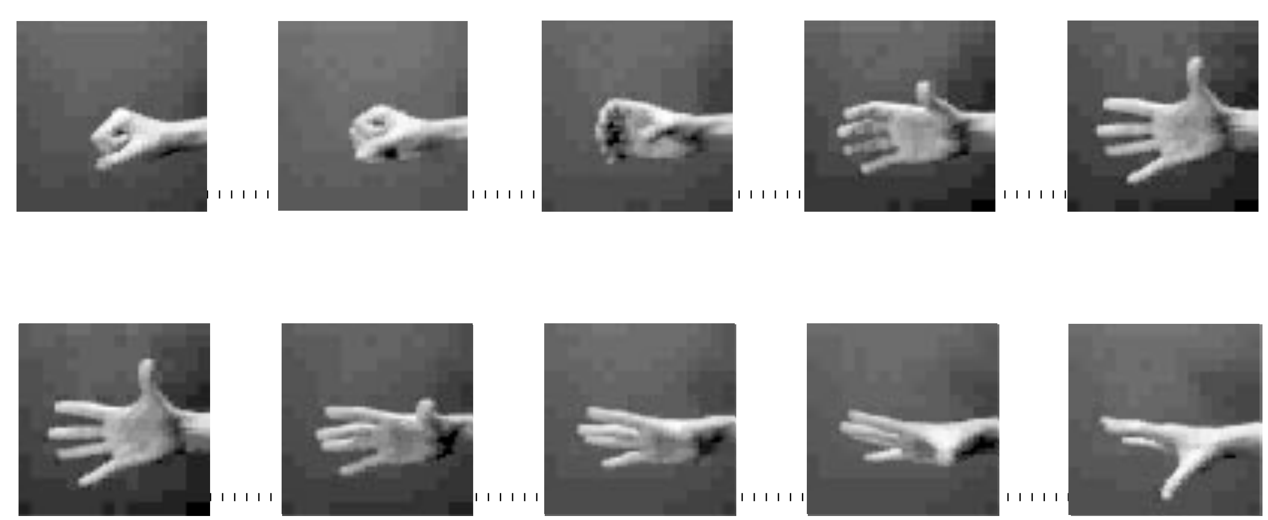


IsoMap examples

- Interpolations along “straight” lines in the embedding space yield realistic, though highly nonlinear, transitions in the image







Scaling-up: Landmark Isomap

de Silva & Tenenbaum '03

Problem

- Isomap does not scale well
- For large N, all-pairs shortest paths computation is too expensive

Scaling-up: Landmark Isomap

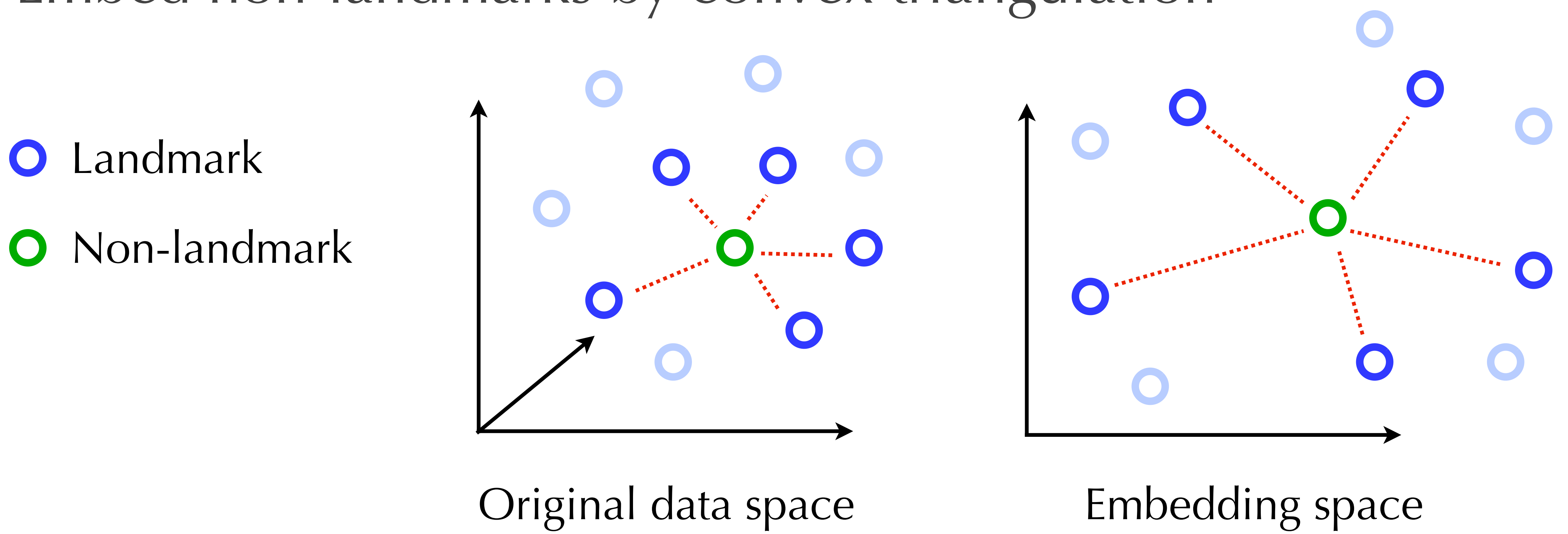
de Silva & Tenenbaum '03

Problem

- Isomap does not scale well
- For large N, all-pairs shortest paths computation is too expensive

Solution

- Compute embedding using a subset of the data (landmarks)
- Embed non-landmarks by convex triangulation

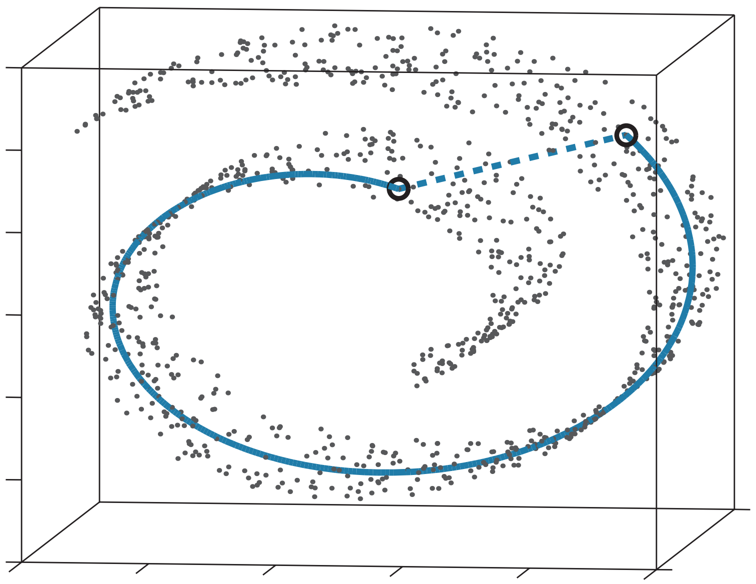


IsoMap strengths

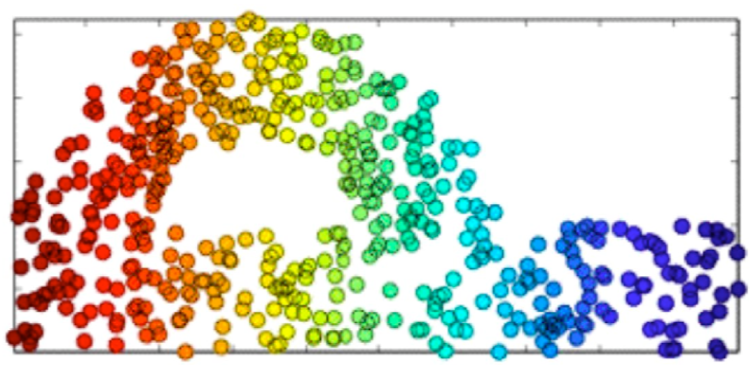
- Strengths inherited from MDS
  - Polynomial time algorithm
  - No local optima
  - Non-iterative
  - Automatic intrinsic dimensionality estimate
- Isomap adds a single heuristic parameter
  - graph neighbourhood size **k**
- Guaranteed asymptotic convergence
  - For data living on a convex submanifold of Euclidean space, and given large enough sample N, Isomap is guaranteed to recover the true manifold, up to a rotation and translation.

IsoMap weaknesses

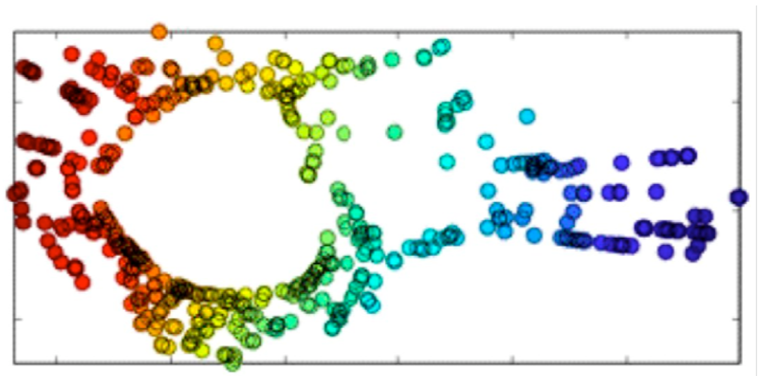
- Sensitive to “short-cuts” due to **k** being too large



- Does not scale well to very large N
  - NxN dense eigenvector problem is expensive
- Convexity assumption
  - Cannot handle manifolds with “holes”



Input



IsoMap embedding

e.g. periodic motion

Nonlinear Dimensionality Reduction

Method 2: Locally Linear Embedding

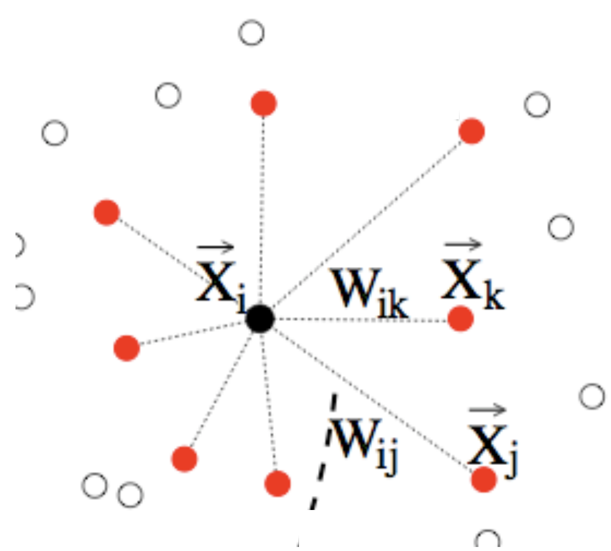
Locally Linear Embedding (LLE)

Roweis & Saul, Science, Dec '00

- "Think locally, fit globally!" - an alternative to Isomap
- LLE aims to preserve local manifold geometry in its embedding

Idea

- Assume manifold is locally linear
  - We expect each D-dim data point to lie on or near a locally linear patch of the manifold
- Characterize each point x_i as a convex linear combination of its k-nearest neighbors x_j
- Seek an embedding that preserves these weights

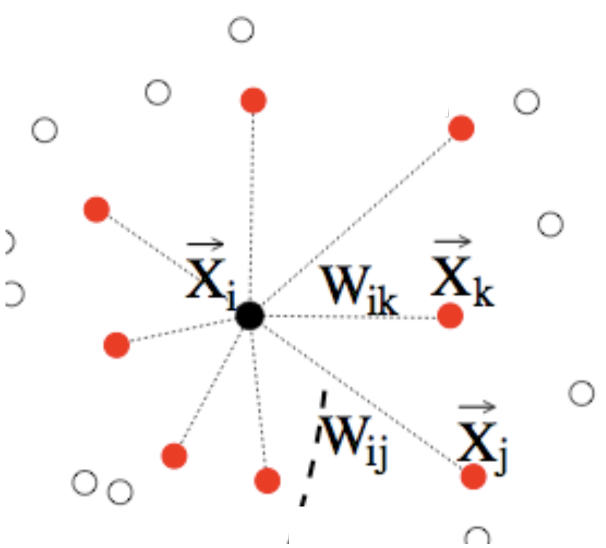


Locally Linear Embedding

- **Step 1:** Compute k-nearest neighbors for each point x_i
  - Same as in Isomap
- **Step 2:** Compute weights W_{ij} that best reconstruct x_i as a convex sum of its neighbors x_j

$$\arg\min_{W} \Phi(W) = \sum_i \left\| \vec{x}_i - \sum_{j \in \mathcal{N}_i} W_{ij} \vec{x}_j \right\|^2$$

$$\text{subject to} \quad \sum_j W_{ij} = 1$$



  - This is easily solved using a Lagrange multiplier
  - Note that local weights are invariant to *translation, rotation and scale*
  - Hence weights should be preserved under a well-behaved embedding

Locally Linear Embedding

- **Step 3:** Choose embedded coordinates y_i that minimize reconstruction error using previously computed weights W_{ij}

$$\arg\min_{\vec{y}} \Theta(\vec{y}) = \sum_i \left\| \vec{y}_i - \sum_{j \in \mathcal{N}_i} W_{ij} \vec{y}_j \right\|^2$$

$$\text{subject to} \qquad \sum_i y_i = 0 \qquad \text{(zero mean)}$$

$$\frac{1}{N} \sum_i y_i y_i^\top = I_d \qquad \text{(unit covariance)}$$

  - Since the embedding is only defined up to an arbitrary translation and scale, the constraints serve to make the problem well-posed

Locally Linear Embedding

- The result is given by the eigenvectors of the matrix Q corresponding to the **d+1** smallest eigenvalues, where

$$Q = (I - W)^\top (I - W)$$

- The bottom eigenvector is the vector $[1\ 1\ 1\ 1]^\top$, an exact null-vector corresponding to a free translation mode.
- Discarding it imposes the zero-mean constraint.
- The remaining **d** eigenvectors give the embedding

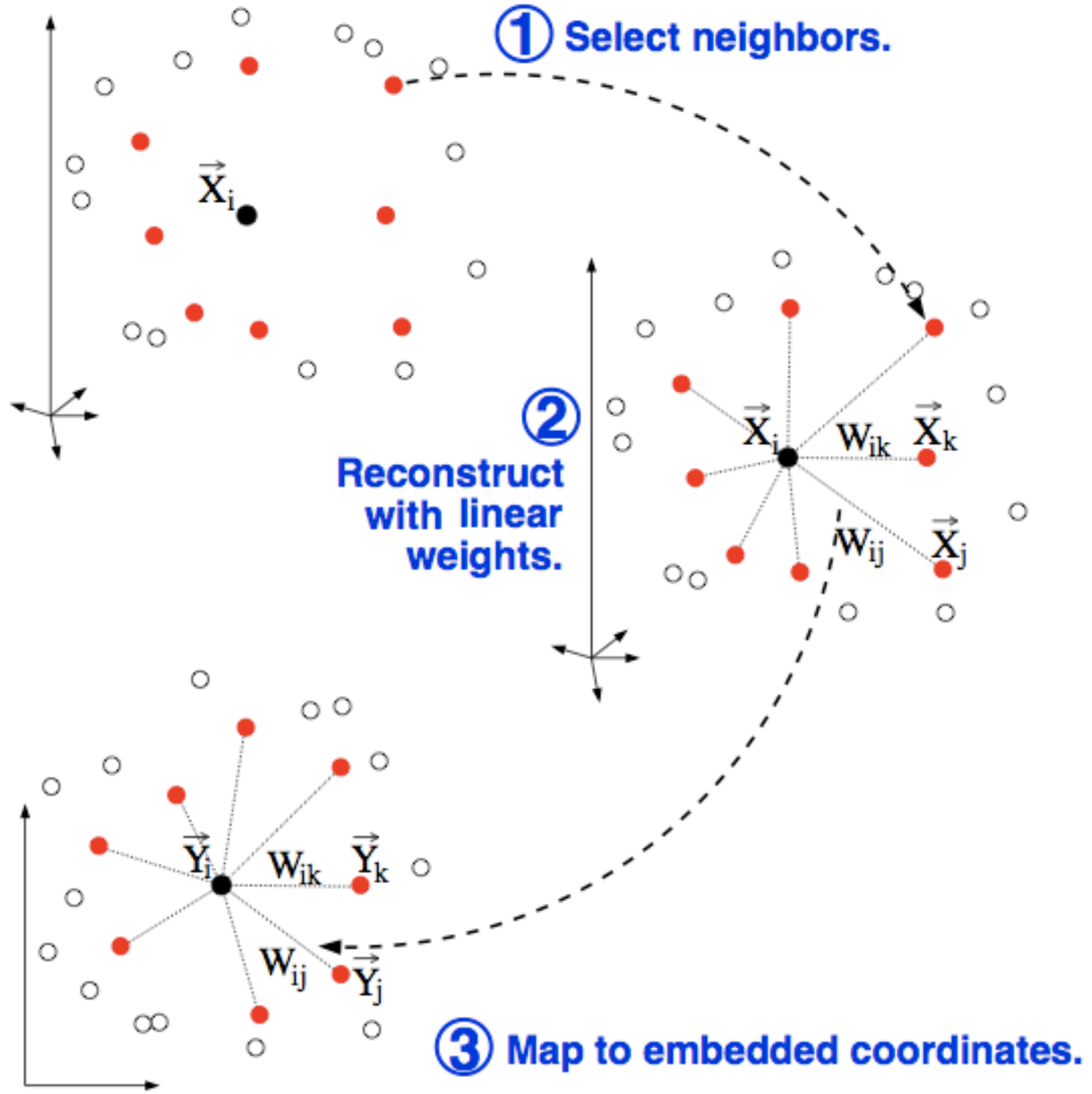
- ***Note : W*** *and hence* ***Q*** *is very sparse (compare to IsoMap* ***G****)*
- *Efficient algorithms exist for large, sparse eigenvector problems*

LLE summary

1. **Compute the neighbors of each data point, $\vec{X}_i$.**

2. **Compute the weights W_{ij} that best reconstruct each data point $\vec{X}_i$ from its neighbors, minimizing the cost in eq. (1) by constrained linear fits.**

3. **Compute the vectors $\vec{Y}_i$ best reconstructed by the weights W_{ij}, minimizing the quadratic form in eq. (2) by its bottom nonzero eigenvectors.**

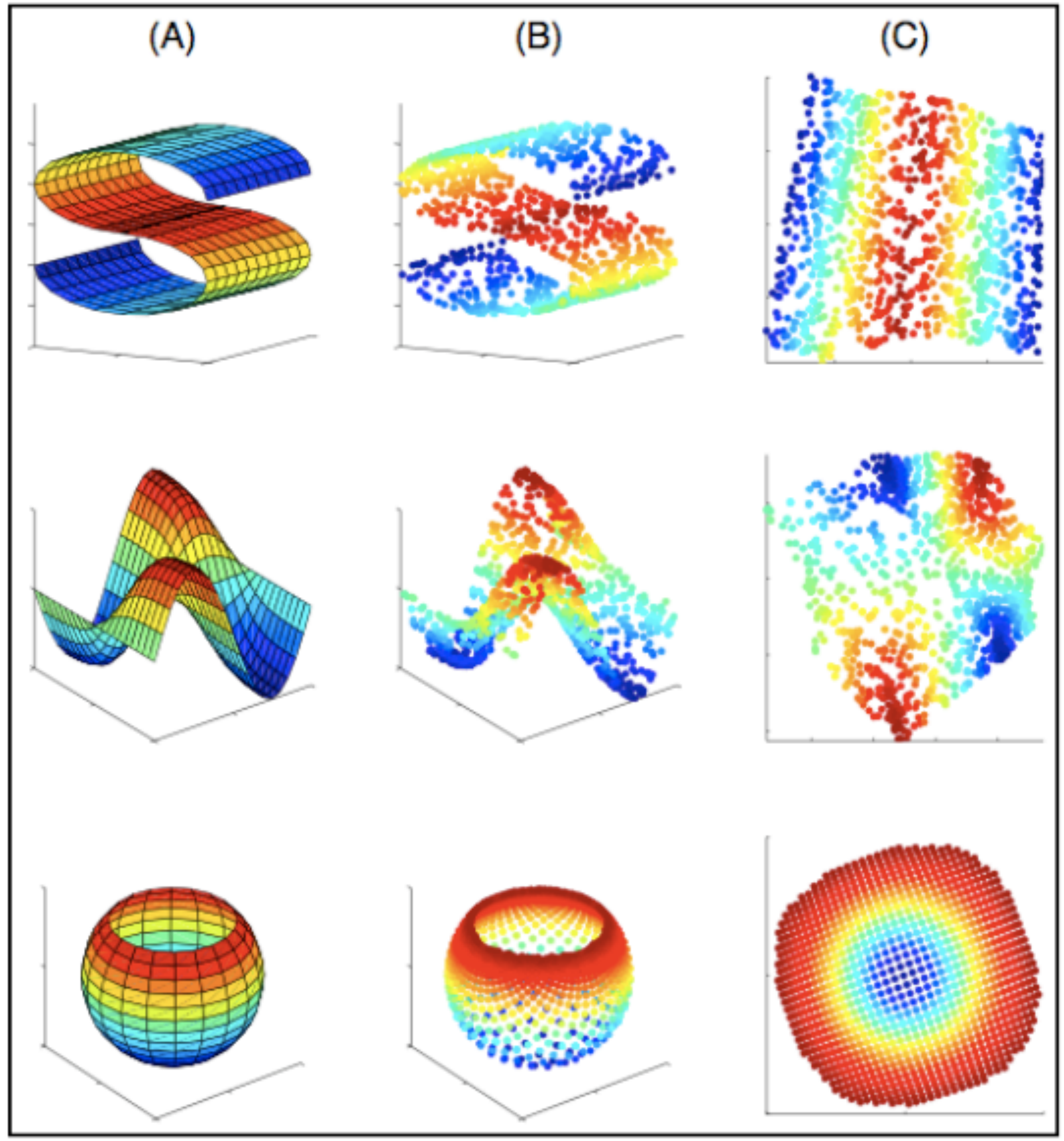


LLE examples

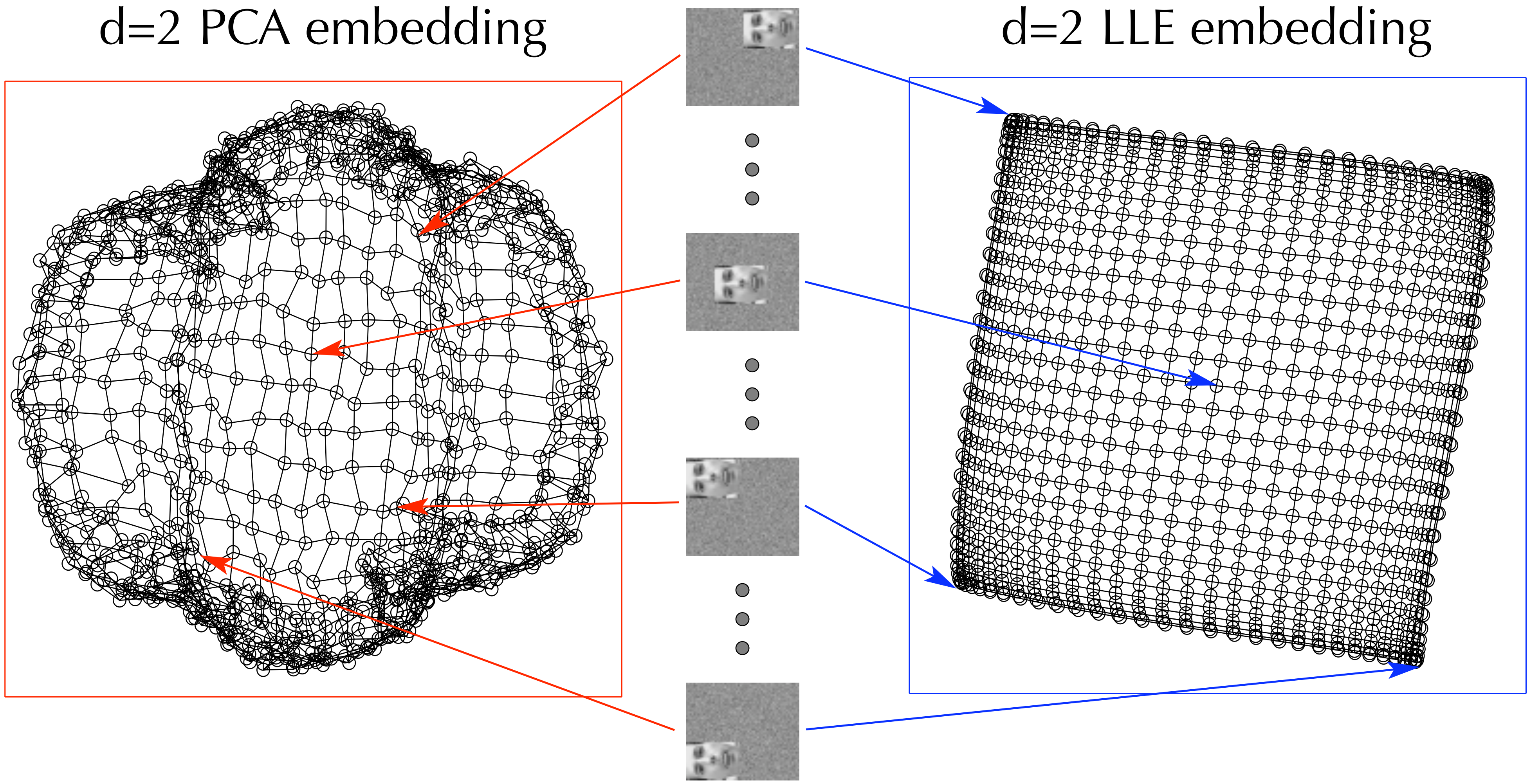
N=1000
inputs

k=8
nearest
neighbors

D=3
d=2
dimensions



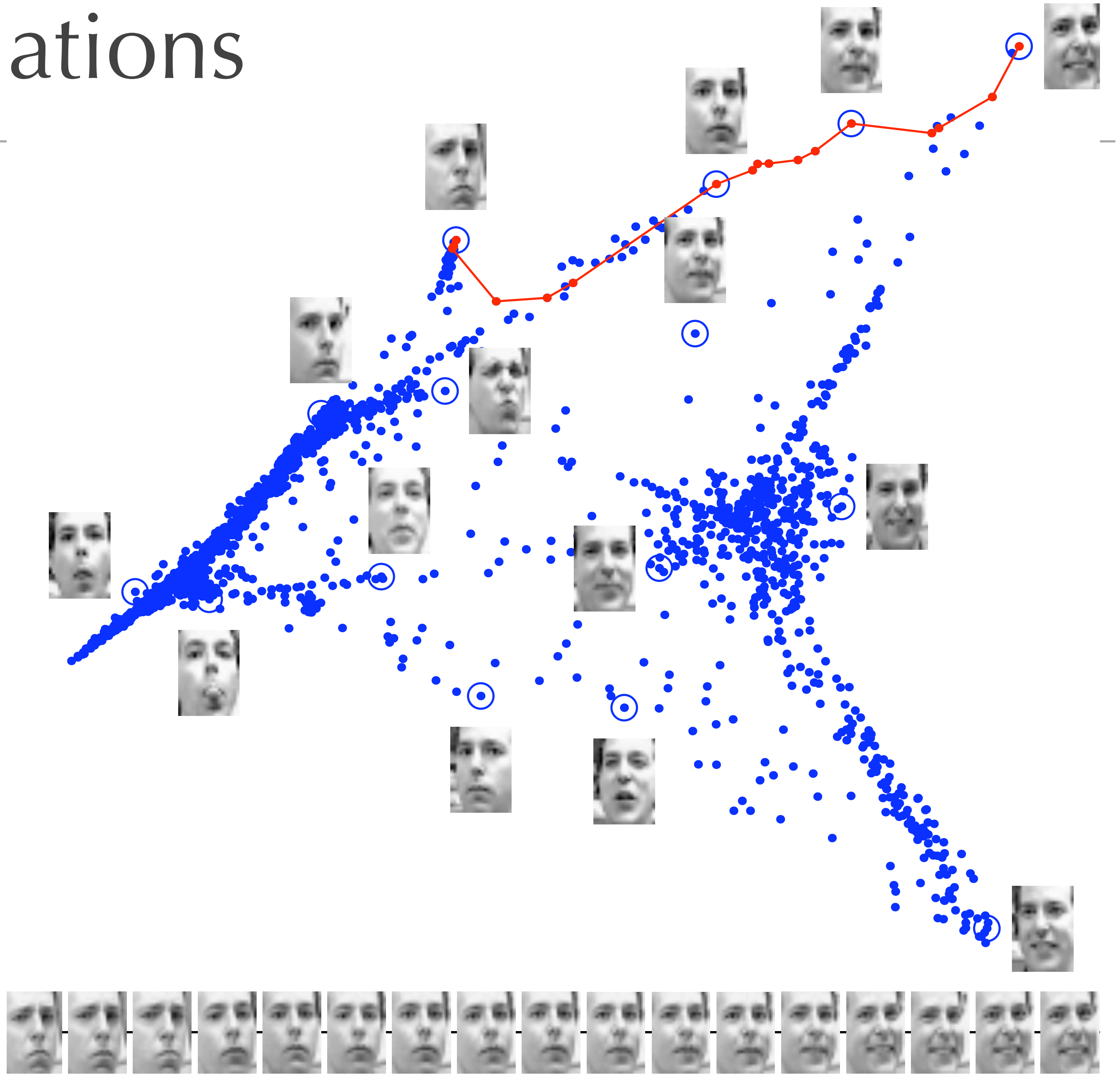
PCA vs LLE example



- Input: 30x30 images of a translating face (N=961)
- PCA fails to recover a meaningful 2-d embedding
- LLE discovers the 2 translational degrees of freedom in the input

LLE example - Face variations

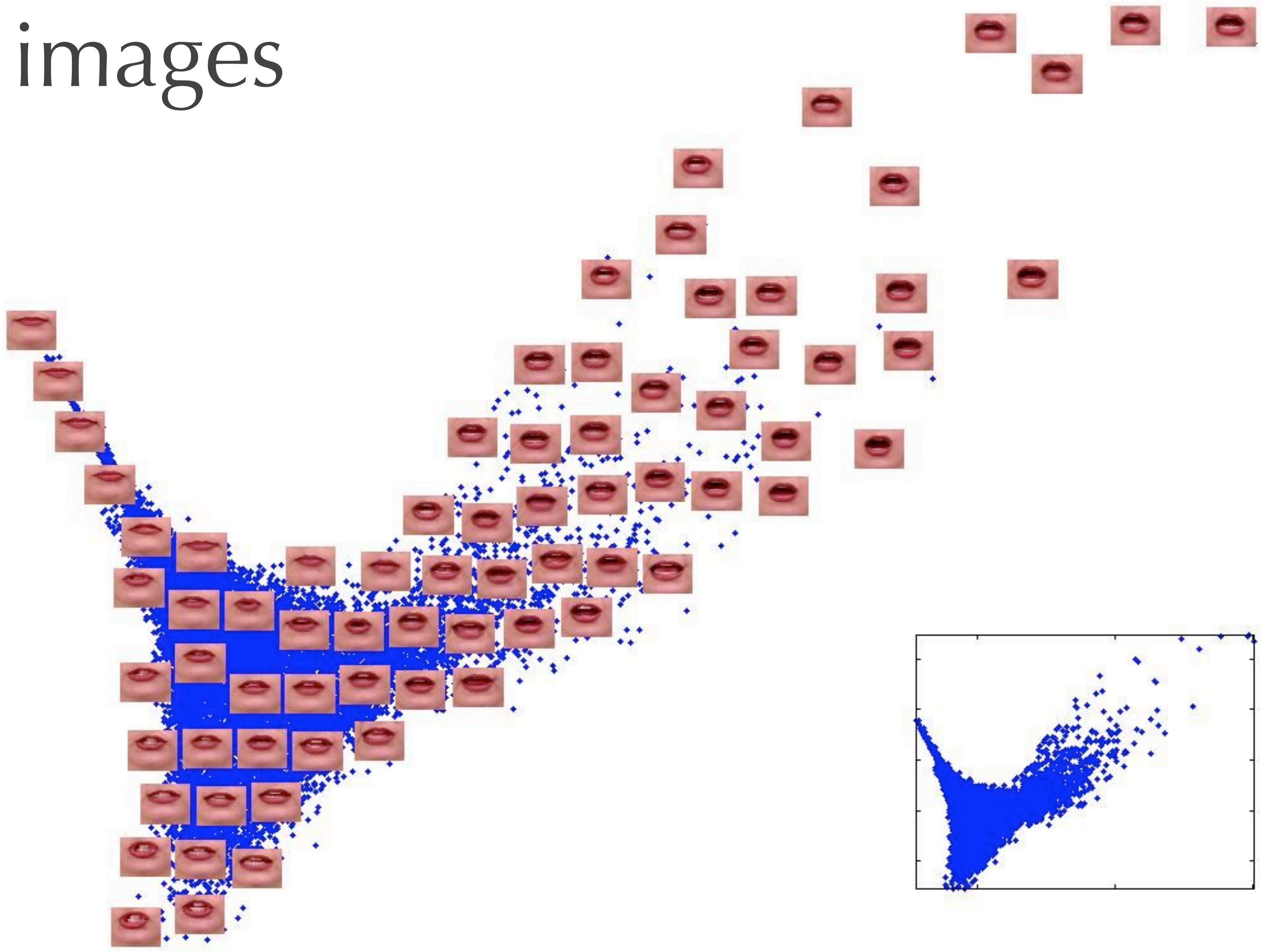
- 20x28 pixel images
- N=1965
- k=12
- d=2



- The 2-d LLE embedding coordinates correspond roughly to variations in pose and expression
- The trajectory (red) corresponds to a realistic facial transition (bottom row)

LLE example - Lips images

- 256x256 pixel images
- N=15960
- k=24
- d=2

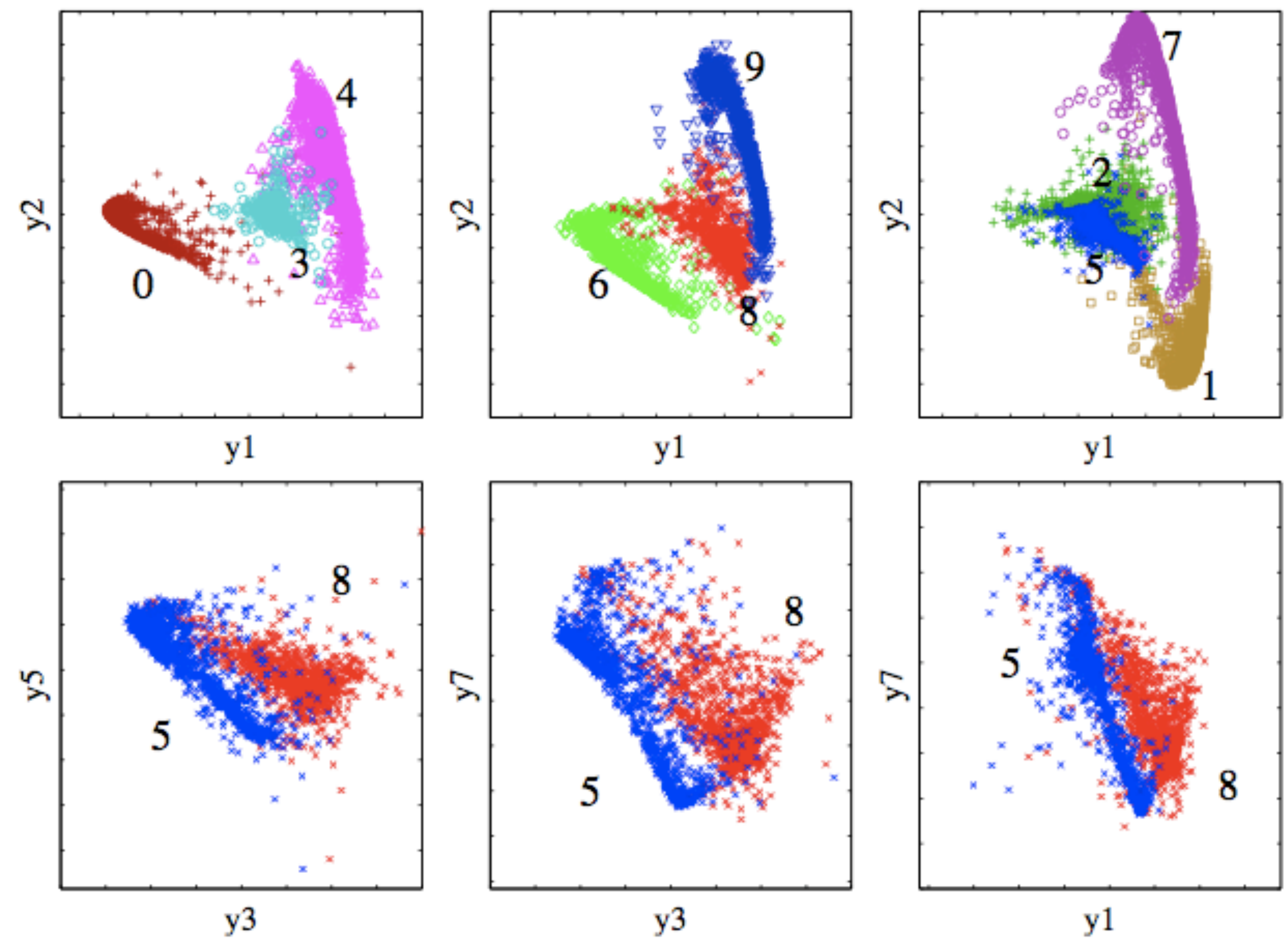


- Trajectories in the 2-d embedding correspond to smooth variations in the mouth configuration
- Note: LLE easily handles the large problem size (N=15960) thanks to sparse weights matrix

LLE example - a pattern classifier

- Recognition of hand-written digits

- 16x16 pixel images (USPS dataset)
- N=11000
- k=?? (author doesn't say)
- d=8



- Most digit classes are easily separable in just the first two embedding dimensions
- A classifier would be easy to construct and visualize

LLE with pairwise distances

- What if we only have pairwise distances $d(X_i,X_j)$ between data points, as was the case with MDS and IsoMap?

- We can use the same trick for expressing dot products in terms of distances when computing the LLE weights W_{ij}

- The neighborhood covariance may be written as

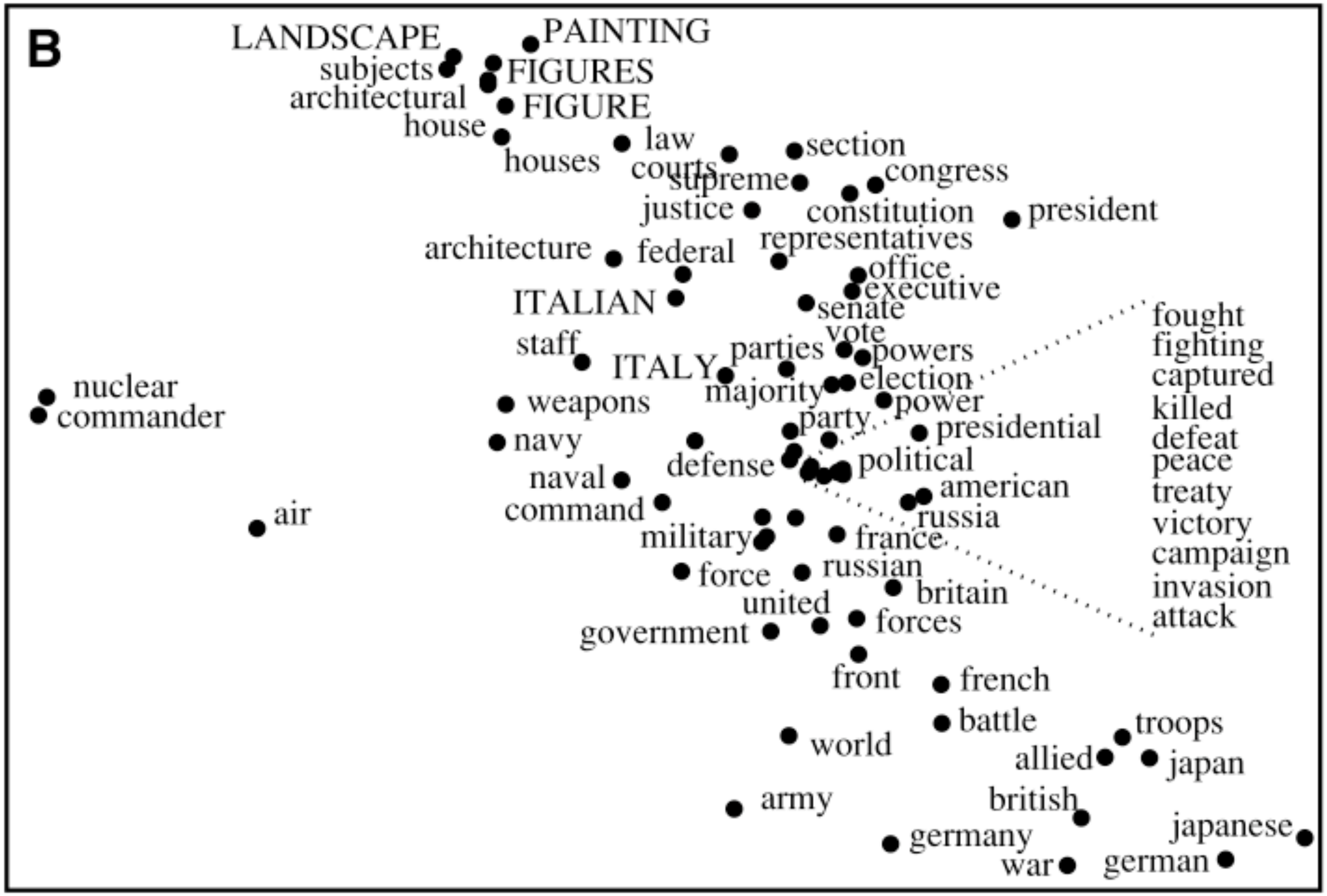
$$C_{jk} = \frac{1}{2}\left(D_j + D_k - D_{jk} - D_0\right)$$

where

$$D_\ell = \sum_z D_{\ell z}$$

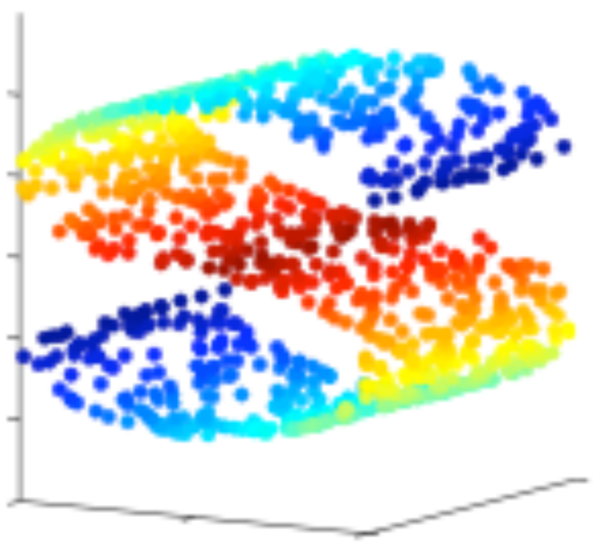
$$D_0 = \sum_{jk} D_{jk}$$

LLE with pairwise distances

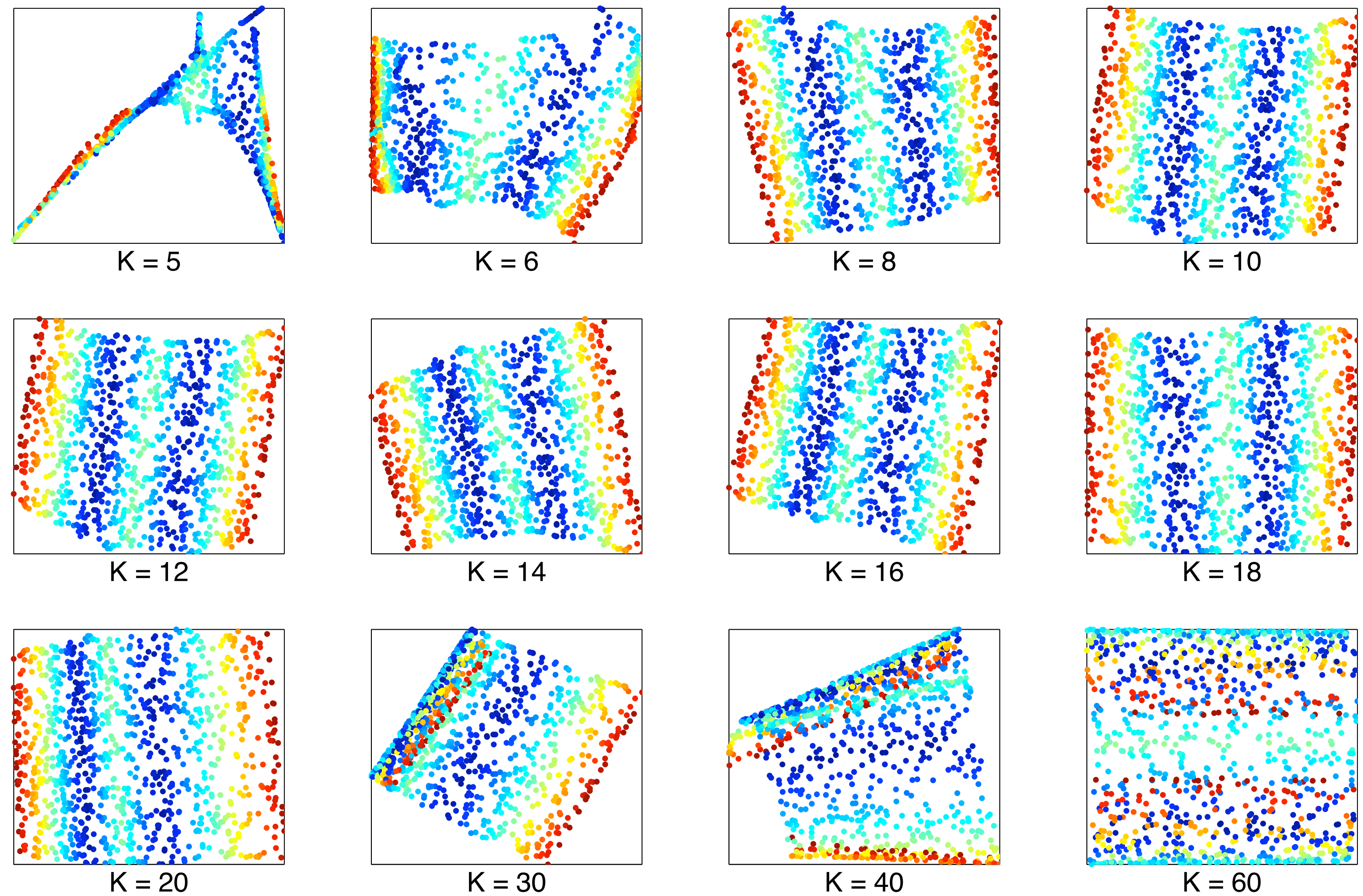


- Input: Histograms of occurrence of 5000 words in 31000 encyclopedia articles
- Distance metric: dot-products between unit-normalized histograms
- k=20
- LLE recovers a continuous semantic embedding

LLE: choosing neighborhood size **k**

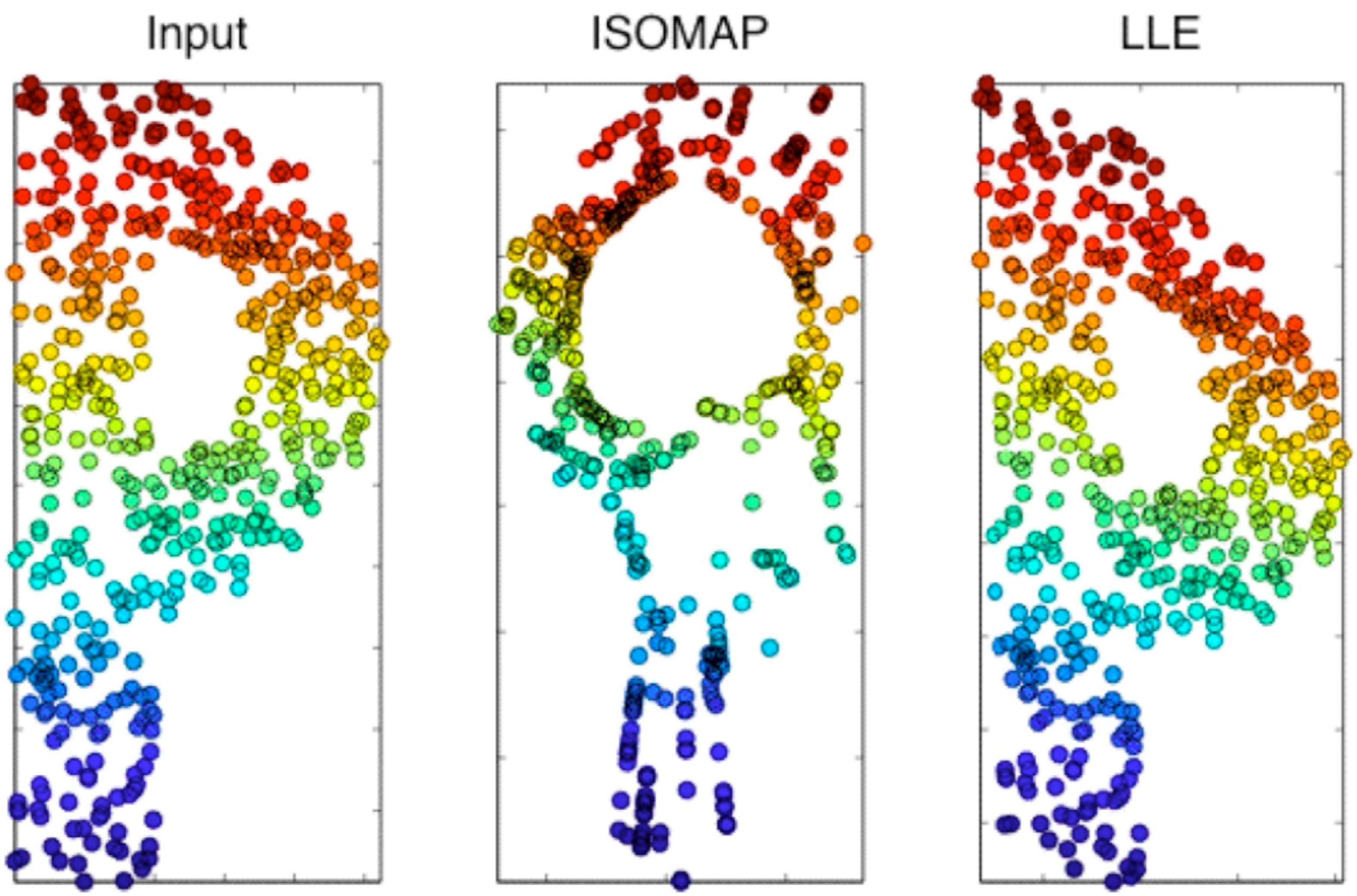


3-d S-manifold



- Neighborhood size **k** is varied in 2-d embedding of S-manifold
- **k** too low - no meaningful structure is recovered
- **k** too high - S is squashed onto a plane, ordering not preserved

LLE: Non-convex manifolds



- LLE handles non-convex manifolds (those with holes) a little better than IsoMap
- Not perfect - we'd prefer this particular 2d-2d embedding to be a simple isometry!

LLE strengths/weaknesses

- Similar strengths to IsoMap
  - Graph-base, eigenvector method
  - Polynomial time algorithm
  - No local optima
  - Non-iterative
  - Single heuristic parameter (neighbourhood size **k)**
- PLUS - Better handling of non-convex manifolds

- BUT - some additional weaknesses
  - Also sensitive to “short-cuts”
  - No asymptotic guarantees
  - No way to estimate intrinsic manifold dimension

IsoMap vs. LLE

IsoMap

- Computes top **d** eigenvectors of a **dense** NxN matrix
- Preserves distances
- Asymptotic guarantee of finding true manifold

LLE

- Computes bottom **d+1** eigenvectors of a **sparse** NxN matrix
- Preserves local linear geometry
- Copes with “holes” rather better

Major “selling point” for LLE :

- LLE avoids the need to compute a dense, all-pair shortest distance matrix
- The LLE eigenvector problem is extremely sparse
- Far more efficient in terms of both time and storage requirements

Application : Clever graphics stuff!

Unwrap Mosaics:
A New Representation for Video Editing

Rav-Acha, Kohli, Rother, Fitzgibbon
SIGGRAPH 2008

http://research.microsoft.com/unwrap/

Recent advances and further reading

- **Linear methods**
  - Principal components analysis (PCA) finds maximum variance subspace.
  - Metric multidimensional scaling (MDS) finds distance-preserving subspace.
- **Graph-based methods**