Unfolding Manifolds: ISOMAP vs. LLE
--几何数据处理初步

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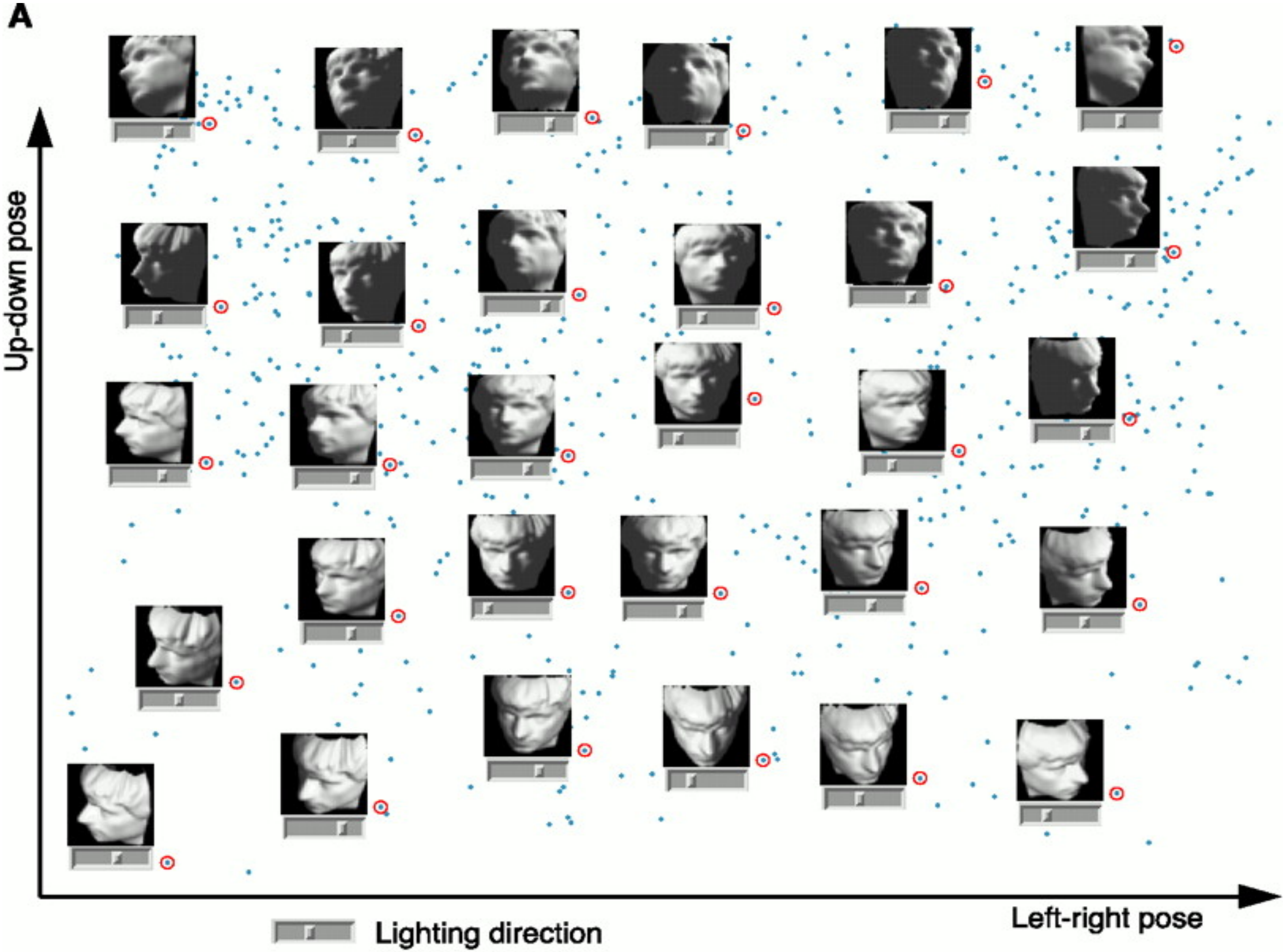
高等统计选讲

2009.10.14


A
Up-down pose
Left-right pose
Lighting direction

Dimensionality Reduction

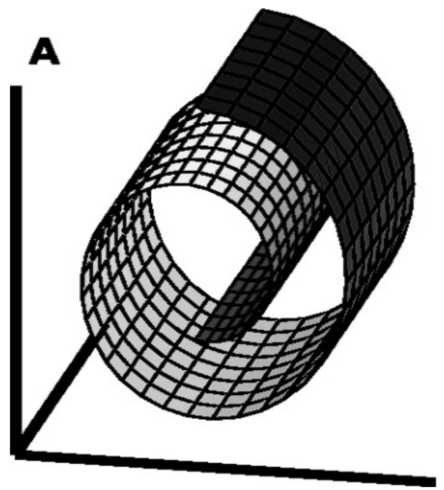
- Need to analyze large amounts multivariate data.
  - Human Faces.
  - Speech Waveforms.
  - Global Climate patterns.
  - Gene Distributions.

- Difficult to visualize data in dimensions just greater than three.

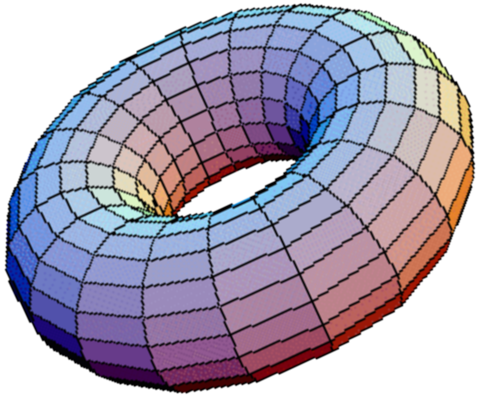
- Discover compact representations of high dimensional data.
  - Visualization.
  - Compression.
  - Better Recognition.
  - Probably meaningful dimensions.

Types of structure in multivariate data..

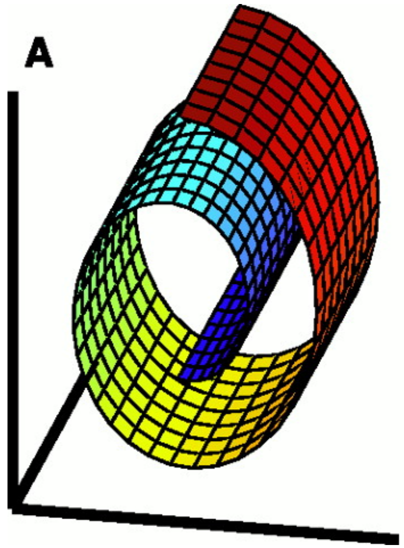
- Clusters.
  - Density Estimation Techniques.
- On or around low Dimensional Manifolds
  - Linear： Principal Component Analysis
  - NonLinear: ISOMAP, LLE, Laplacian Eigenmap, Diffusion Map, etc.



Concept of Manifolds



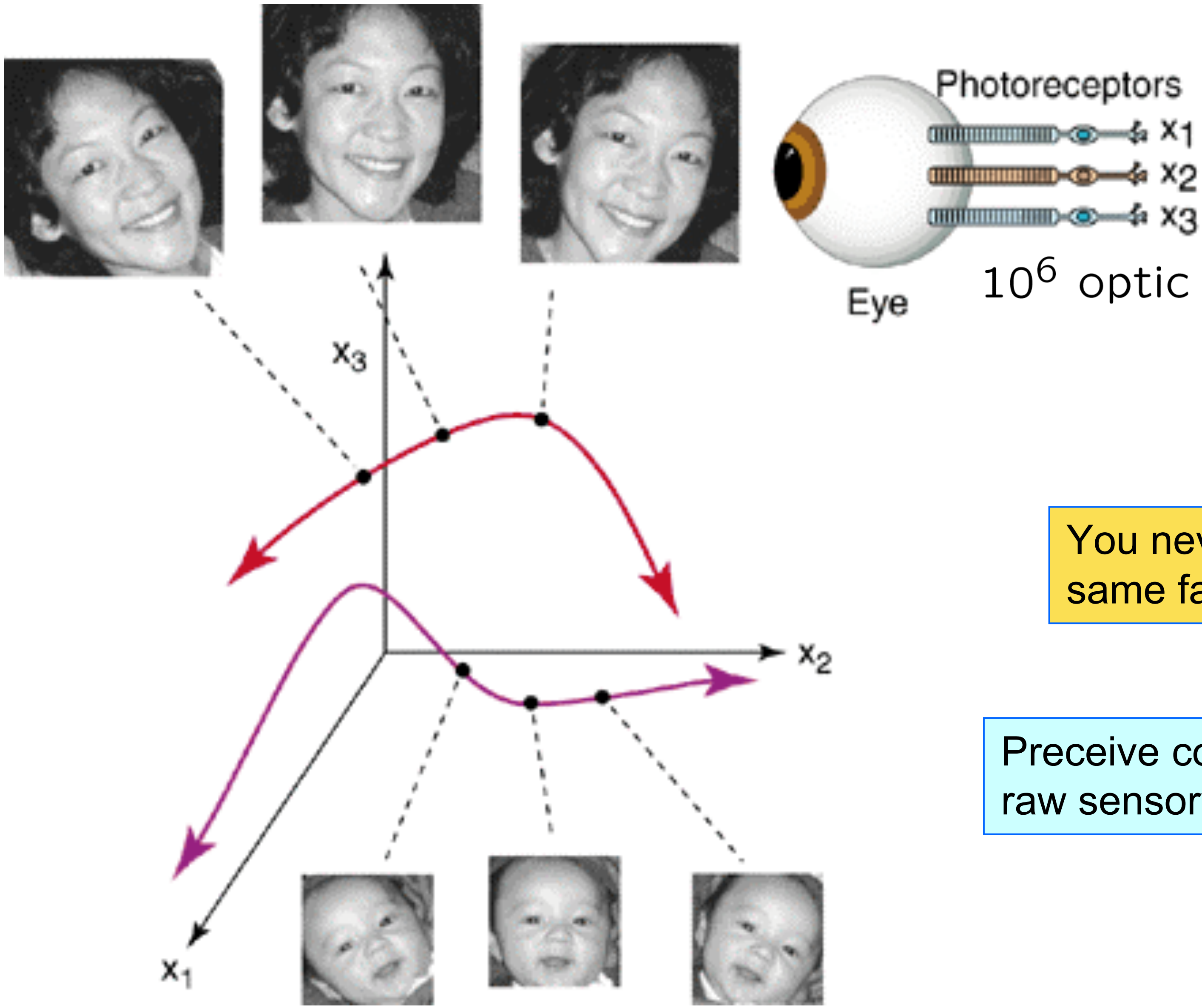
- *“A manifold is a topological space which is locally Euclidean.”*
- In general, any object which is nearly "flat" on small scales is a manifold.
- Euclidean space is a simplest example of a manifold.
- Concept of submanifold.
- Manifolds arise naturally whenever there is a smooth variation of parameters [like pose of the face in previous example]
- The dimension of a manifold is the minimum integer number of co-ordinates necessary to identify each point in that manifold.



Concept of Dimensionality Reduction:

Embed data in a higher dimensional space to a lower dimensional manifold

Manifolds of Perception..Human Visual System

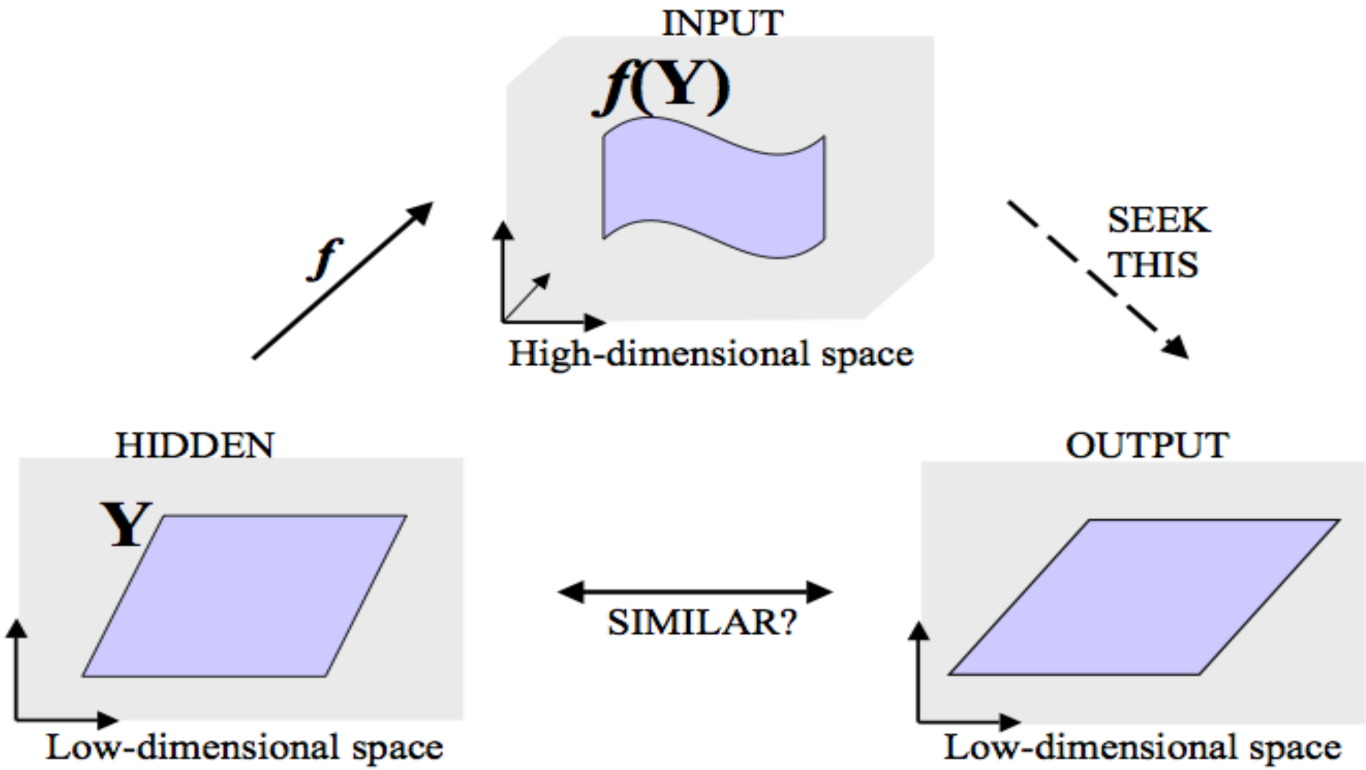


10^6 optic nerve fibres

You never see the same face twice.

Preceive constancy when raw sensory inputs are in flux..

Generative Models in Manifold Learning

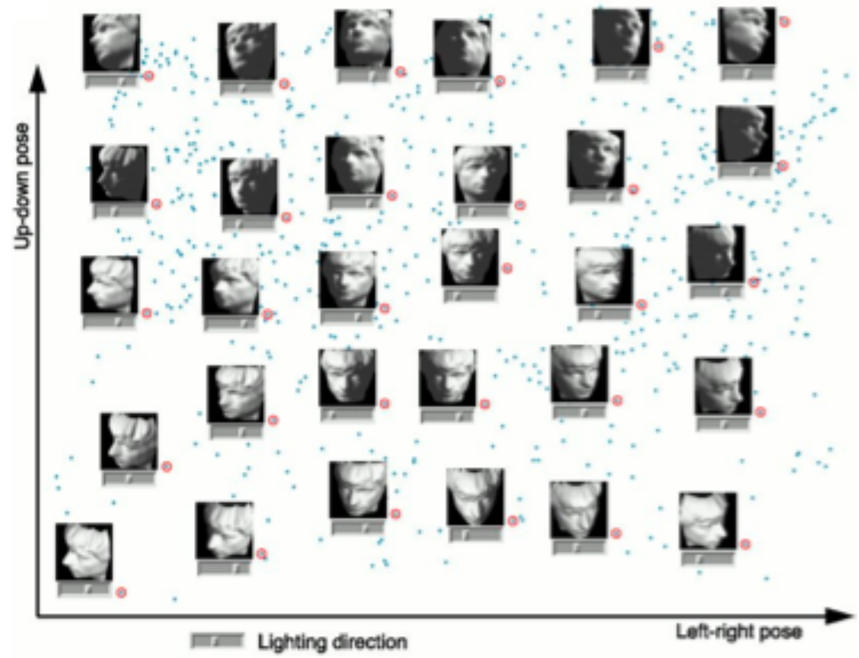


Example: faces

- Given input:
  - randomly ordered sequence of images

  - varied in pose and lighting

- Desired output:
  - Intrinsic dimensionality: 3
  - Low-dimensional representation:

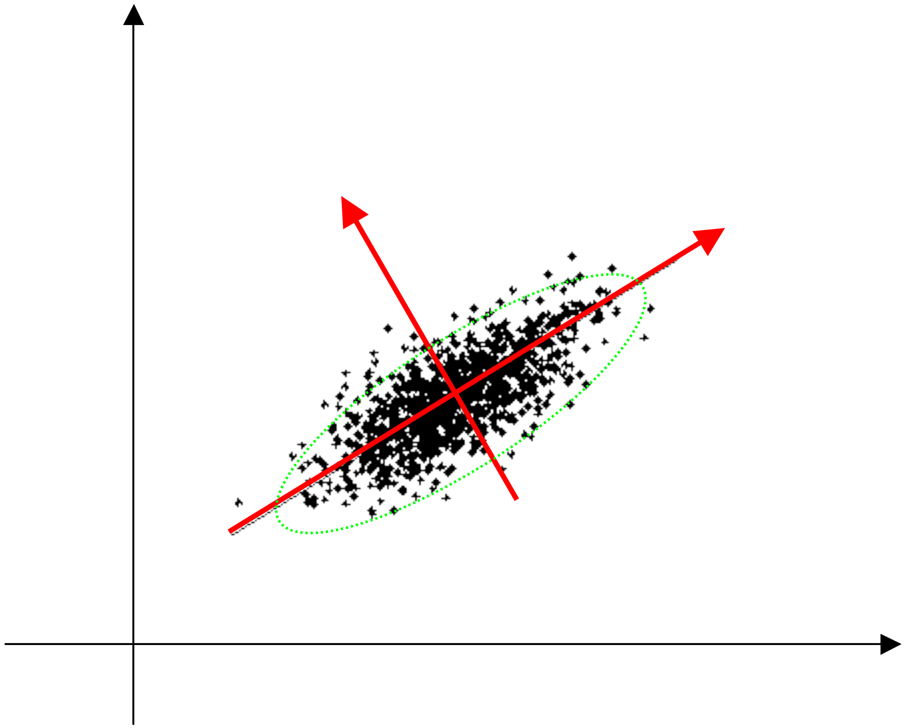


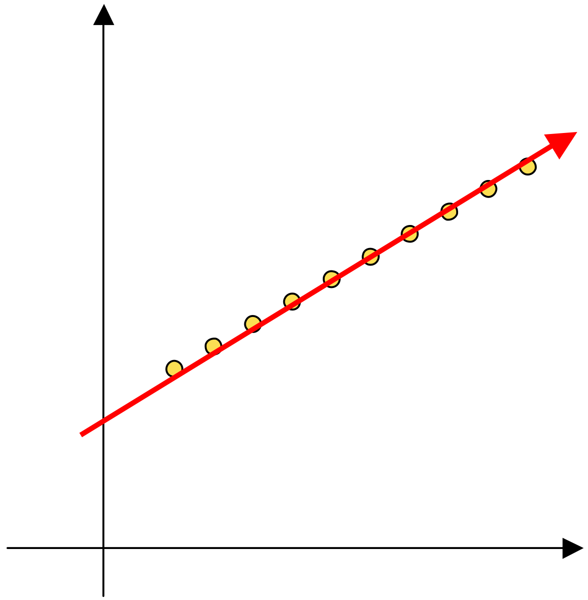
Linear methods..

- Principal Component Analysis (PCA)

$$X_{D\times N} = [X_1|X_2|....|X_N]$$

EigenValue Decomposition of XX^T

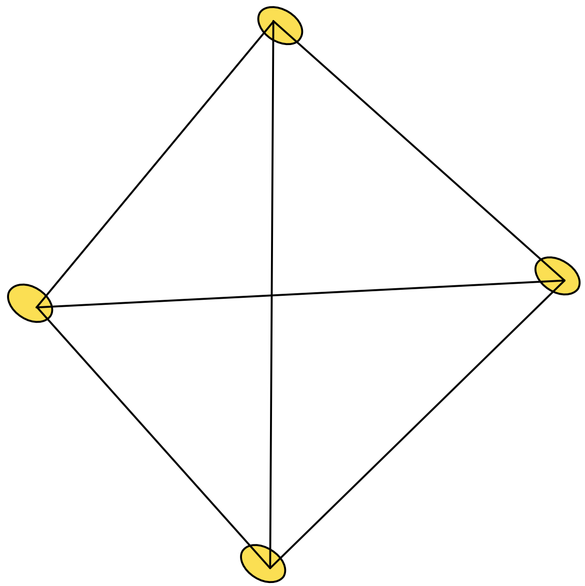




One Dimensional Manifold

MultiDimensional Scaling..

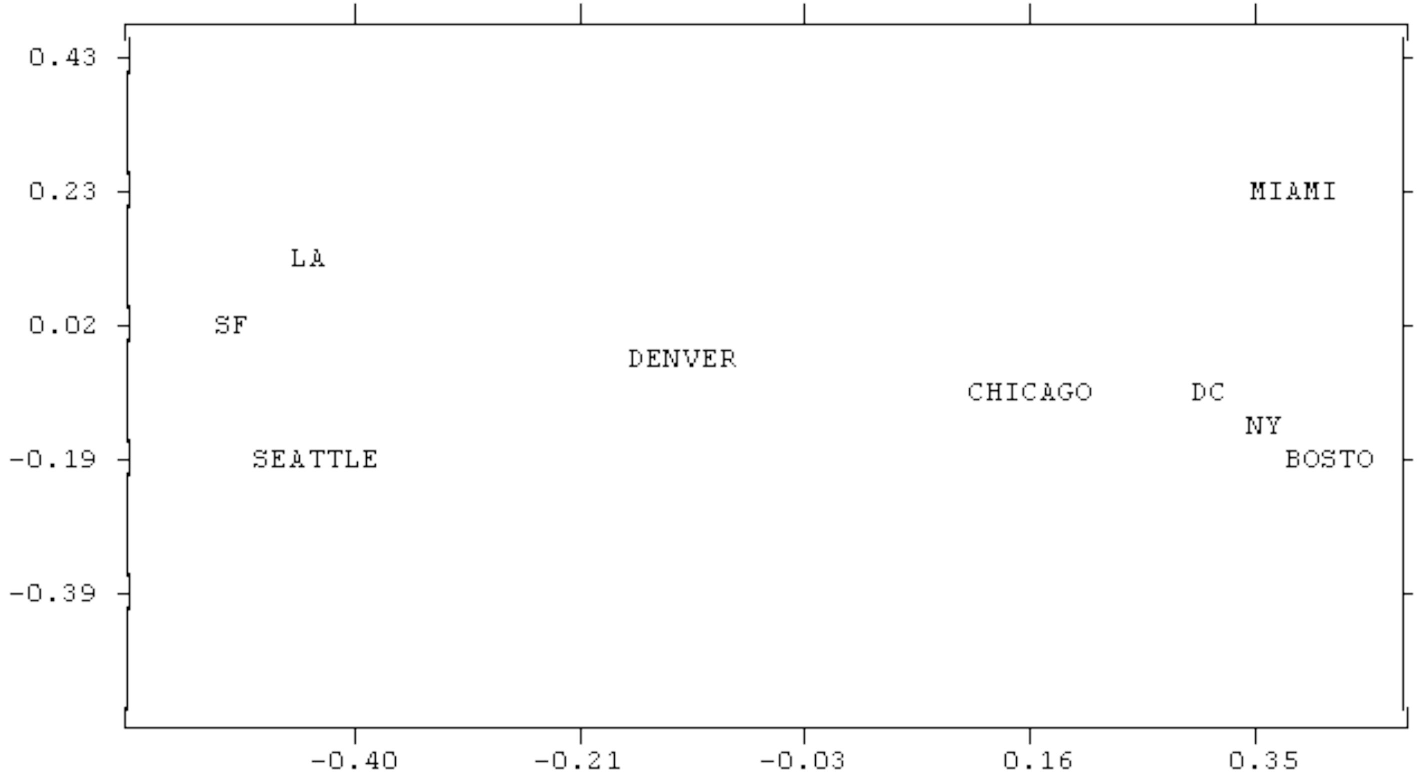
- Here we are given pairwise distances instead of the actual data points.
  - First convert the pairwise distance matrix into the dot product matrix XX^T
  - After that same as PCA.



If we preserve the pairwise distances do we preserve the structure??

Example of MDS…

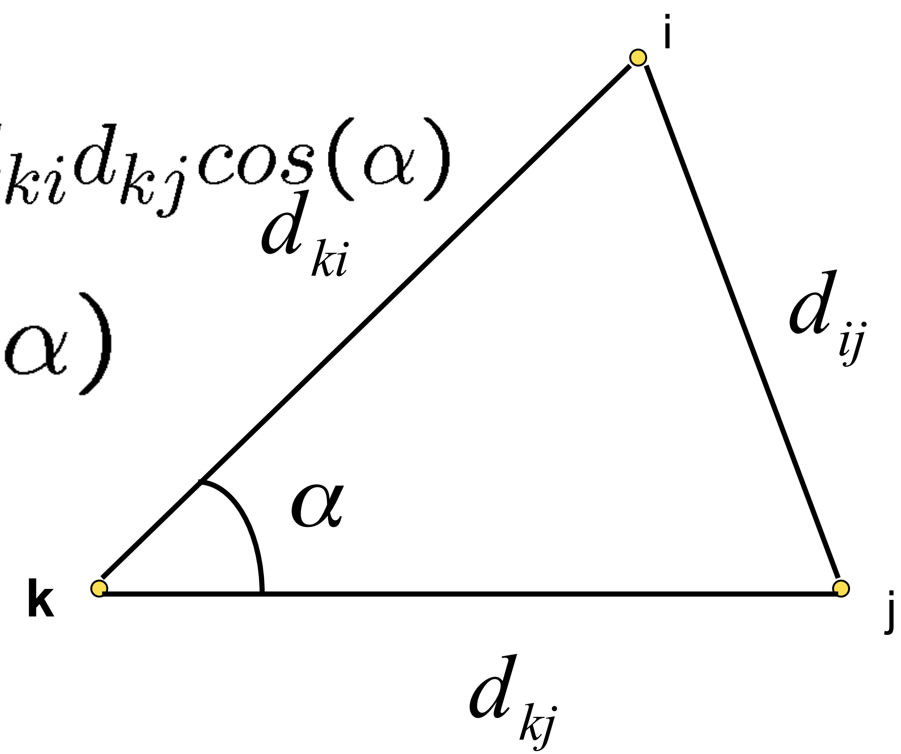
		1 BOST	2 NY	3 DC	4 MIAM	5 CHIC	6 SEAT	7 SF	8 LA	9 DENV
1	BOSTON	0	206	429	1504	963	2976	3095	2979	1949
2	NY	206	0	233	1308	802	2815	2934	2786	1771
3	DC	429	233	0	1075	671	2684	2799	2631	1616
4	MIAMI	1504	1308	1075	0	1329	3273	3053	2687	2037
5	CHICAGO	963	802	671	1329	0	2013	2142	2054	996
6	SEATTLE	2976	2815	2684	3273	2013	0	808	1131	1307
7	SF	3095	2934	2799	3053	2142	808	0	379	1235
8	LA	2979	2786	2631	2687	2054	1131	379	0	1059
9	DENVER	1949	1771	1616	2037	996	1307	1235	1059	0



How to get dot product matrix from pairwise distance matrix?

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

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



$$b_{ij} = \frac{1}{2}(d_{ki}^2 + d_{kj}^2 - d_{ij}^2)$$

MDS..

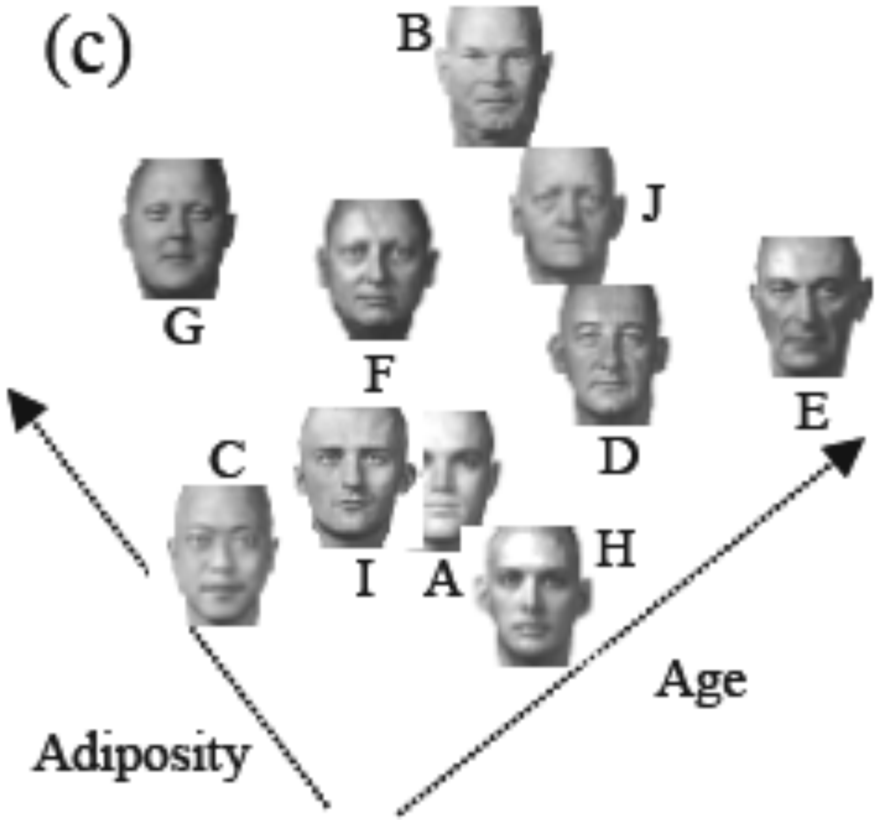
- MDS—origin as one of the points and orientation arbitrary.

Centroid as origin

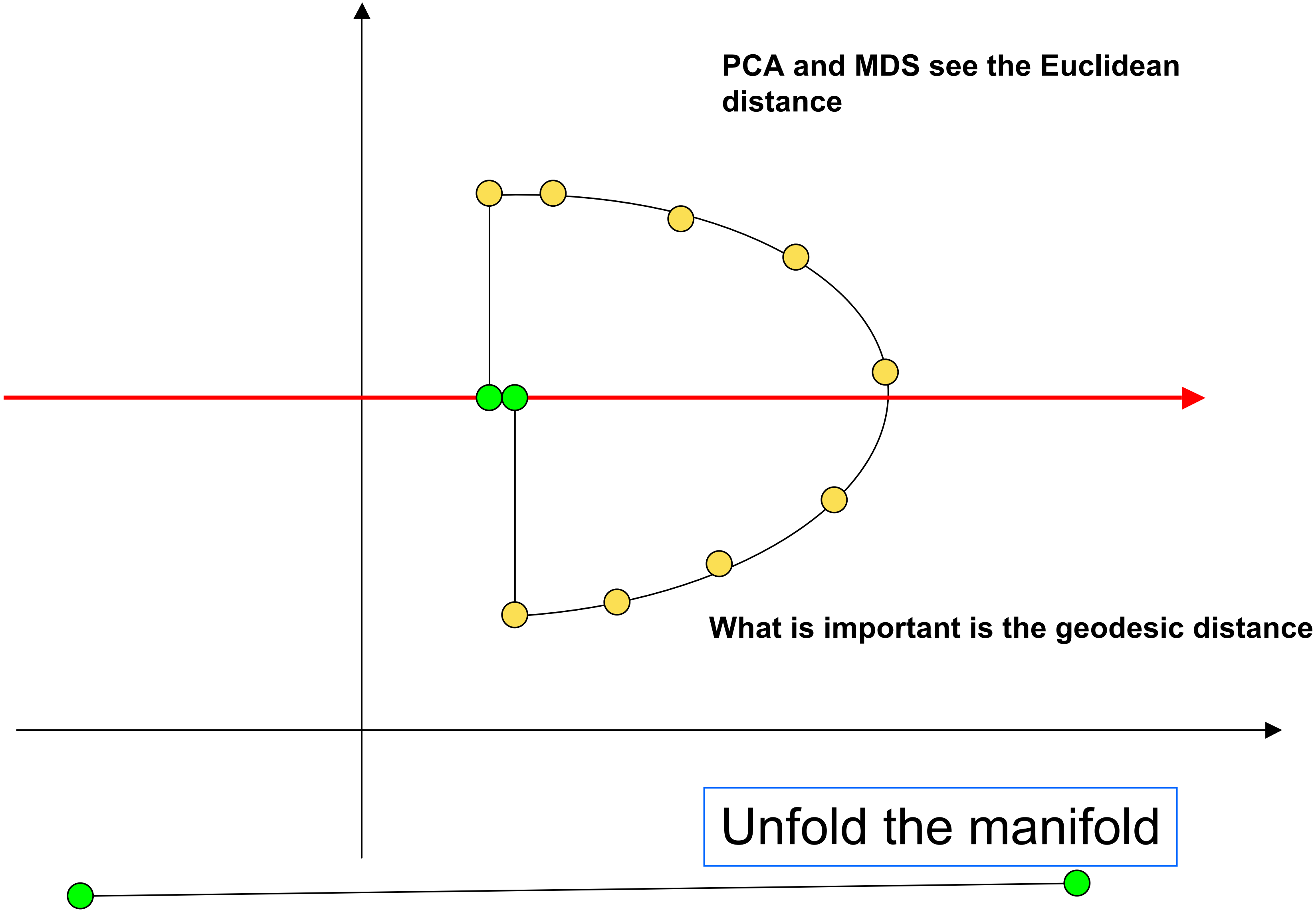
$$b_{ij}^{*} = -\frac{1}{2}\left[d_{ij}^{2} - \frac{1}{N}\sum_{l=1}^{N} d_{il}^{2} - \frac{1}{N}\sum_{m=1}^{N} d_{mj}^{2} + \frac{1}{N^{2}}\sum_{o=1}^{N}\sum_{p=1}^{N} d_{op}^{2}\right]$$

MDS is more general..

- Instead of pairwise distances we can use paiwise "dissimilarities".
- When the distances are Euclidean MDS is equivalent to PCA.
- Eg. Face recognition, wine tasting
- Can get the significant cognitive dimensions.

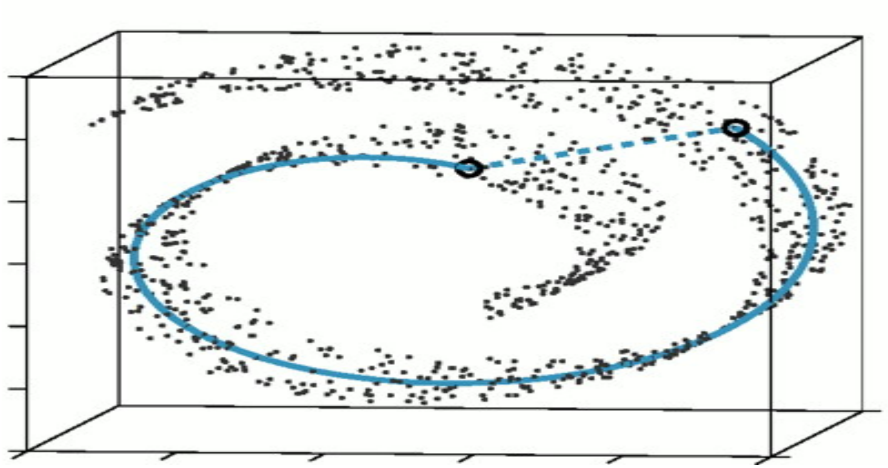


Nonlinear Manifolds..



Intrinsic Description..

- ***To preserve structure, preserve the geodesic distance and not the euclidean distance.***



Two Basic Geometric Embedding Methods

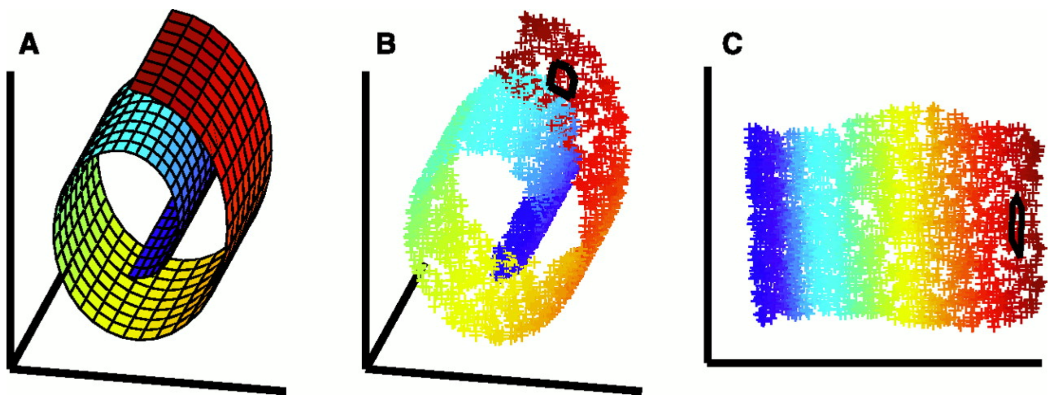
- Tenenbaum et.al's Isomap Algorithm
  - Global approach.
  - On a low dimensional embedding
    - Nearby points should be nearby.
    - Farway points should be faraway.

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

Isomap

- **Estimate the geodesic distance between faraway points.**
- For neighboring points Euclidean distance is a good approximation to the geodesic distance.
- For farway 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

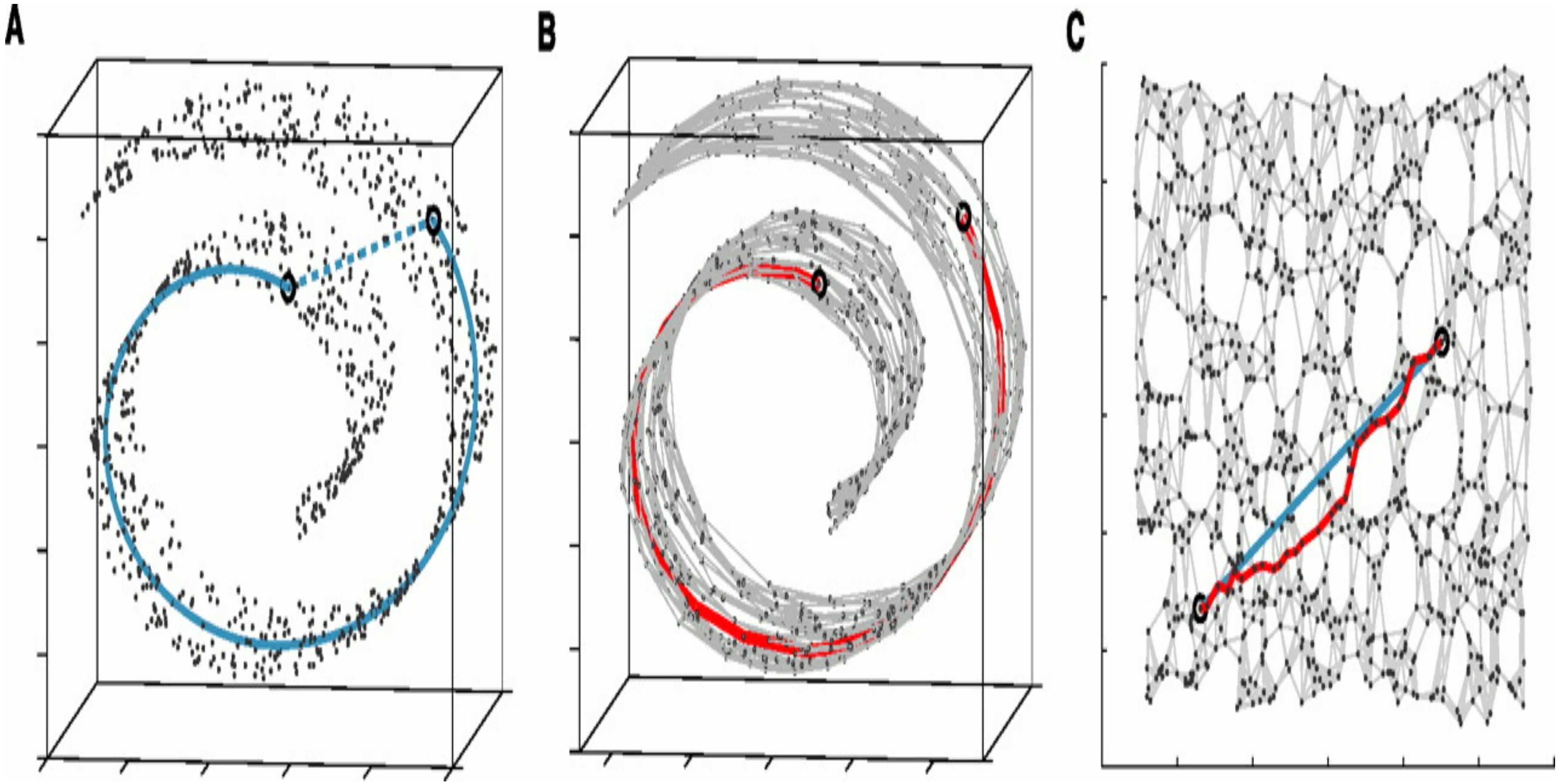
Once we have all pairwise geodesic distances use classical metric MDS

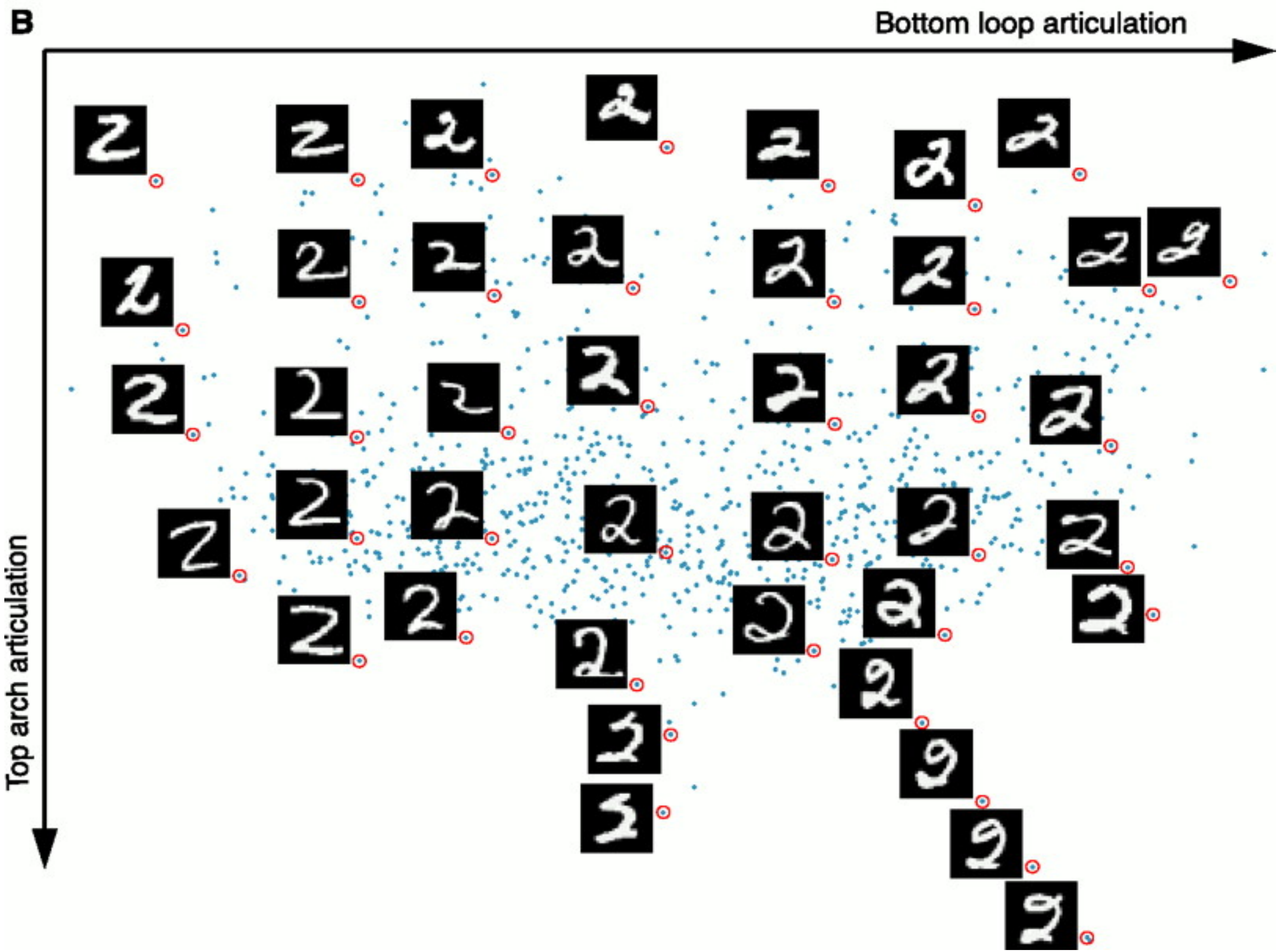


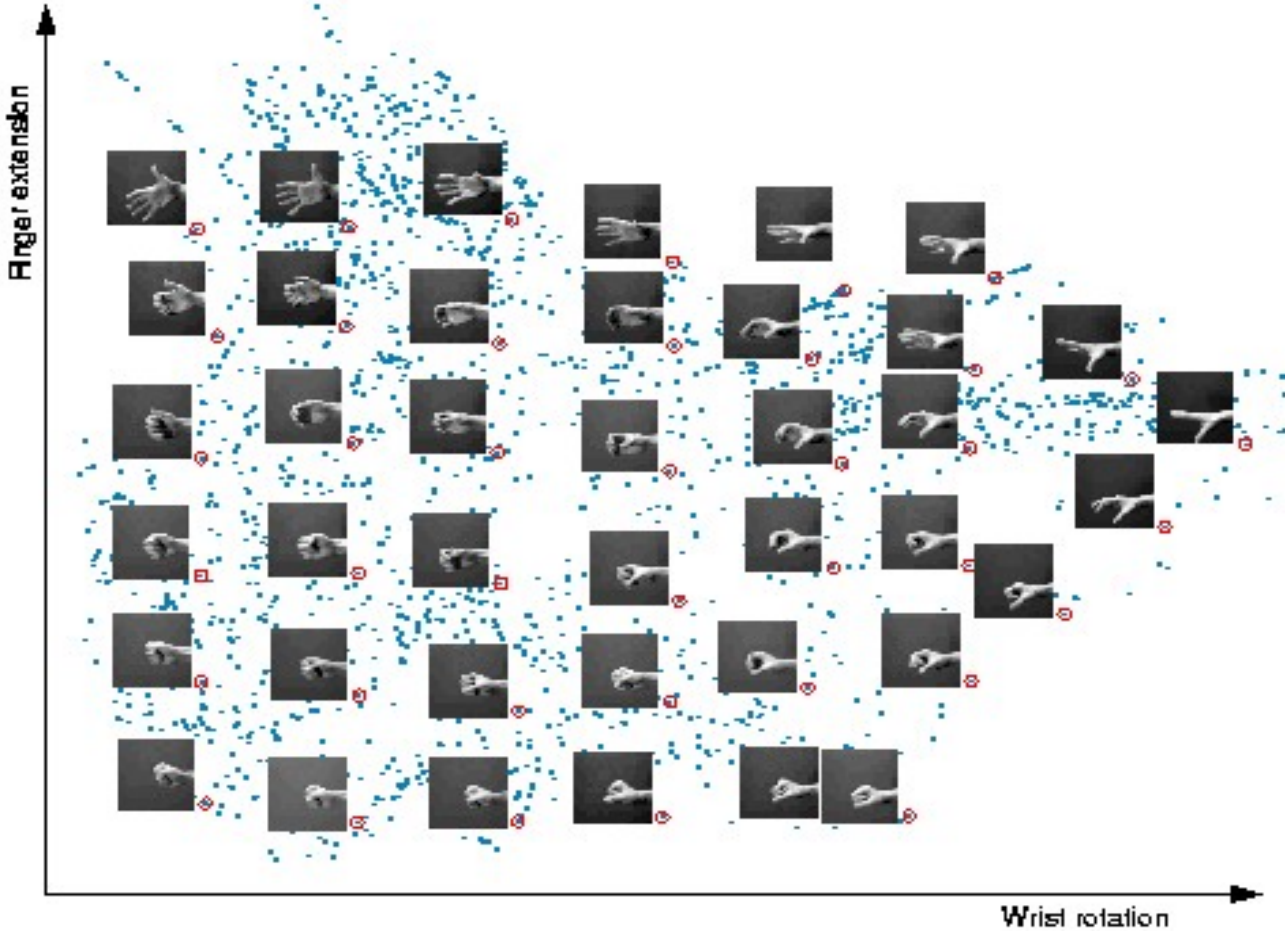
Isomap - Algorithm

- Determine the neighbors.
  - All points in a fixed radius.
  - K nearest neighbors
- Construct a neighborhood graph.
  - Each point is connected to the other if it is a K nearest neighbor.
  - Edge Length equals the Euclidean distance
- Compute the shortest paths between two nodes
  - Floyd's Algorithm
  - Djkastra's ALgorithm
- Construct a lower dimensional embedding.
  - Classical MDS

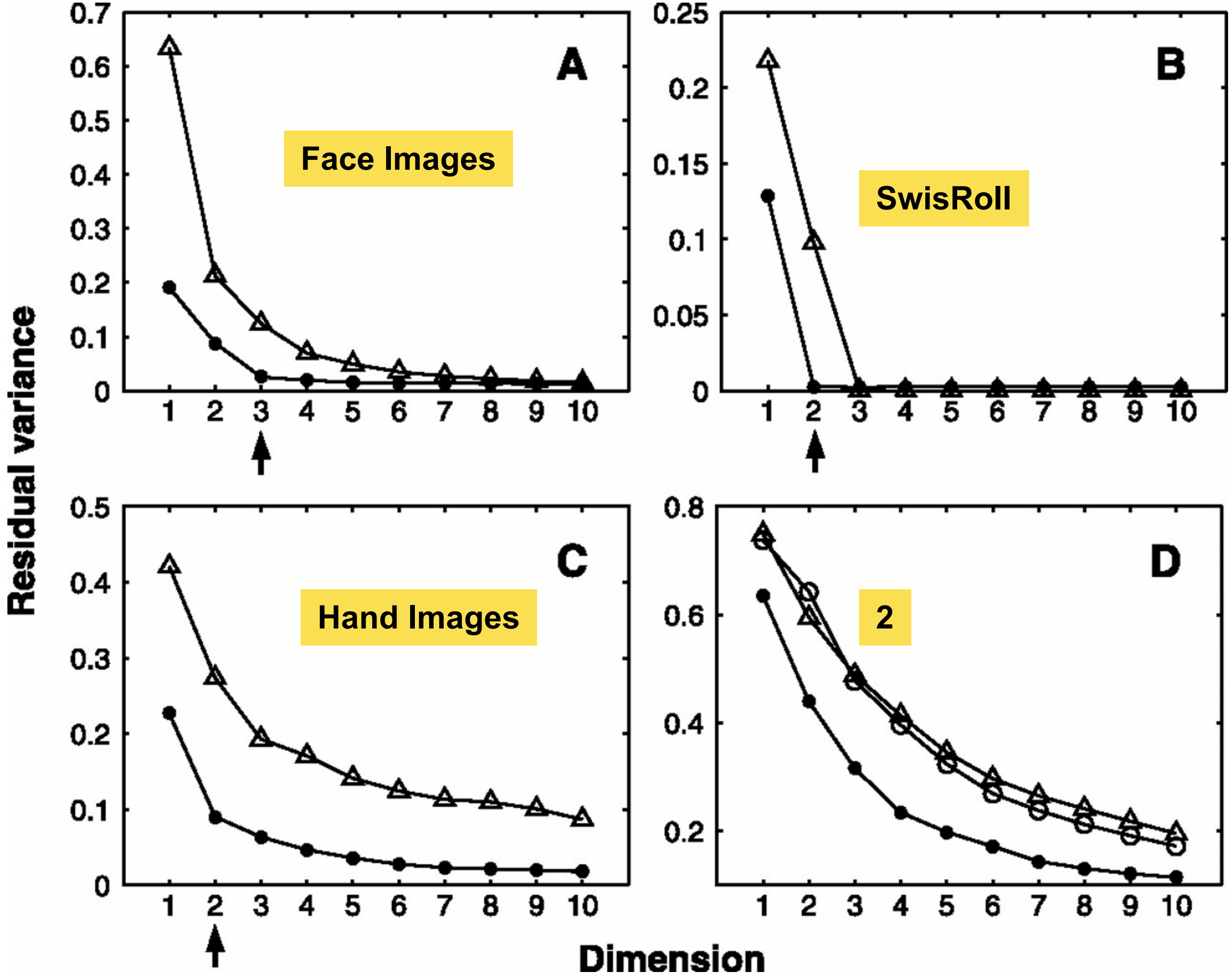
Isomap




B
Bottom loop articulation
Top arch articulation


Finger extension
Wrist rotation

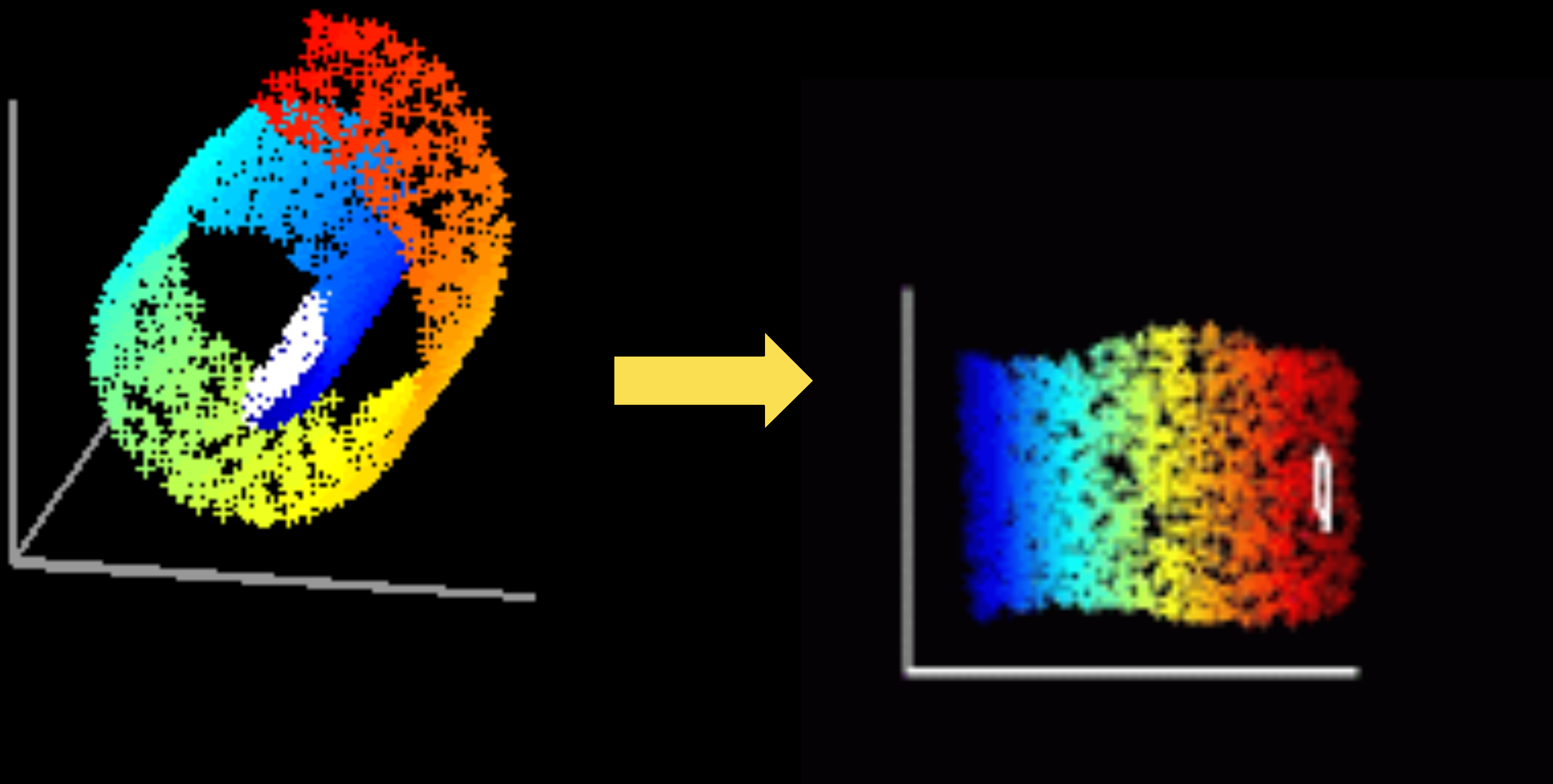
Residual Variance



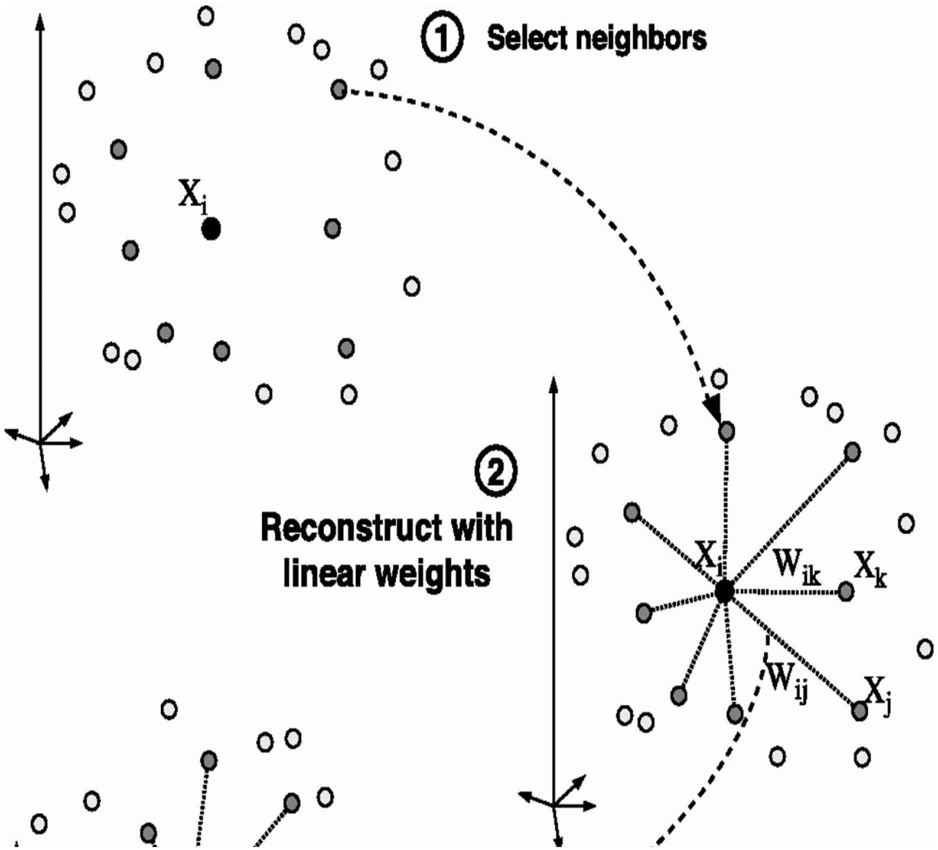
Locally Linear Embedding

manifold is a topological space which is locally Euclidean

Fit Locally , Think Globally



Fit Locally…



We expect each data point and its neighbours to lie on or close to a locally linear patch of the manifold.

Each point can be written as a linear combination of its neighbors.
The weights choosen to minimize the reconstruction Error.

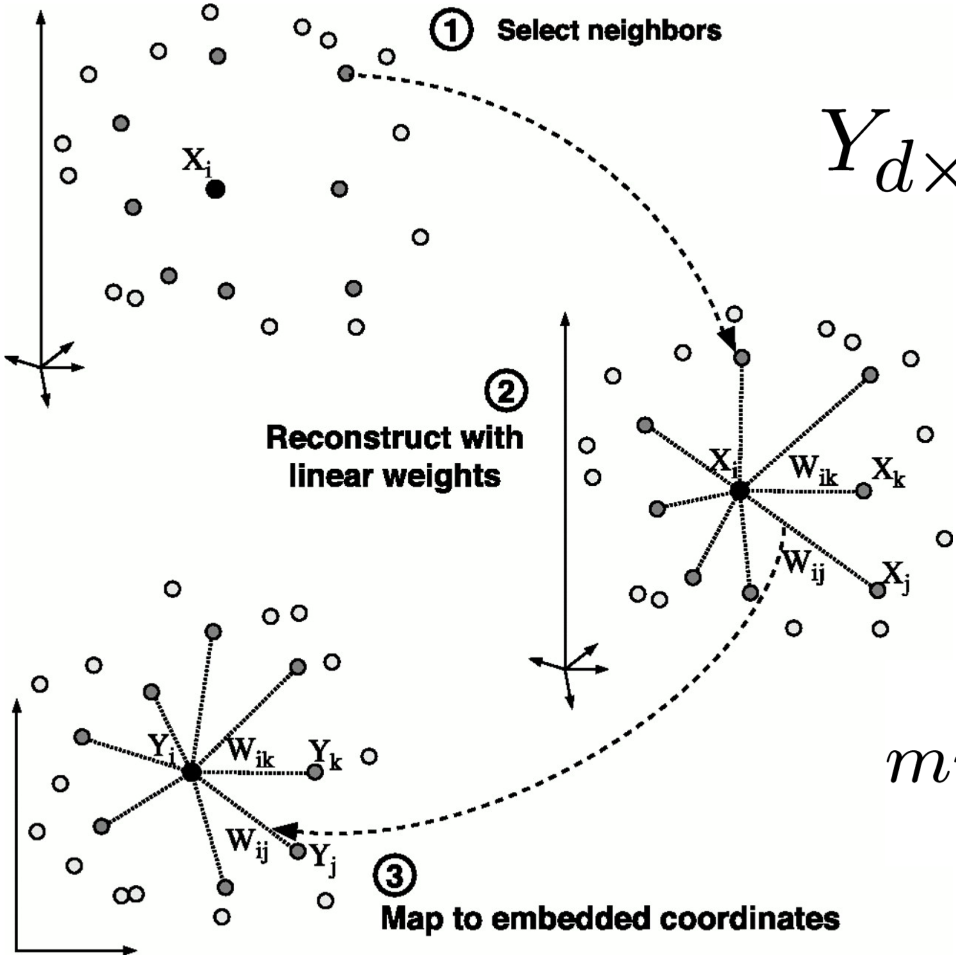
$$min_W \parallel X_i - \sum_{j=1}^{K} W_{ij} X_j \parallel^2 \qquad (1)$$

Derivation on board

Important property...

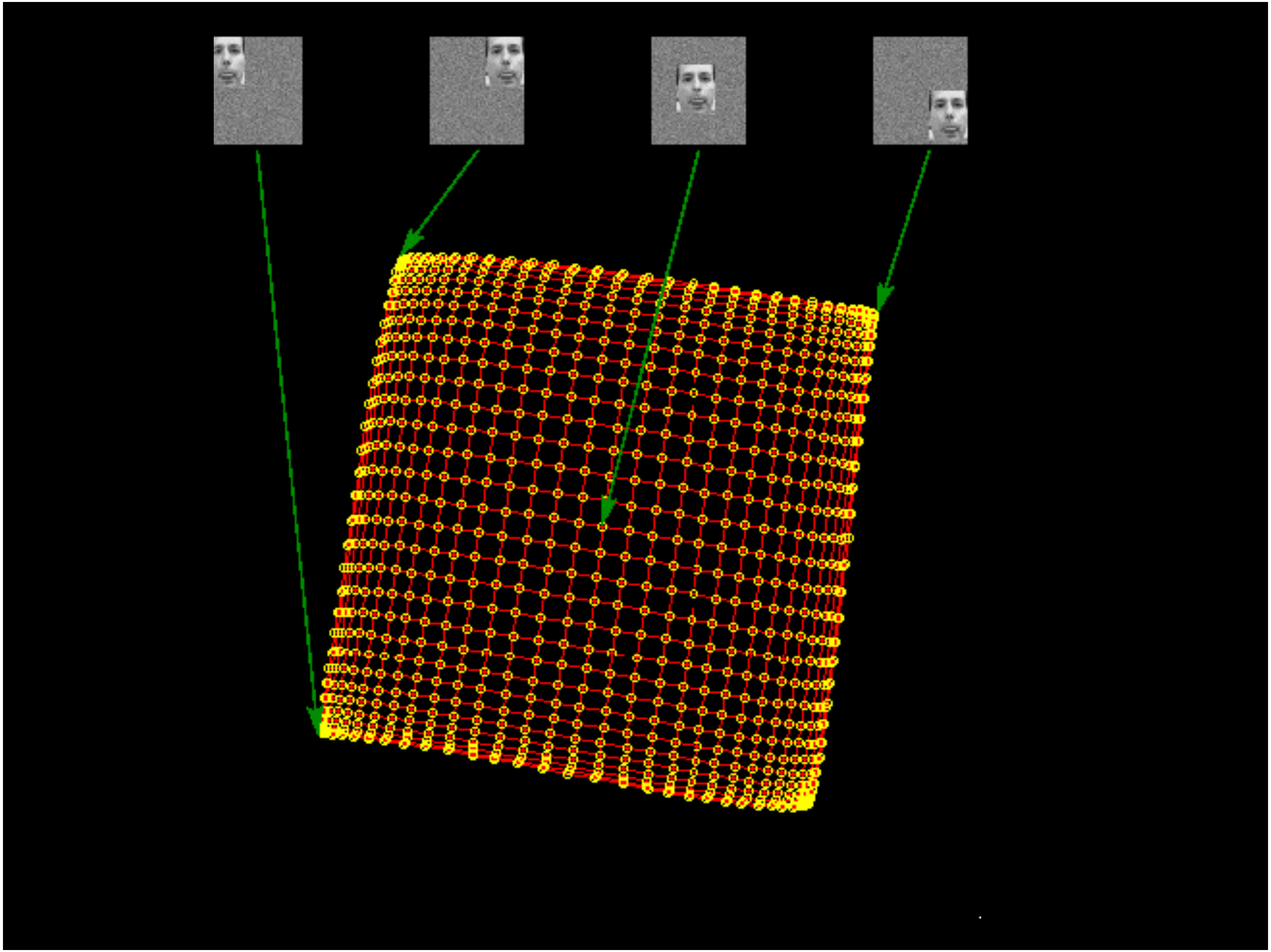
- The weights that minimize the reconstruction errors are invariant to rotation, rescaling and translation of the data points.
  - Invariance to translation is enforced by adding the constraint that the weights sum to one.
- **The same weights that reconstruct the datapoints in D dimensions should reconstruct it in the manifold in d dimensions.**
  - The weights characterize the intrinsic geometric properties of each neighborhood.

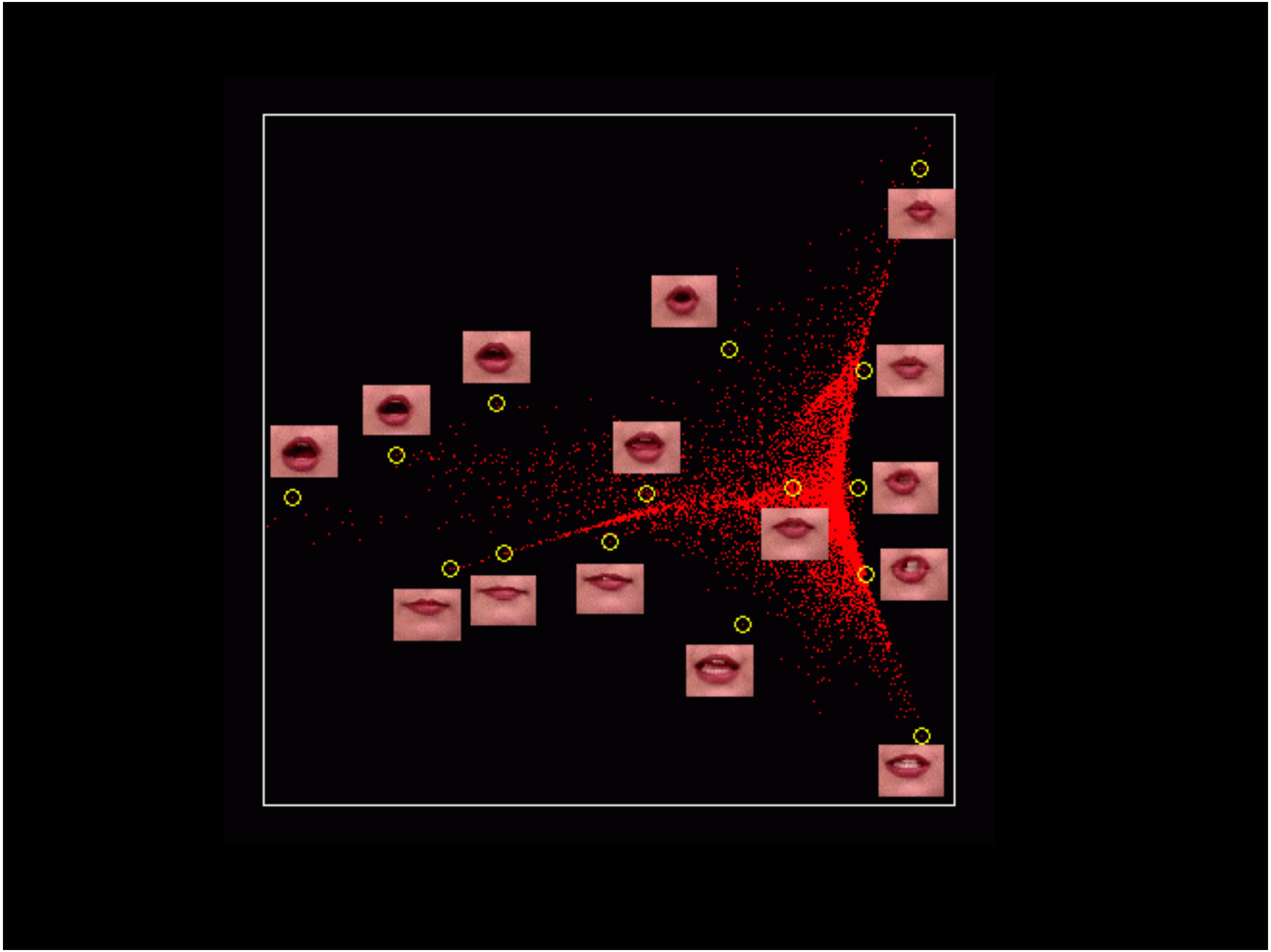
Think Globally...

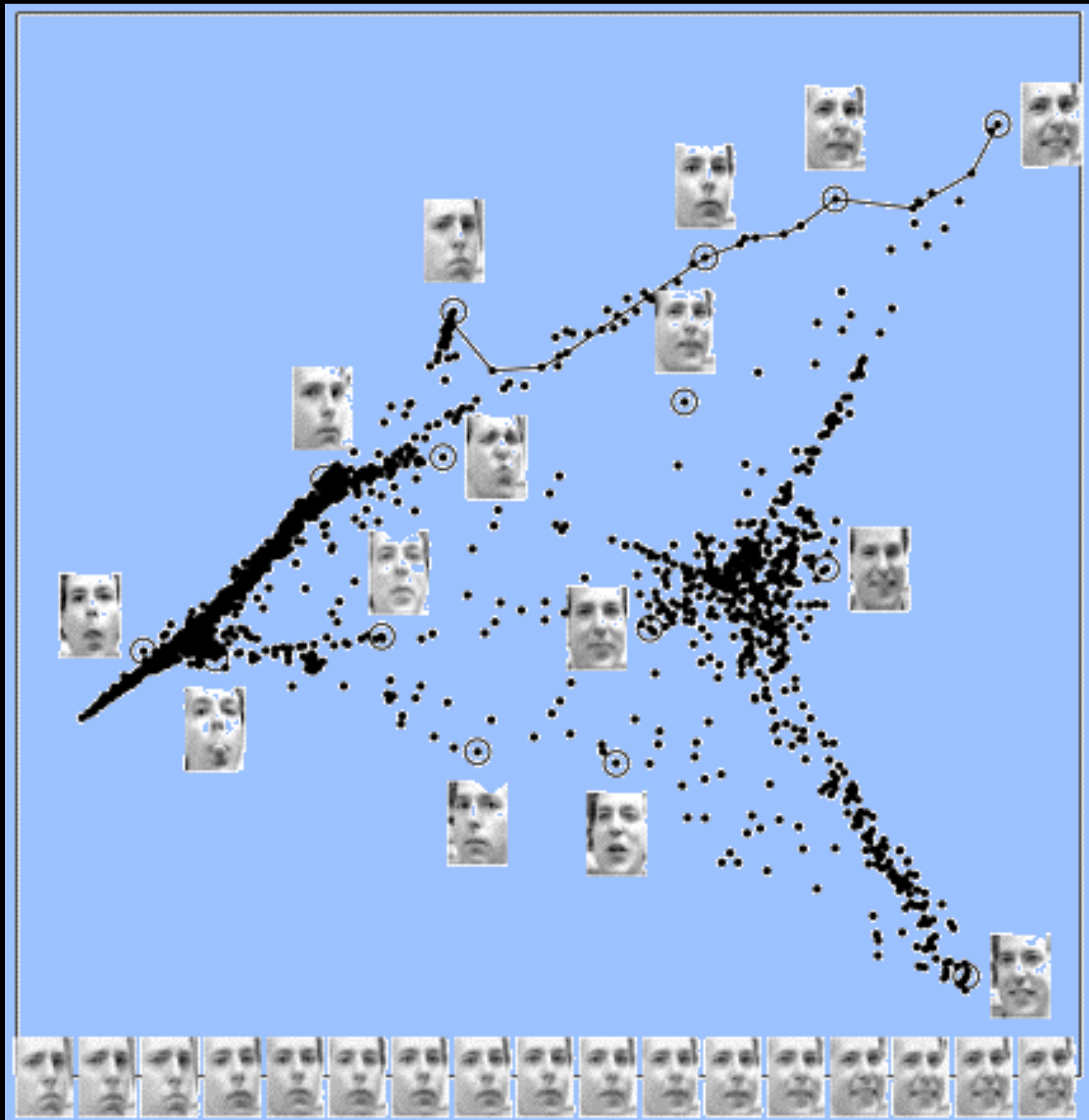


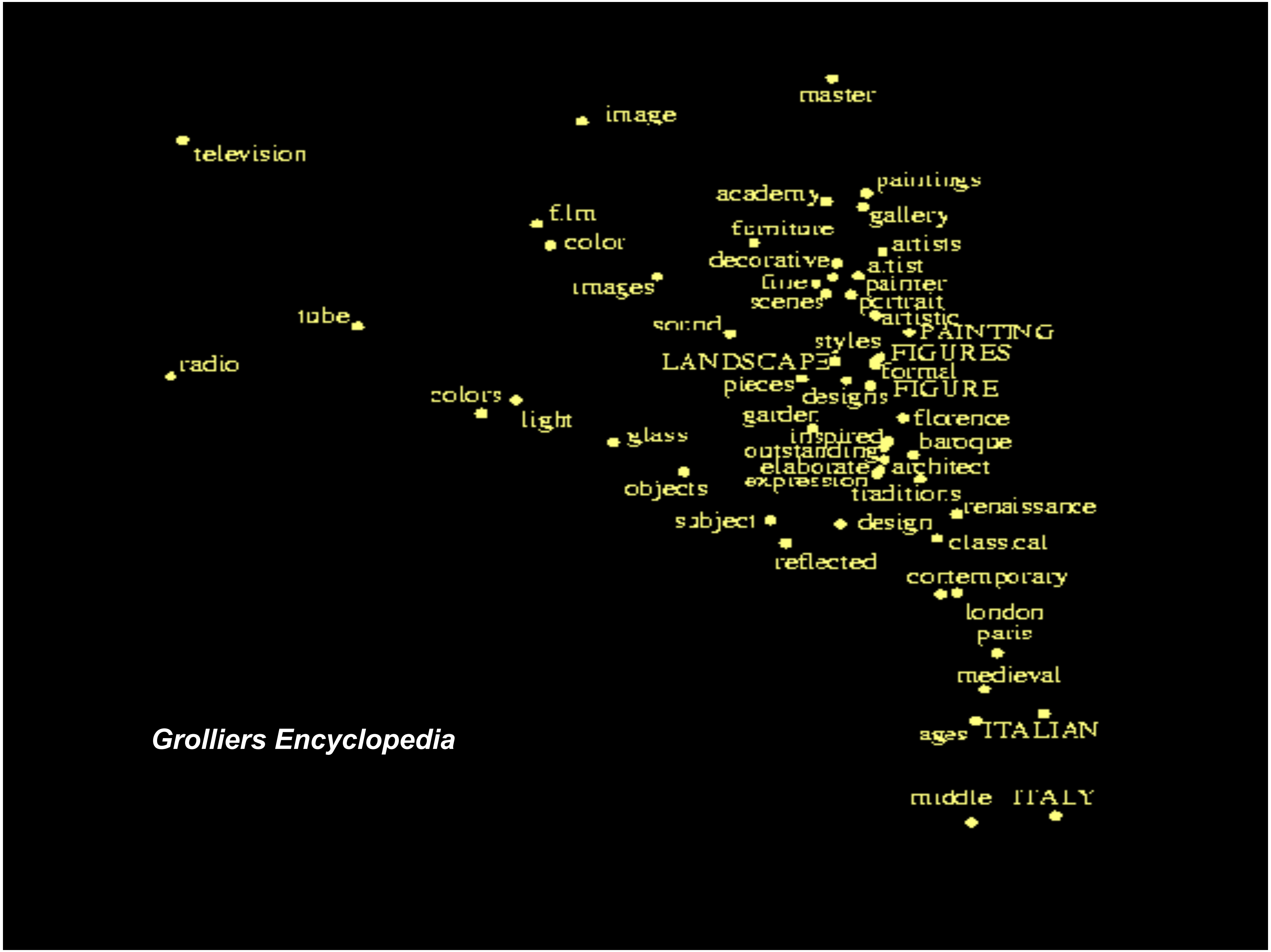
$$Y_{d \times N} = [Y_1 | Y_2 | ... | Y_N]$$

$$min_Y \sum_{i=1}^{N} \parallel Y_i - Y W_i \parallel^2$$





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Summary..

ISOMAP	LLE
Do MDS on the geodesic distance matrix.	Model local neighborhoods as linear a patches and then embed in a lower dimensional manifold.
Global approach	Local approach
Might not work for nonconvex manifolds with holes	Nonconvex manifolds with holes
Extensions: Conformal & Isometric ISOMAP	Extensions: Hessian Eigenmaps, Laplacian Eigenmaps etc.

Both needs manifold finely sampled.

Conformal & Isometric Embedding

Y d-dimensional domain in Euclidean space R^D

$f : Y -> R^D$ smooth embedding

Recover Y and f based on a given set of x_i in R^D.

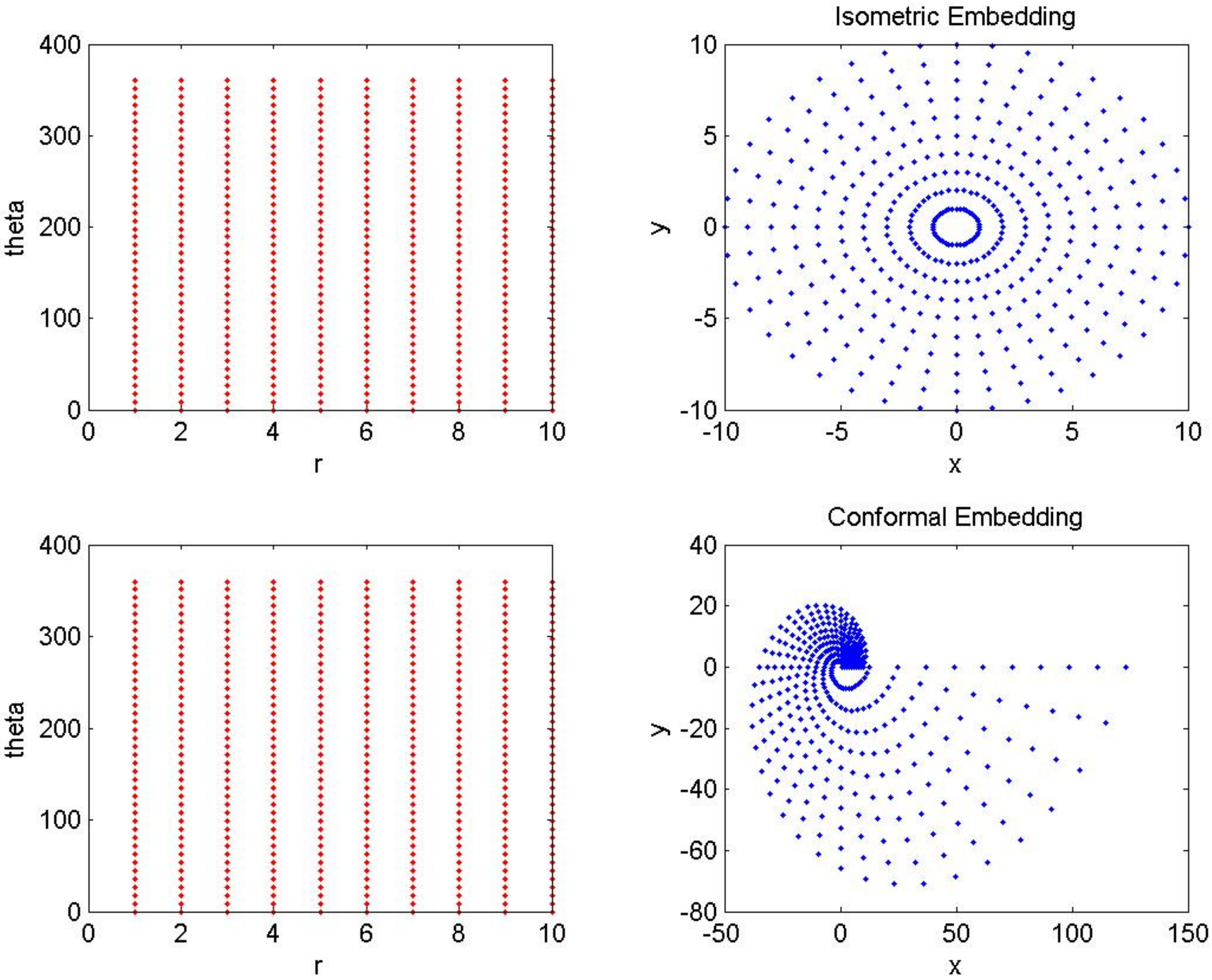
f is an isometric embedding if f preserves infinitesimal lengths and angles.

f is a conformal embedding if f preserves infinitesimal angles.

At every point y there is a scalar $s(y) > 0$ such that the infintesimal vectors at y get magnified in length by a factor $s(y)$.

Isometric Mapping and C-Isomap

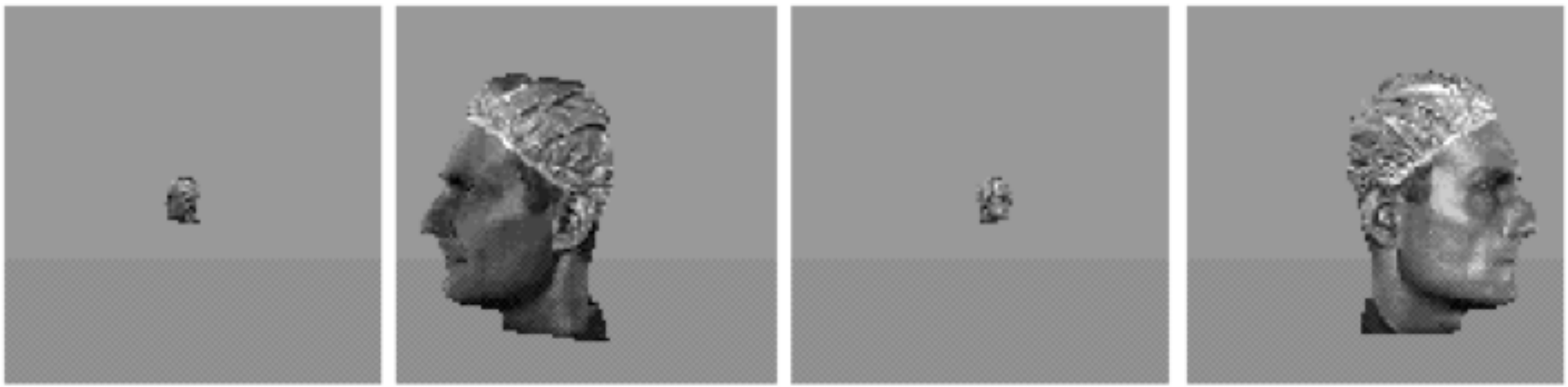
- Isometric mapping
  - Intrinsically flat manifold
  - Invariants??
    - Geodesic distances are reserved.
    - Metric space under geodesic distance.
- Conformal Embedding
  - Locally isometric upto a scale factor s(y)
  - Estimate s(y) and rescale.
  - C-Isomap
  - Original data should be uniformly dense



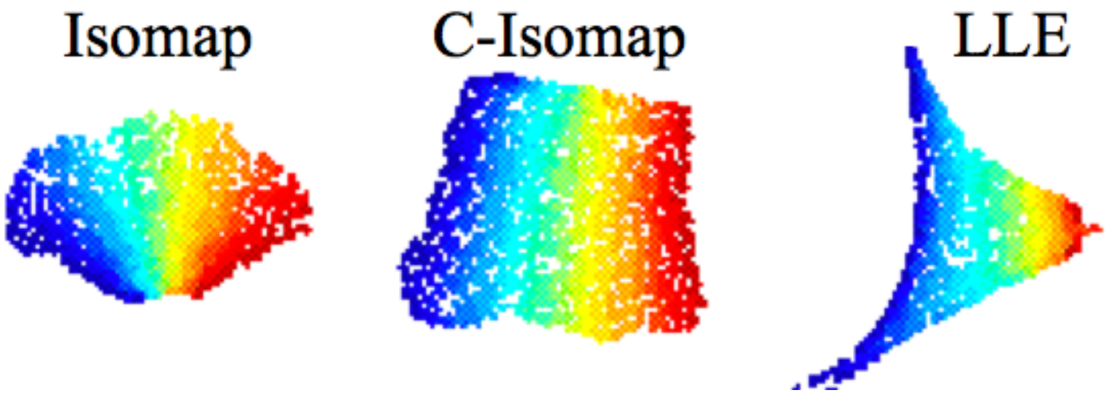
Isometric Embedding
Conformal Embedding
theta
r
x
y

C-Isomap

- C-Isomap is similar to Isomap, but the graph weights are renormalised.
- Suitable when observed effect of parameter variation is not constant over the manifold.



More Example: C-Isomap



- C-Isomap succeeds when
  - Y is a convex subsets of Euclidean space
  - Data are densely sampled, uniformly over Y
  - F is a conformal embedding

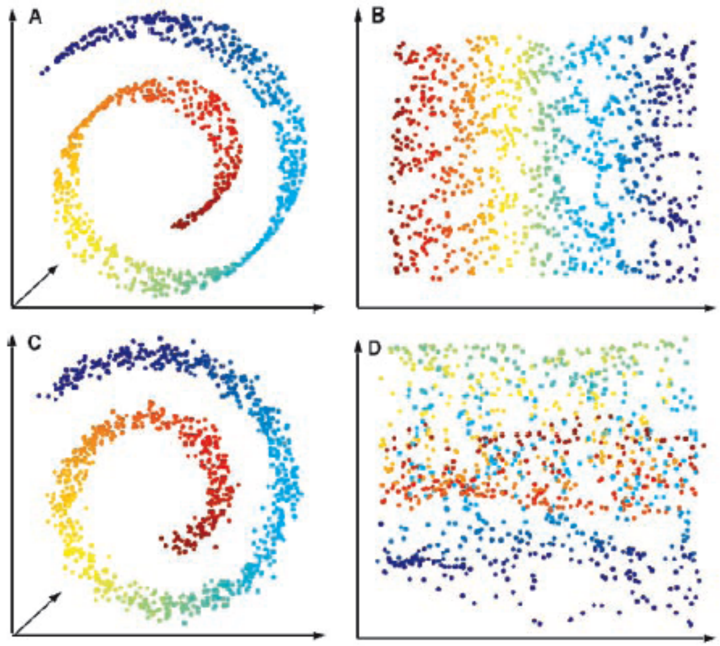
Short Circuit Problem???

Unstable?

Only free parameter is

How many neighbours?

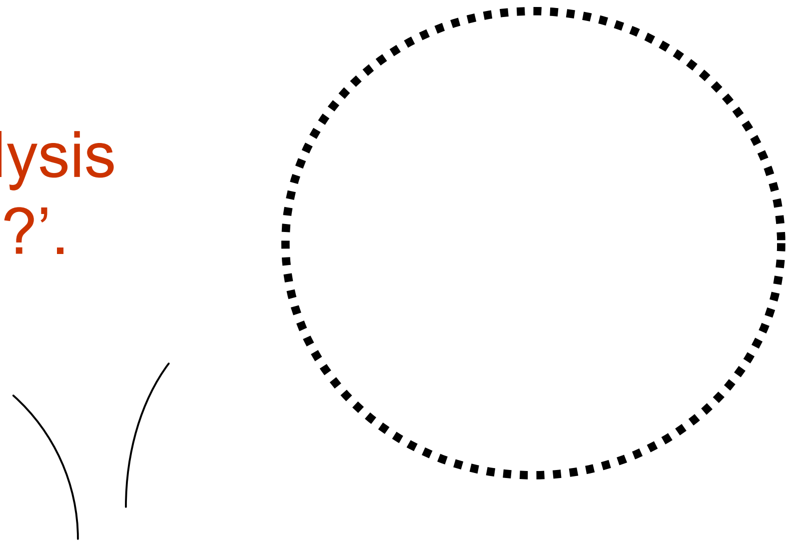
– How to choose neighborhoods.
    - Susceptible to short-circuit errors if neighborhood is larger than the folds in the manifold.
    - If small we get isolated patches.



???

- Isomap might not work on closed manifold, manifolds with holes?
- Noisy Data?
- Sparse Data?

Develop Multiscale analysis to solve some of those '?'.



Acknowledgement

- Slides stolen from Vikas C. Raykar, Vin de Silva, et al.