

ISOMAP and LLE



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2014.

Matlab Dimensionality Reduction Toolbox

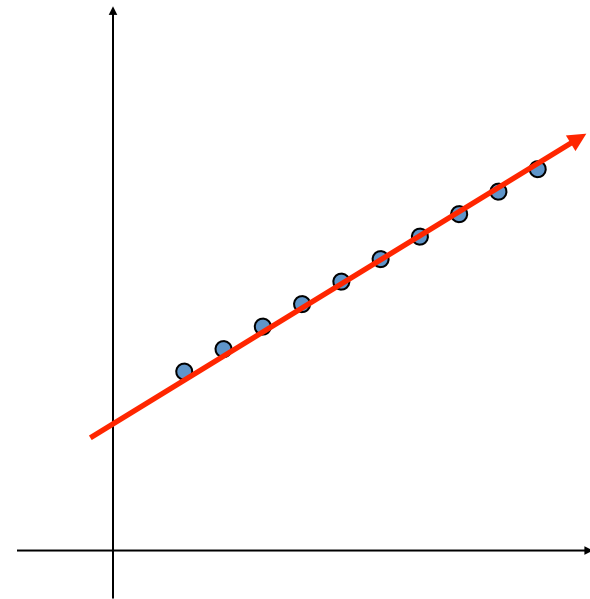
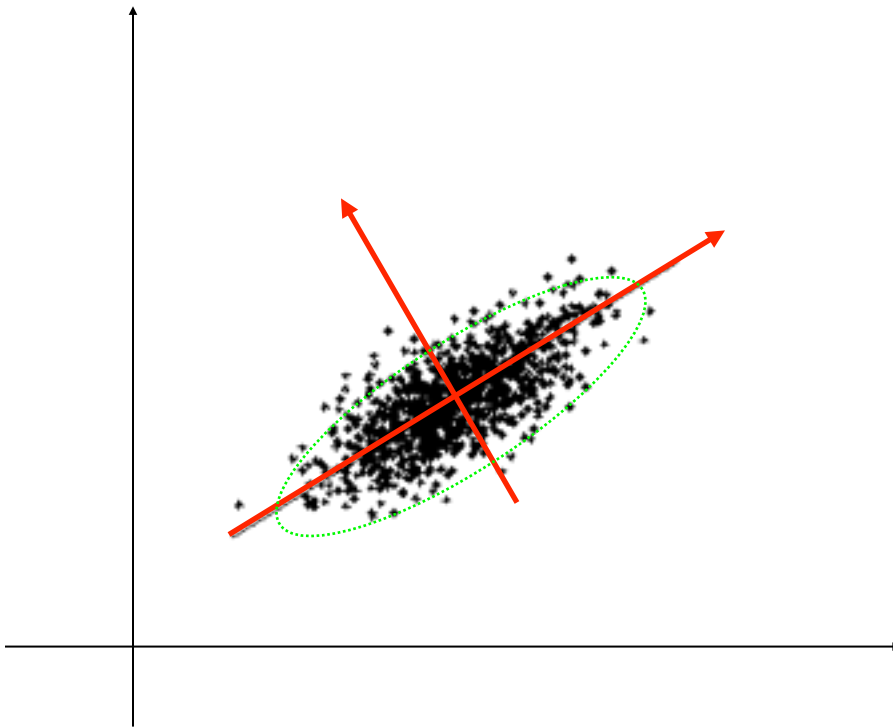
- http://homepage.tudelft.nl/19j49/Matlab_Toolbox_for_Dimensionality_Reduction.html
- drtoolbox contains:
 - Principal Component Analysis (PCA), Probabilistic PC
 - Factor Analysis (FA), Sammon mapping, Linear Discriminant Analysis (LDA)
 - Multidimensional scaling (MDS), Isomap, Landmark Isomap
 - Local Linear Embedding (LLE), Laplacian Eigenmaps, Hessian LLE, Conformal Eigenmaps
 - Local Tangent Space Alignment (LTSA), Maximum Variance Unfolding (extension of LLE)
 - Landmark MVU (LandmarkMVU), Fast Maximum Variance Unfolding (FastMVU)
 - Kernel PCA
 - Diffusion maps
 - ...

Recall: PCA

- Principal Component Analysis (PCA)

$$X_{p \times n} = [X_1 \quad X_2 \quad \dots \quad X_n]$$

EigenValue Decomposition of XX^T

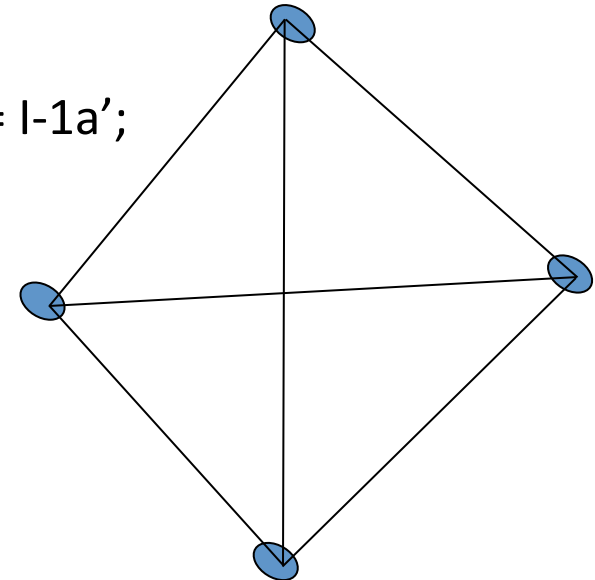


One Dimensional
Manifold

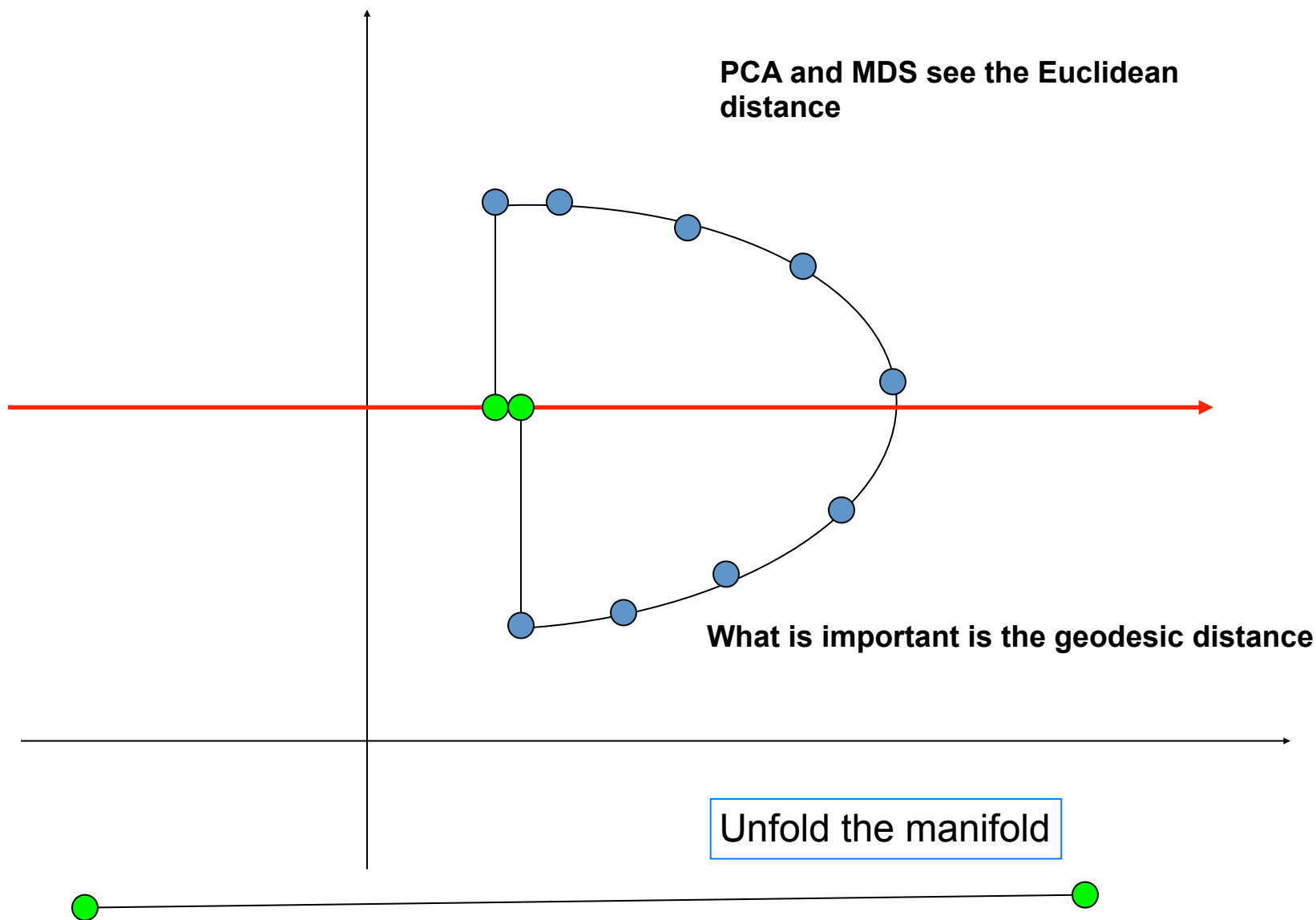
Recall: MDS

- Given pairwise distances D , where $D_{ij} = d_{ij}^2$, the squared distance between point i and j
 - Convert the pairwise distance matrix D (c.n.d.) into the dot product matrix B (p.s.d.)
 - $B_{ij}(a) = -.5 H(a) D H'(a)$, Hölder matrix $H(a) = I - 1a'$;
 - $a = 1_k$: $B_{ij} = -.5 (D_{ij} - D_{ik} - D_{jk})$
 - $a = 1/n$: $B_{ij} = -\frac{1}{2} \left(D_{ij} - \frac{1}{N} \sum_{s=1}^N D_{sj} - \frac{1}{N} \sum_{t=1}^N D_{it} + \frac{1}{N^2} \sum_{s,t=1}^N D_{st} \right)$
 - Eigendecomposition of $B = YY^T$

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

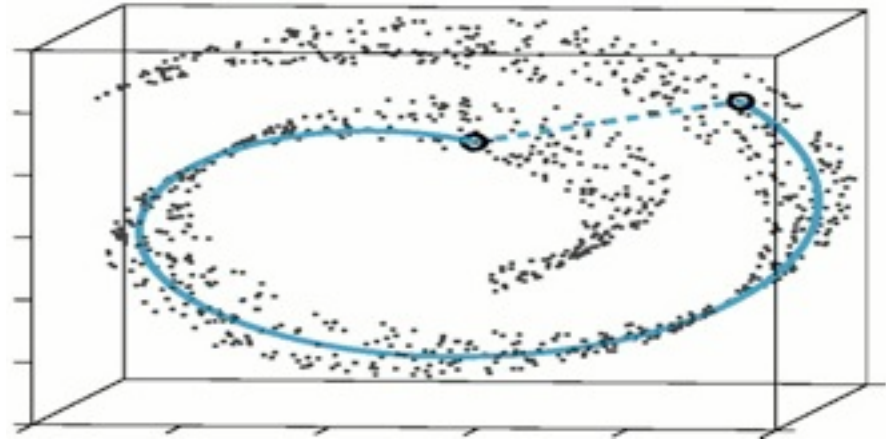


Nonlinear Manifolds..



Intrinsic Description..

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



Manifold Learning

Learning when data $\sim \mathcal{M} \subset \mathbb{R}^N$

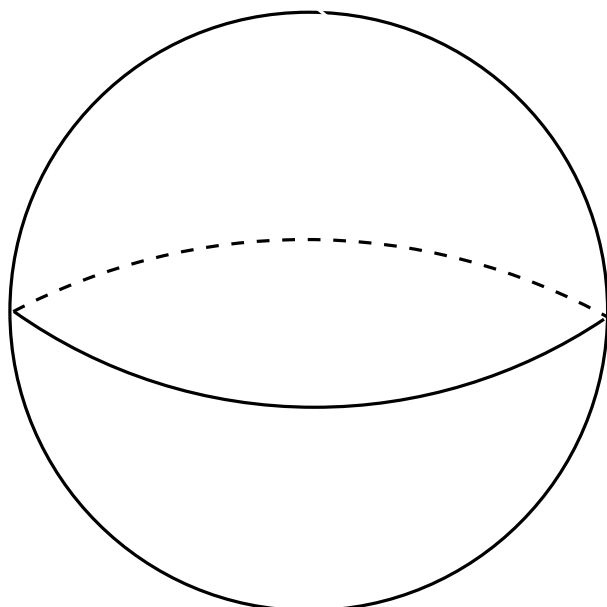
- Clustering: $\mathcal{M} \rightarrow \{1, \dots, k\}$
connected components, min cut
- Classification/Regression: $\mathcal{M} \rightarrow \{-1, +1\}$ or $\mathcal{M} \rightarrow \mathbb{R}$
 P on $\mathcal{M} \times \{-1, +1\}$ or P on $\mathcal{M} \times \mathbb{R}$
- Dimensionality Reduction: $f : \mathcal{M} \rightarrow \mathbb{R}^n$ $n \ll N$
- \mathcal{M} unknown: what can you learn about \mathcal{M} from data?
e.g. dimensionality, connected components
holes, handles, homology
curvature, geodesics

All you wanna know about
differential geometry but
were afraid to ask, in 9 easy

Embedded (sub-)Manifolds

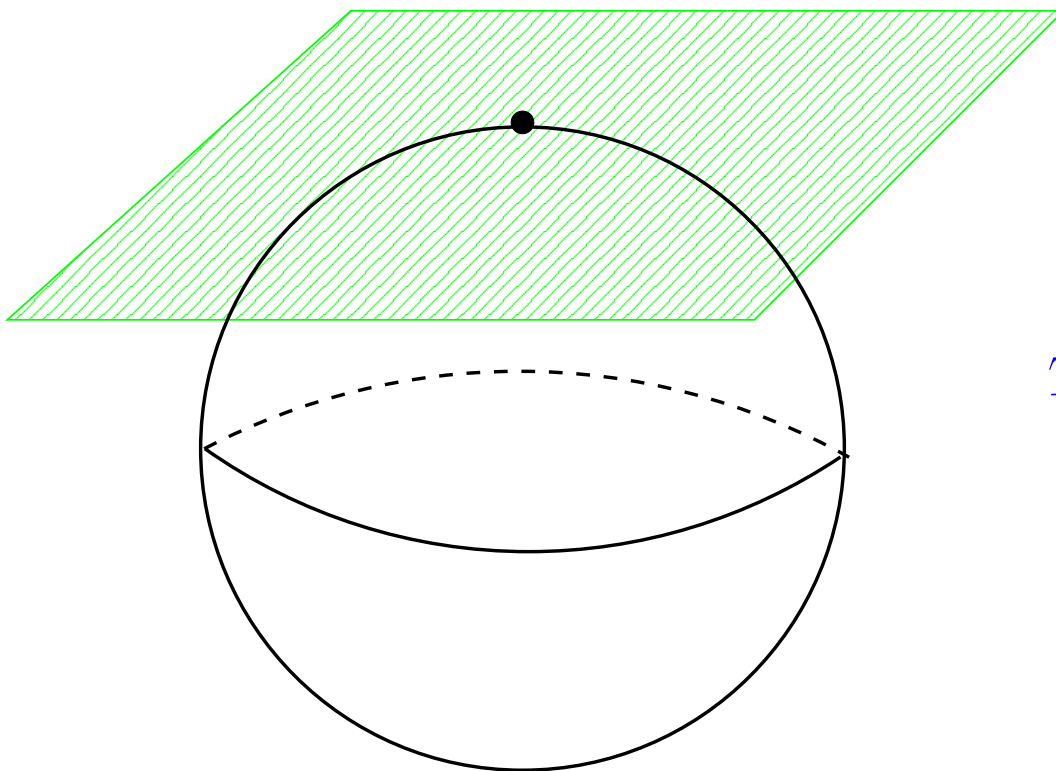
$$\mathcal{M}^k \subset \mathbb{R}^N$$

Locally (not globally) looks like Euclidean space.



$$S^2 \subset \mathbb{R}^3$$

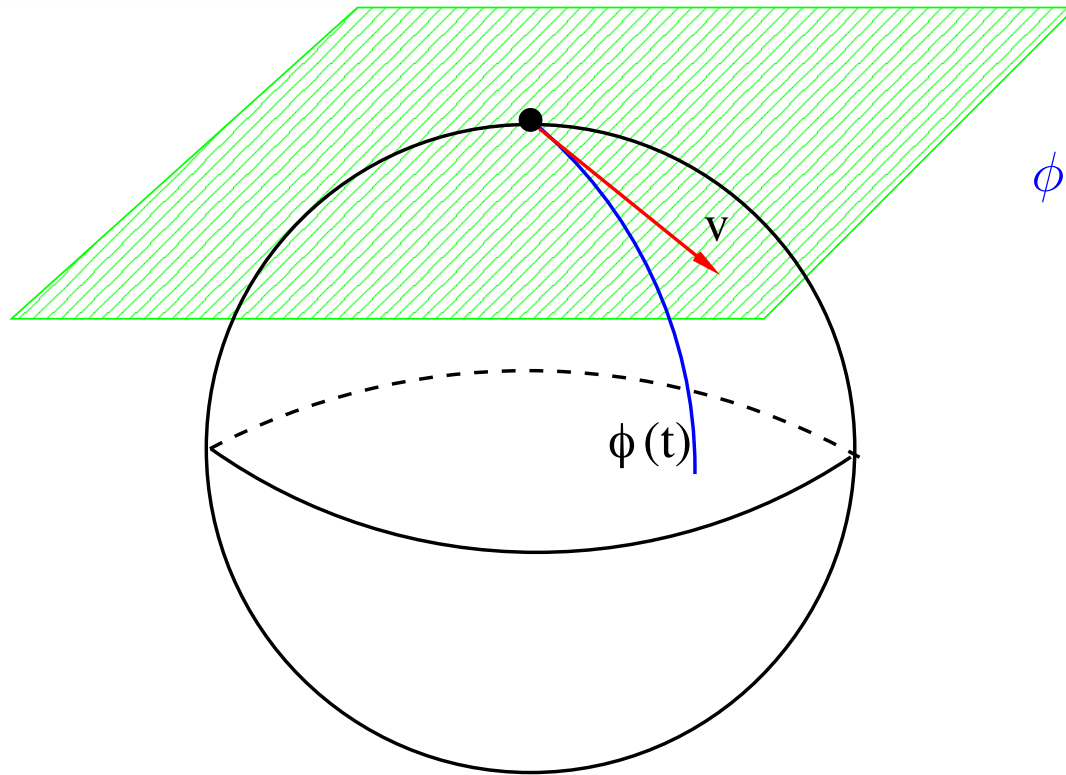
Tangent Space



$$T_p \mathcal{M}^k \subset \mathbb{R}^N$$

k -dimensional affine subspace of \mathbb{R}^N .

Tangent Vectors and Curves



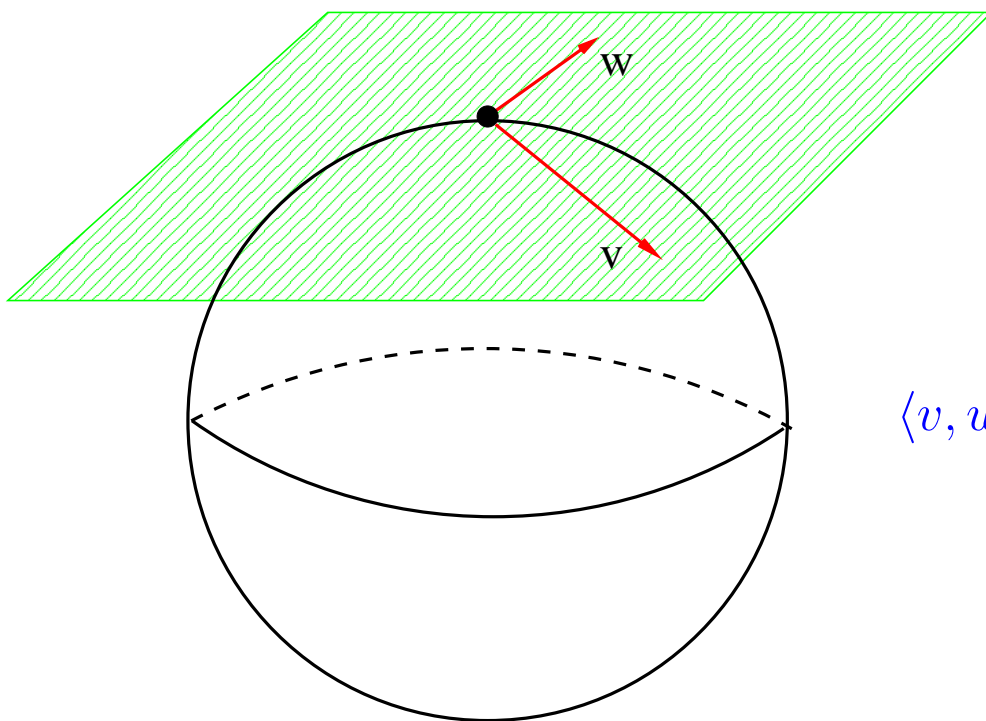
$$\phi(t) : \mathbb{R} \rightarrow \mathcal{M}^k$$

$$\left. \frac{d\phi(t)}{dt} \right|_0 = v$$

Tangent vectors \longleftrightarrow curves.

Riemannian Geometry

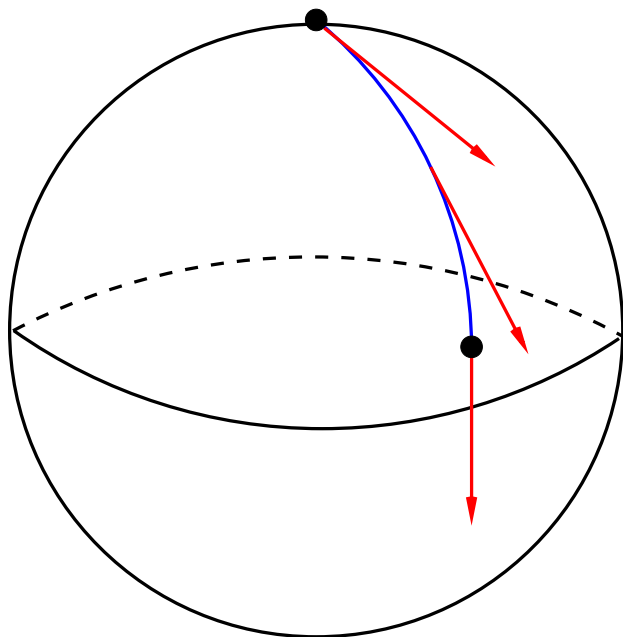
Norms and **angles** in tangent space.



$$\langle v, w \rangle$$

$$\|v\|, \|w\|$$

Geodesics



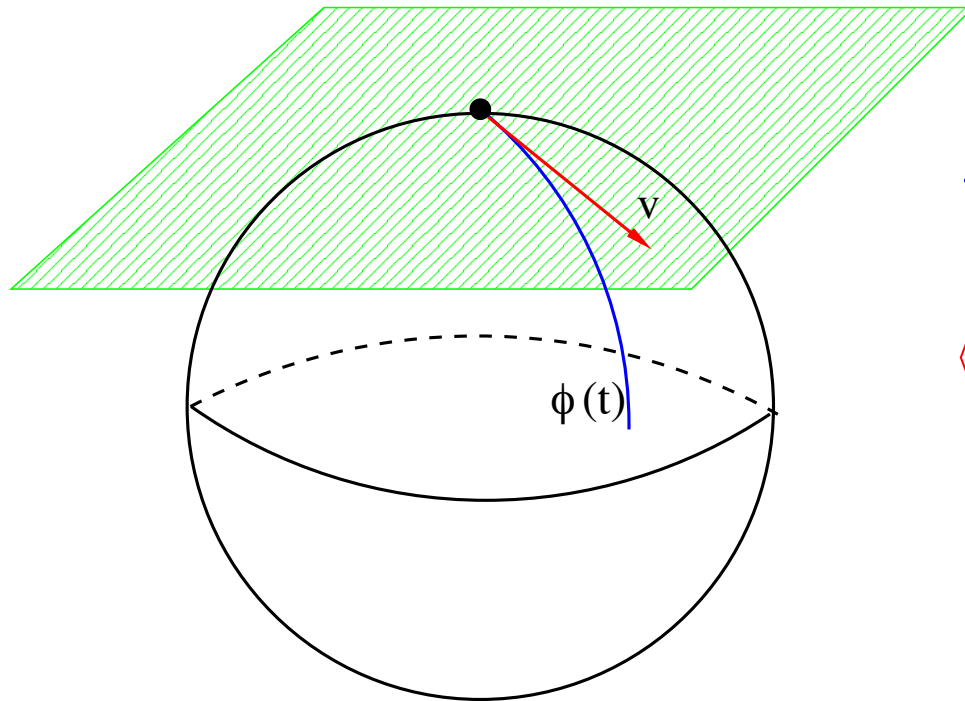
$$\phi(t) : [0, 1] \rightarrow \mathcal{M}^k$$

$$l(\phi) = \int_0^1 \left\| \frac{d\phi}{dt} \right\| dt$$

Can measure length using **norm** in tangent space.

Geodesic — shortest curve between two points.

Gradients



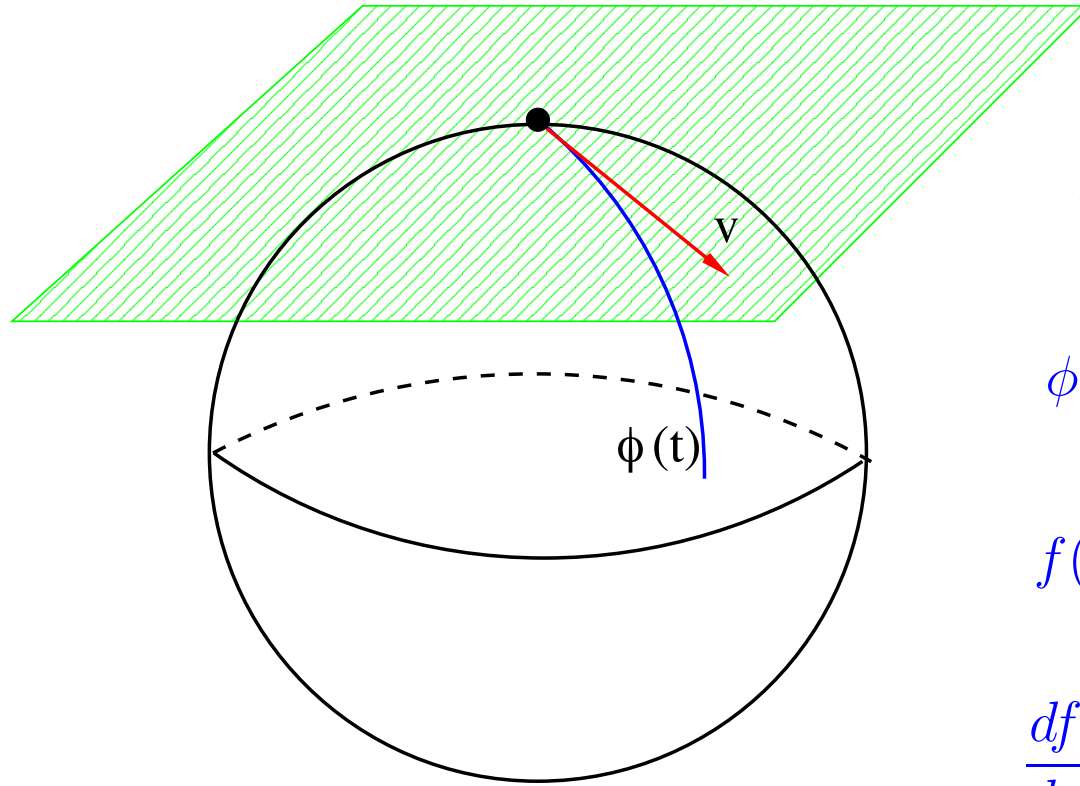
$$f : \mathcal{M}^k \rightarrow \mathbb{R}$$

$$\langle \nabla f, v \rangle \equiv \frac{df}{dv}$$

Tangent vectors $\langle \text{---} \rangle$ Directional derivatives.

Gradient points in the direction of maximum change.

Tangent Vectors vs. Derivatives



$$f : \mathcal{M}^k \rightarrow \mathbb{R}$$

$$\phi(t) : \mathbb{R} \rightarrow \mathcal{M}^k$$

$$f(\phi(t)) : \mathbb{R} \rightarrow \mathbb{R}$$

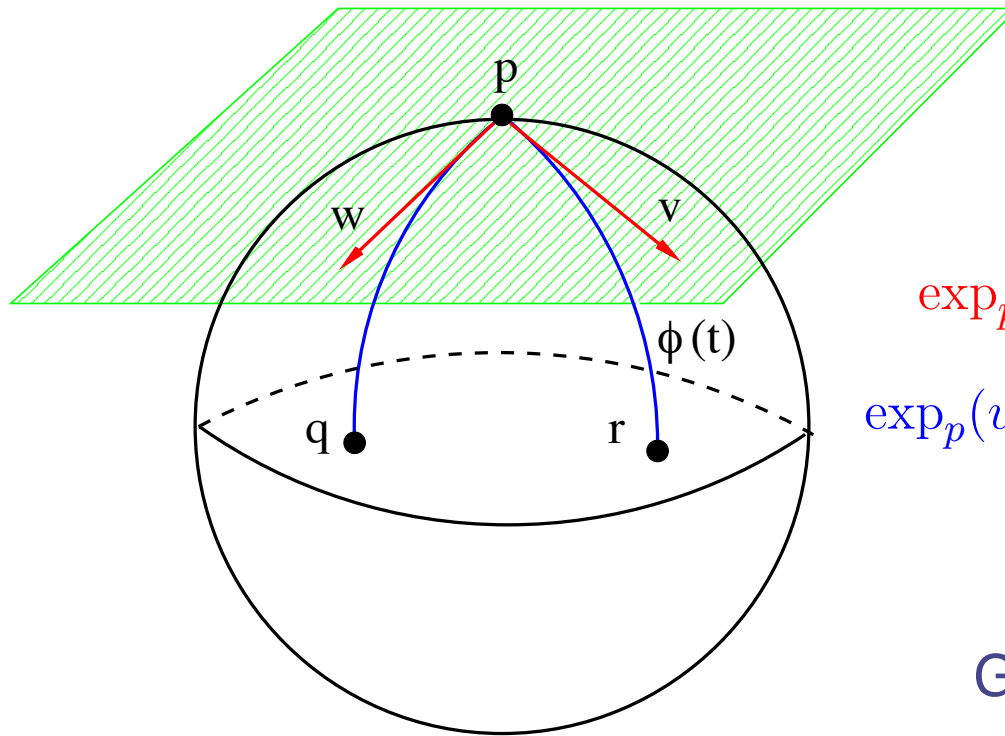
$$\frac{df}{dv} = \left. \frac{df(\phi(t))}{dt} \right|_0$$

Tangent vectors

<— — —>

Directional derivatives.

Exponential Maps



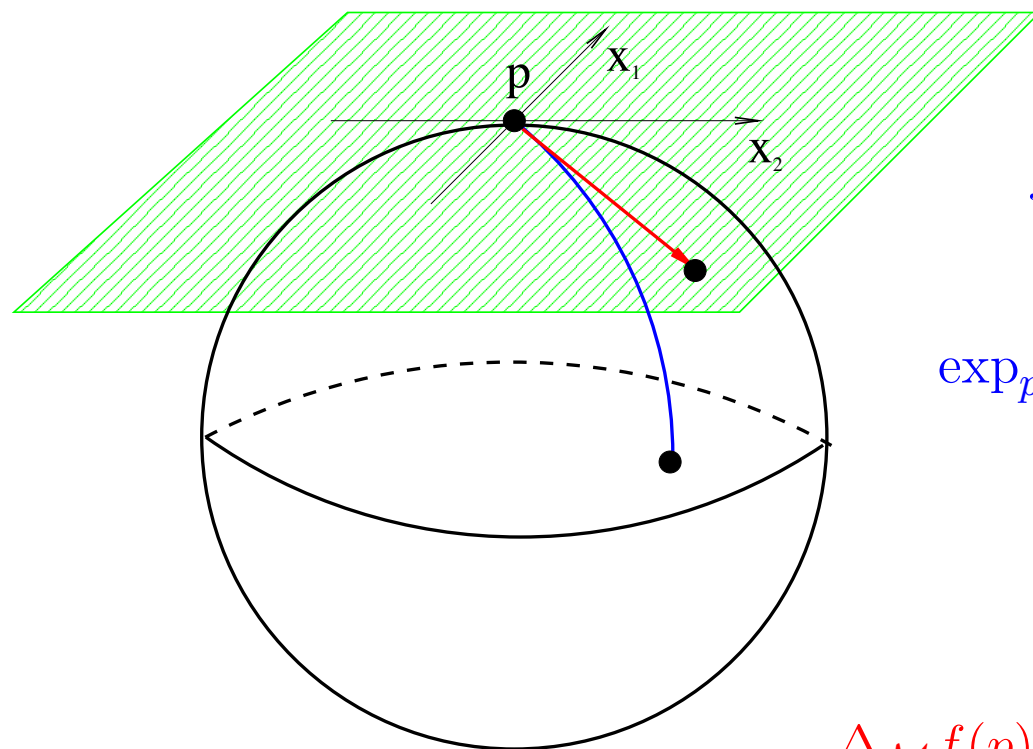
$$\exp_p : T_p \mathcal{M}^k \rightarrow \mathcal{M}^k$$

$$\exp_p(v) = r \quad \exp_p(w) = q$$

Geodesic $\phi(t)$

$$\phi(0) = p, \quad \phi(\|v\|) = q \quad \left. \frac{d\phi(t)}{dt} \right|_0 = v$$

Laplacian-Beltrami Operator



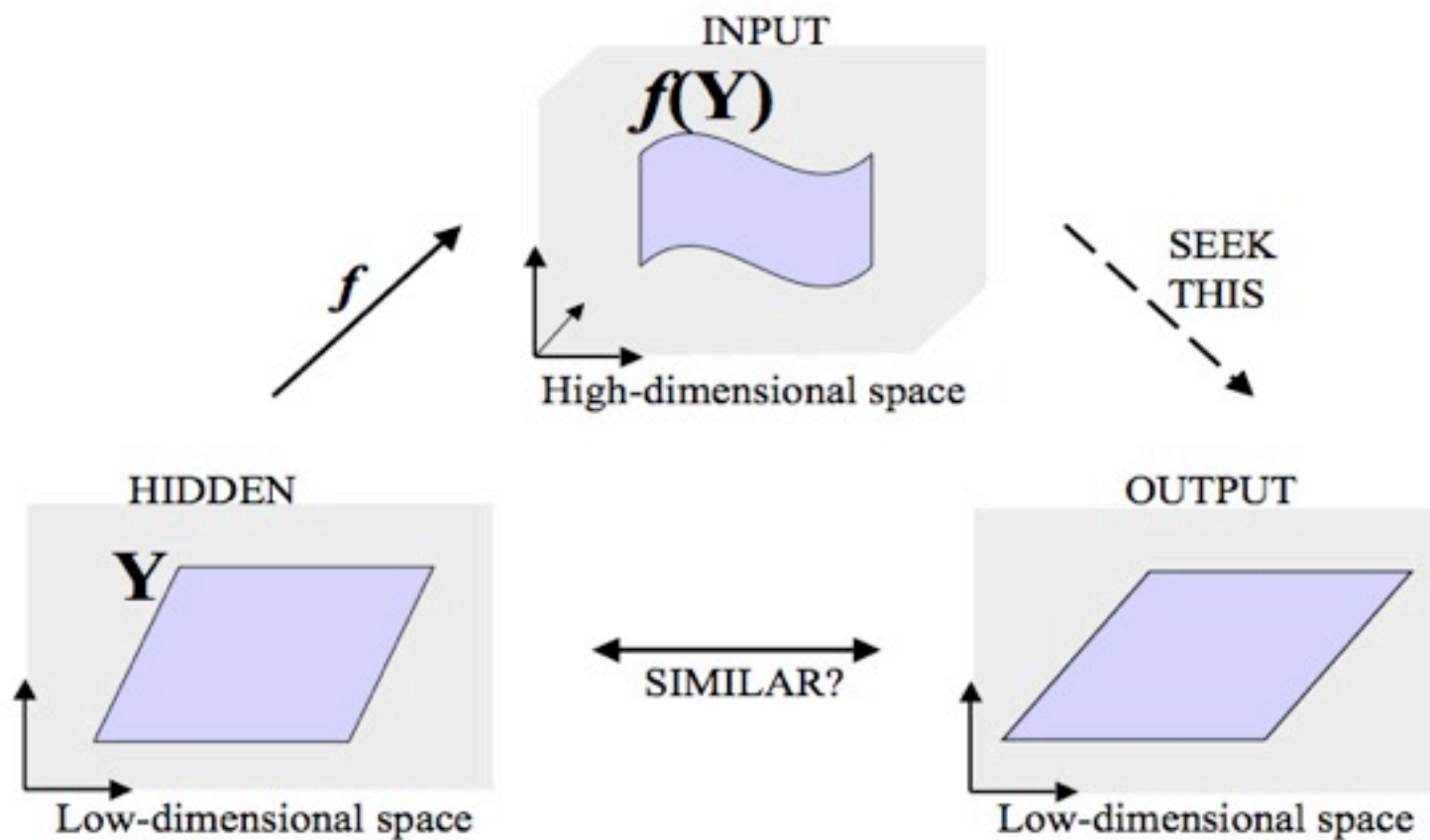
$$f : \mathcal{M}^k \rightarrow \mathbb{R}$$

$$\exp_p : T_p \mathcal{M}^k \rightarrow \mathcal{M}^k$$

$$\Delta_{\mathcal{M}} f(p) \equiv \sum_i \frac{\partial^2 f(\exp_p(x))}{\partial x_i^2}$$

Orthonormal coordinate system.

Generative Models in Manifold Learning



Spectral Geometric Embedding

Given $x_1, \dots, x_n \in \mathcal{M} \subset \mathbb{R}^N$,

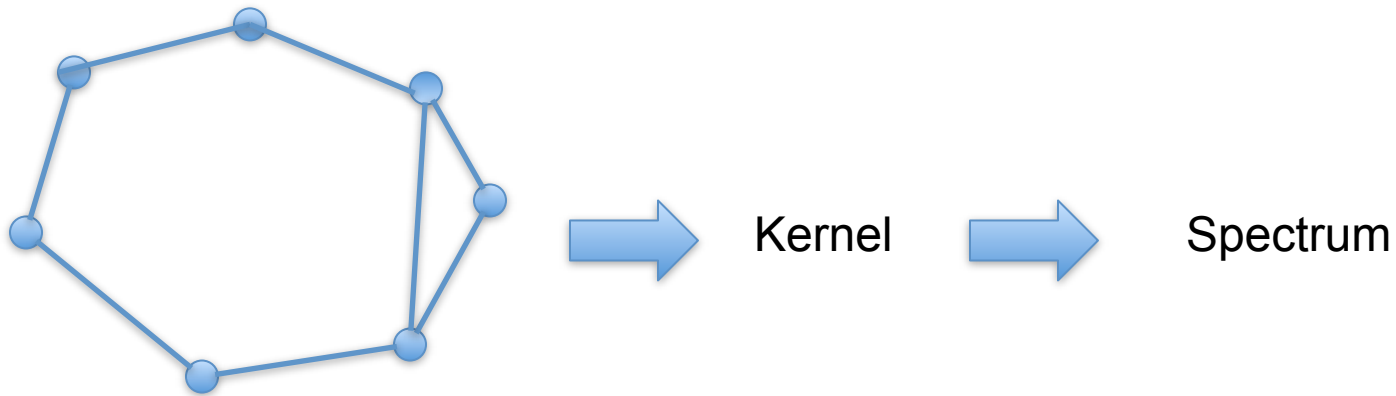
Find $y_1, \dots, y_n \in \mathbb{R}^d$ where $d \ll N$

- ISOMAP (Tenenbaum, et al, 00)
- LLE (Roweis, Saul, 00)
- Laplacian Eigenmaps (Belkin, Niyogi, 01)
- Local Tangent Space Alignment (Zhang, Zha, 02)
- Hessian Eigenmaps (Donoho, Grimes, 02)
- Diffusion Maps (Coifman, Lafon, et al, 04)

Related: Kernel PCA (Schoelkopf, et al, 98)

Meta-Algorithm

- Construct a neighborhood graph
- Construct a positive semi-definite kernel
- Find the spectrum decomposition



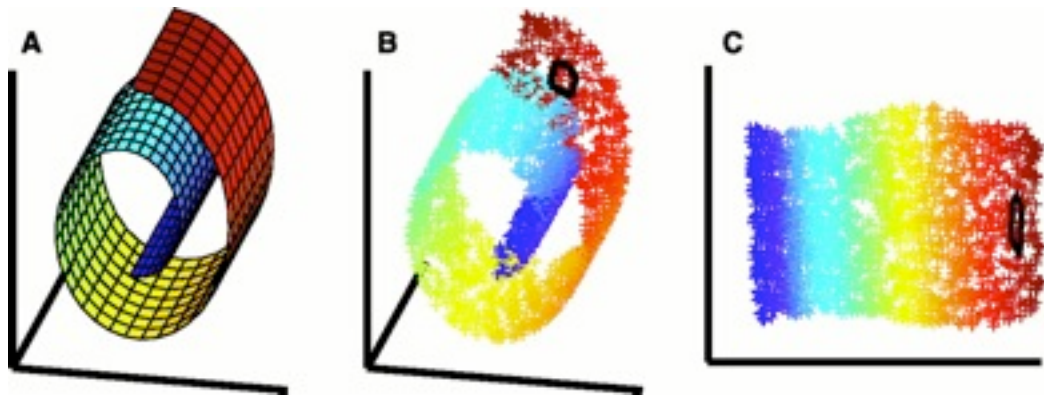
Two Basic Geometric Embedding Methods: Science 2000

- Tenenbaum-de Silva-Langford **Isomap** Algorithm
 - Global approach.
 - On a low dimensional embedding
 - Nearby points should be nearby.
 - Faraway points should be faraway.
- Roweis-Saul **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 **faraway** 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

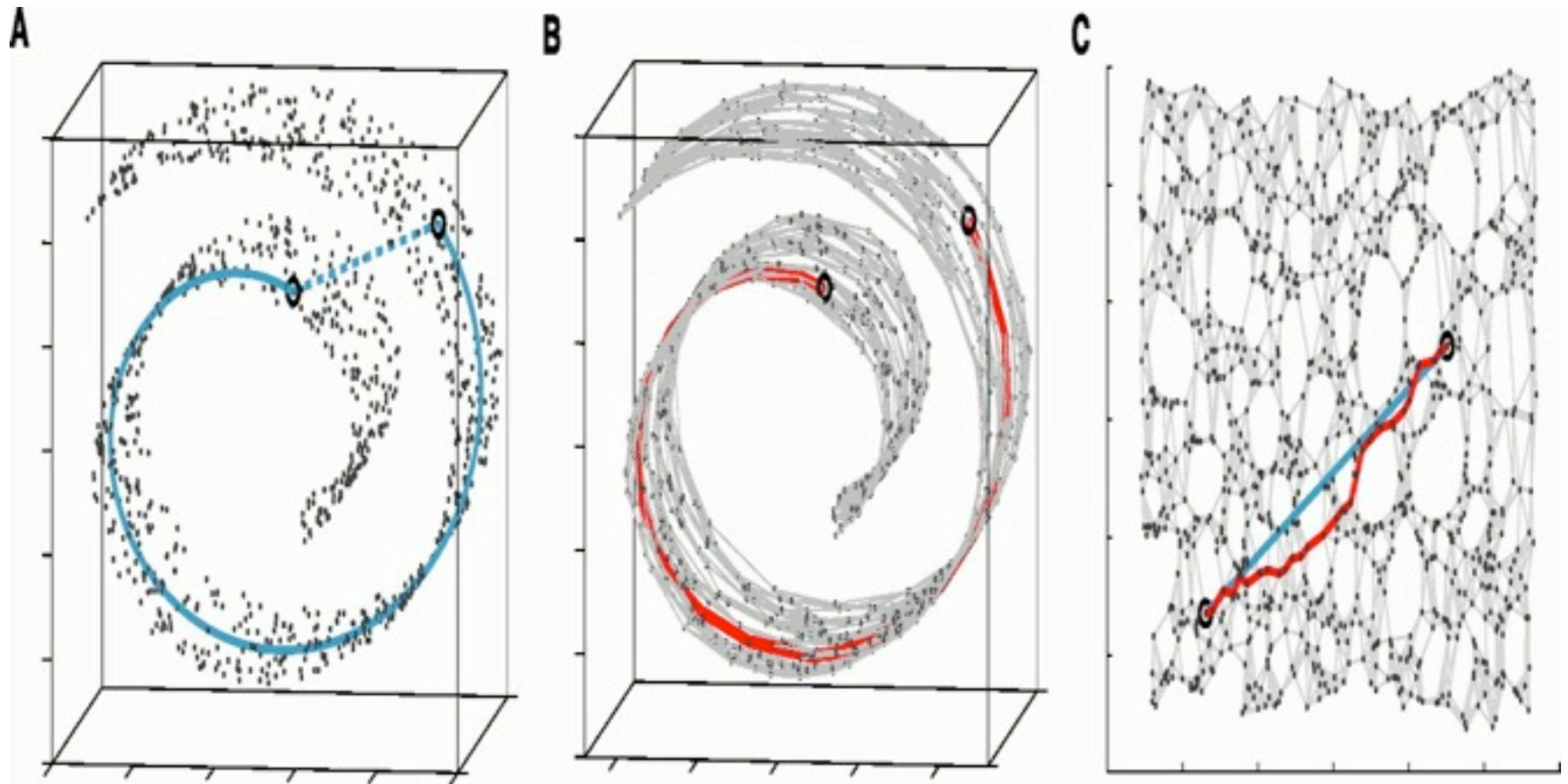
Once we have all pairwise geodesic distances use **classical metric MDS**



Isomap - Algorithm

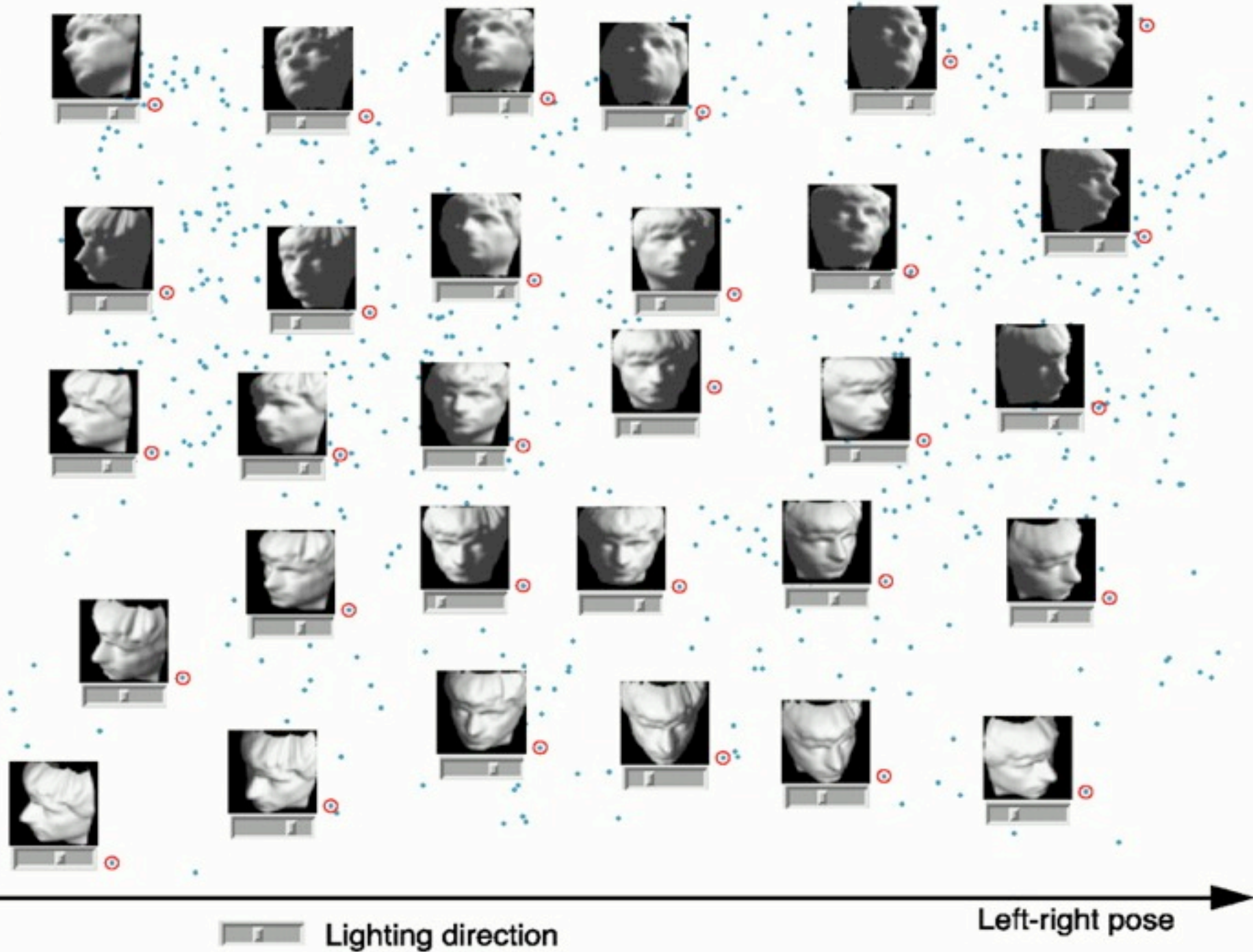
- Construct an n-by-n neighborhood graph
 - connecting points whose distances are within a fixed radius.
 - K nearest neighbor graph
- Compute the **shortest path (geodesic) distances** between nodes: D
 - Floyd's Algorithm ($O(N^3)$)
 - Dijkstra's Algorithm ($O(kN^2 \log N)$)
- Construct a lower dimensional embedding.
 - Classical MDS ($K = -0.5 H D H' = U S U'$)

Isomap



A

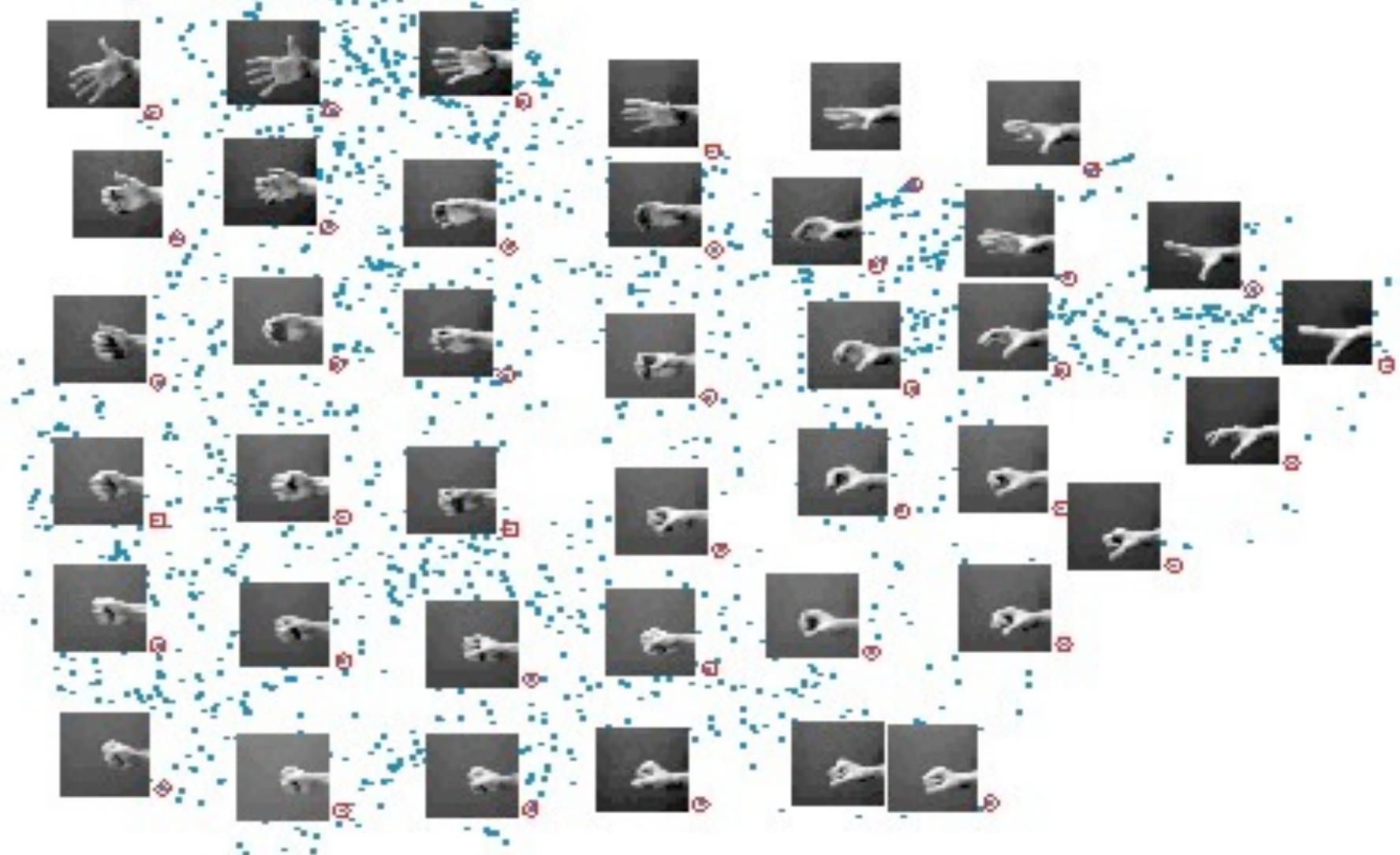
Up-down pose



Lighting direction

Left-right pose

Anger extension

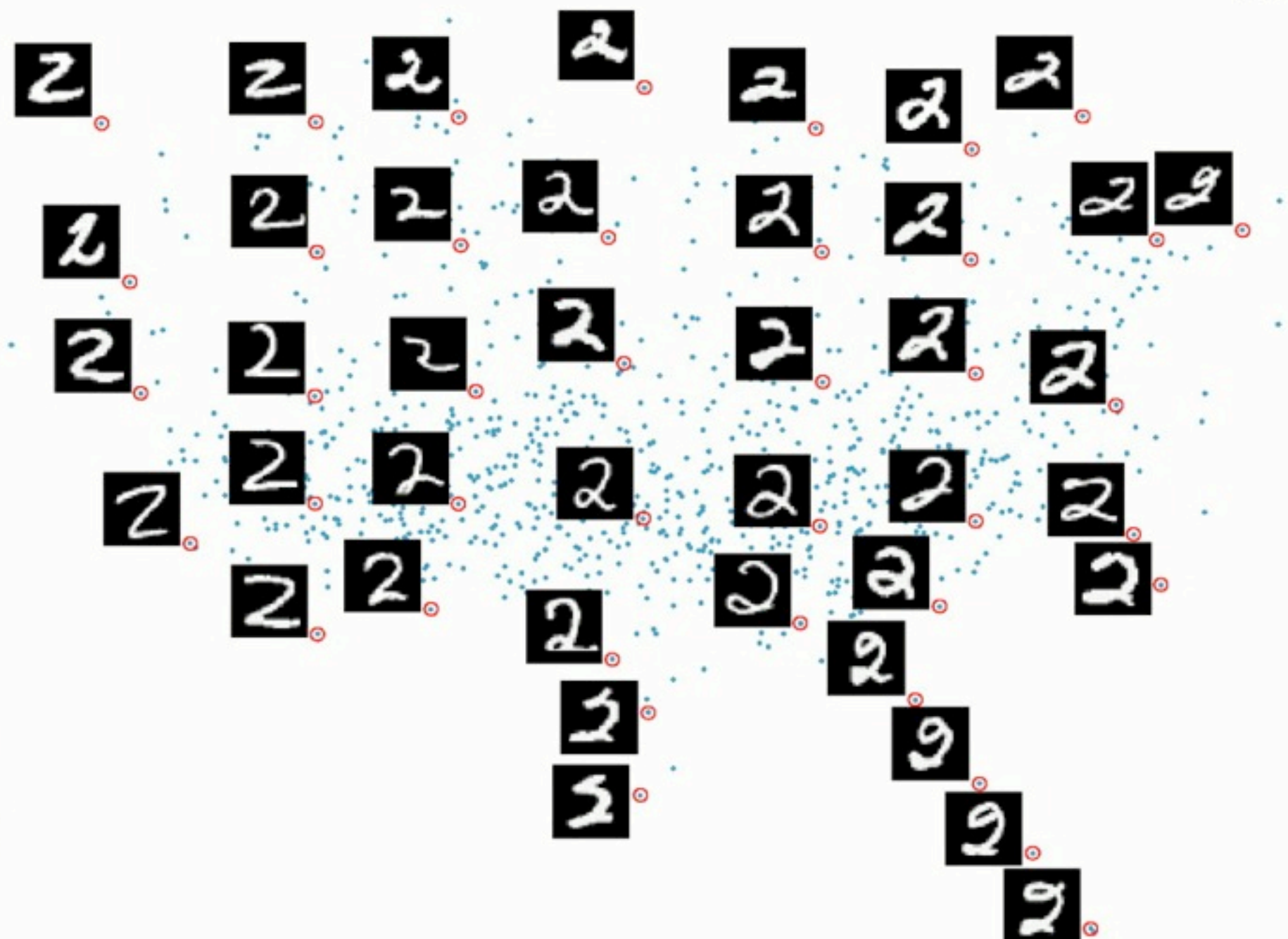


Wrist rotation

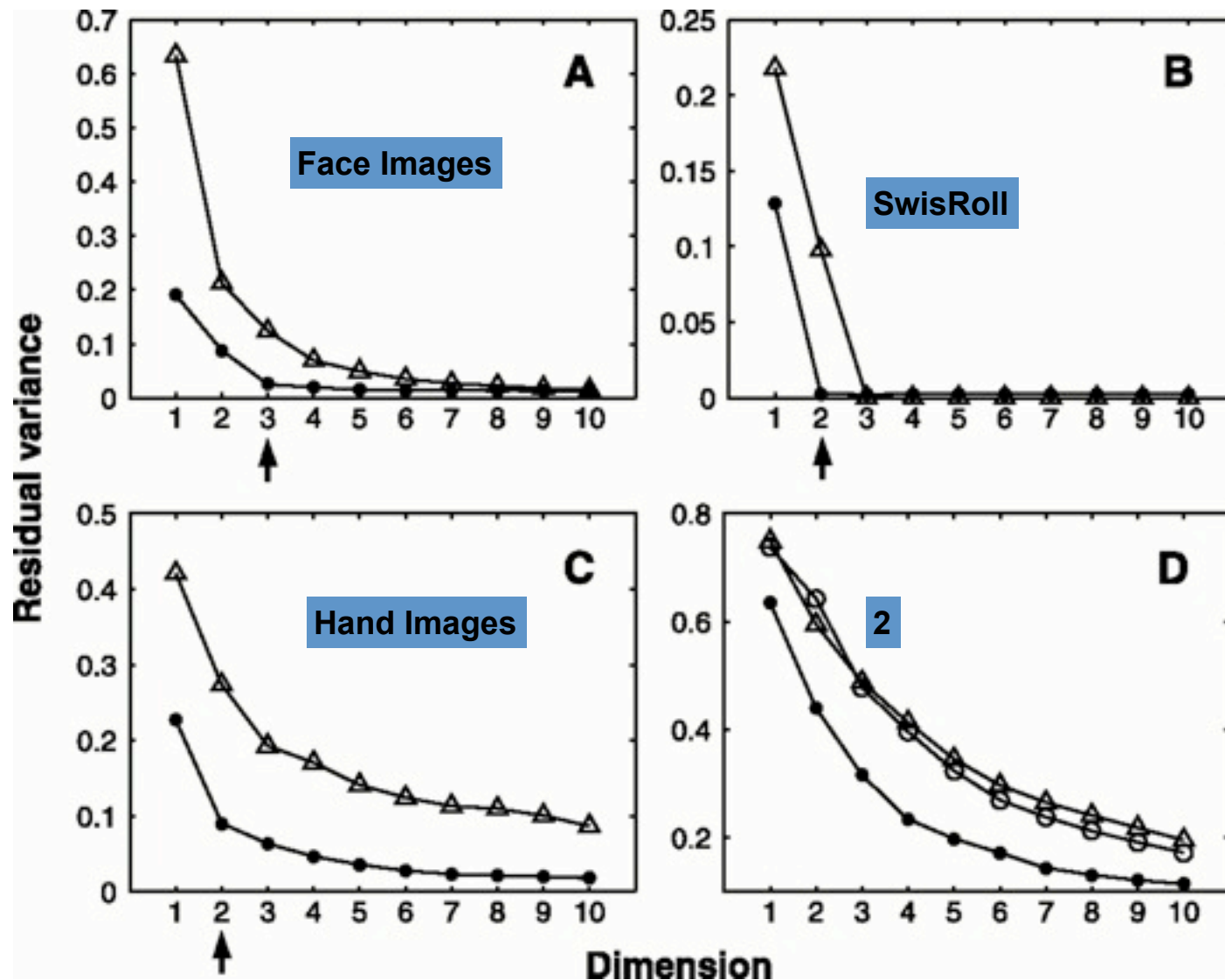
B

Bottom loop articulation →

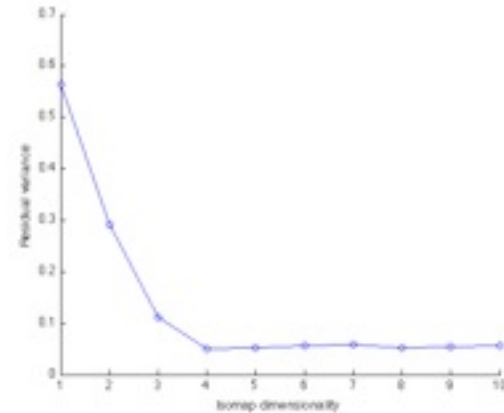
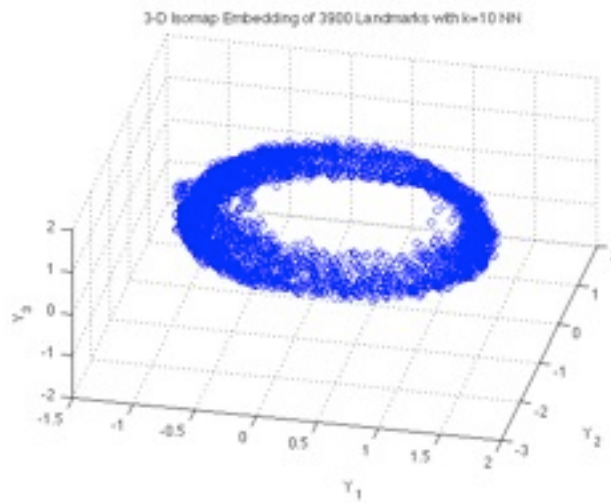
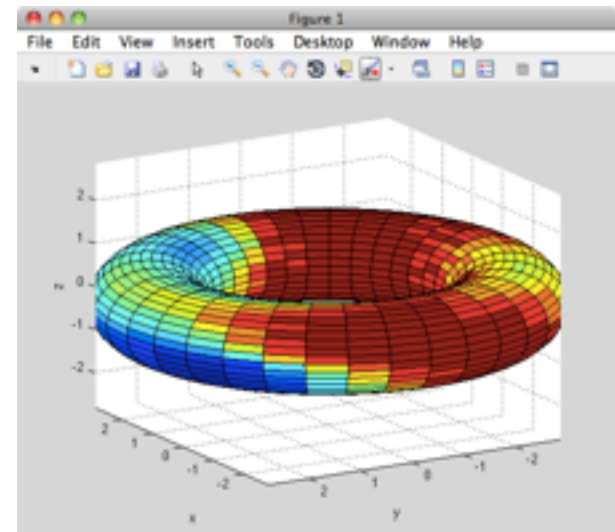
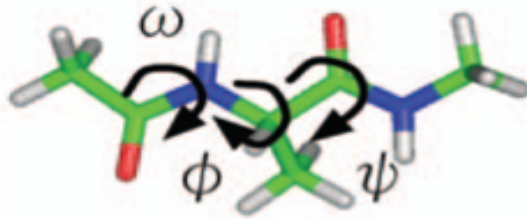
Top arch articulation ↓



Residual Variance vs. Intrinsic Dimension



ISOMAP on Alanine-dipeptide



ISOMAP 3D embedding with RMSD metric on 3900 Kcenters

Convergence of ISOMAP

- ISOMAP has provable convergence guarantees;
- Given that $\{x_i\}$ is sampled sufficiently dense, graph shortest path distance will approximate closely the original geodesic distance as measured in manifold M ;
- But ISOMAP may suffer from nonconvexity such as holes on manifolds

Two step approximations

- Convergence proof hinges on the idea that we can approximate geodesic distance in M by short Euclidean distance hops.

Let's define the following for two points $x, y \in M$:

$$d_M(x, y) = \inf_{\gamma} \{length(\gamma)\}$$

$$d_G(x, y) = \min_P (\|x_0 - x_1\| + \dots + \|x_{p-1} - x_p\|)$$

$$d_S(x, y) = \min_P (d_M(x_0, x_1) + \dots + d_M(x_{p-1}, x_p))$$

where γ varies over the set of smooth arcs connecting x to y in M and P varies over all paths along the edges of G starting at data point $x = x_0$ and ending at $y = x_p$.

- We will show $d_M \approx d_S$ and $d_S \approx d_G$, which will imply the desired result that $d_G \approx d_M$.

Main Theorem

[Bernstein, de Silva, Langford, and

Theorem 1: Let M be a compact submanifold of \mathbf{R}^n and let $\{x_i\}$ be a finite set of data points in M . We are given a graph G on $\{x_i\}$ and positive real numbers $\lambda_1, \lambda_2 < 1$ and $\delta, \epsilon > 0$. Suppose:

1. G contains all edges (x_i, x_j) of length $\|x_i - x_j\| \leq \epsilon$.
2. The data set $\{x_i\}$ satisfies a δ -sampling condition – for every point $m \in M$ there exists an x_i such that $d_M(m, x_i) < \delta$.
3. M is *geodesically convex* – the shortest curve joining any two points on the surface is a geodesic curve.
4. $\epsilon < (2/\pi)r_0\sqrt{24\lambda_1}$, where r_0 is the *minimum radius of curvature of M* – $\frac{1}{r_0} = \max_{\gamma, t} \|\gamma''(t)\|$ where γ varies over all unit-speed geodesics in M .
5. $\epsilon < s_0$, where s_0 is the *minimum branch separation of M* – the largest positive number for which $\|x - y\| < s_0$ implies $d_M(x, y) \leq \pi r_0$.
6. $\delta < \lambda_2\epsilon/4$.

Then the following is valid for all $x, y \in M$,

$$(1 - \lambda_1)d_M(x, y) \leq d_G(x, y) \leq (1 + \lambda_2)d_M(x, y)$$

Probabilistic Result

- ▶ So, short Euclidean distance hops along G approximate well actual geodesic distance as measured in M .
- ▶ What were the main assumptions we made? The biggest one was the δ -sampling density condition.
- ▶ A probabilistic version of the Main Theorem can be shown where each point x_i is drawn from a density function. Then the approximation bounds will hold with high probability. Here's a truncated version of what the theorem looks like now:

Asymptotic Convergence Theorem: Given $\lambda_1, \lambda_2, \mu > 0$ then for density function α sufficiently large:

$$1 - \lambda_1 \leq \frac{d_G(x, y)}{d_M(x, y)} \leq 1 + \lambda_2$$

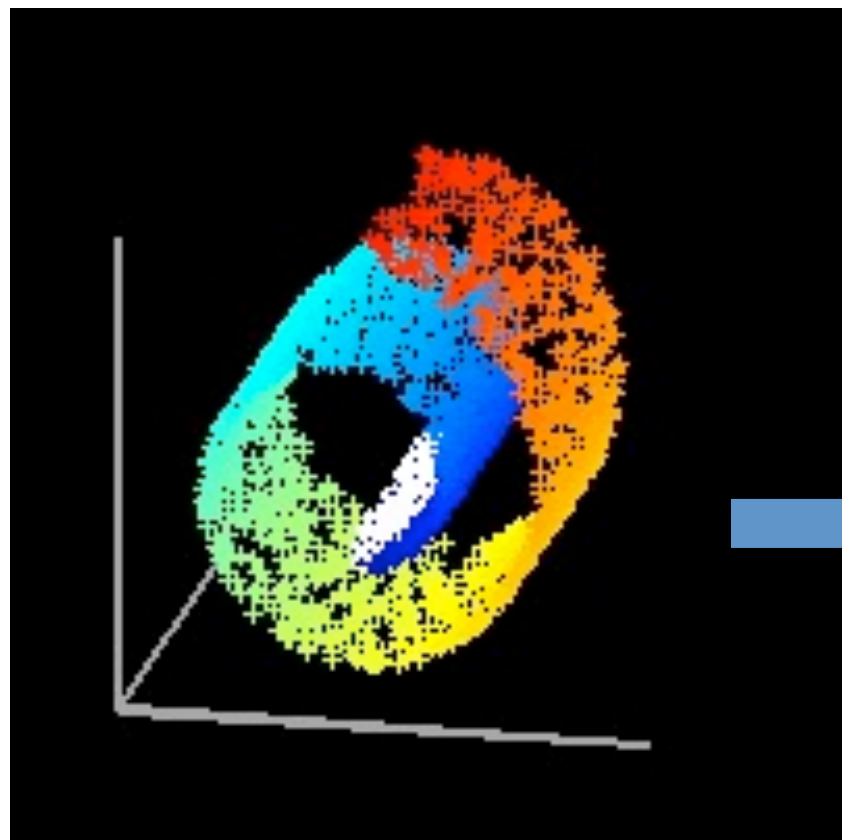
will hold with probability at least $1 - \mu$ for any two data points x, y .

A Shortcoming of ISOMAP

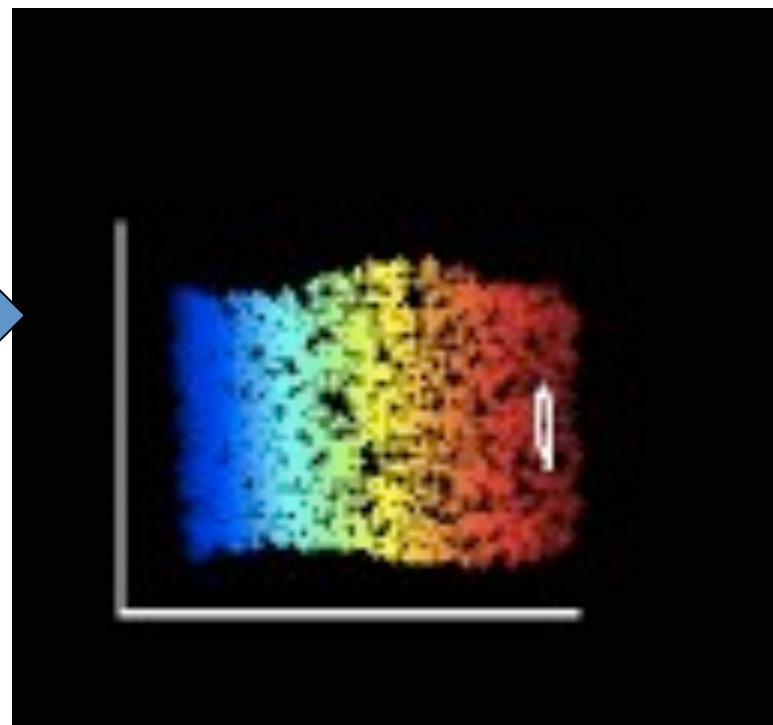
- One need to compute pairwise shortest path between **all** sample pairs (i,j)
 - Global
 - Non-sparse
 - Cubic complexity $O(N^3)$

Locally Linear Embedding

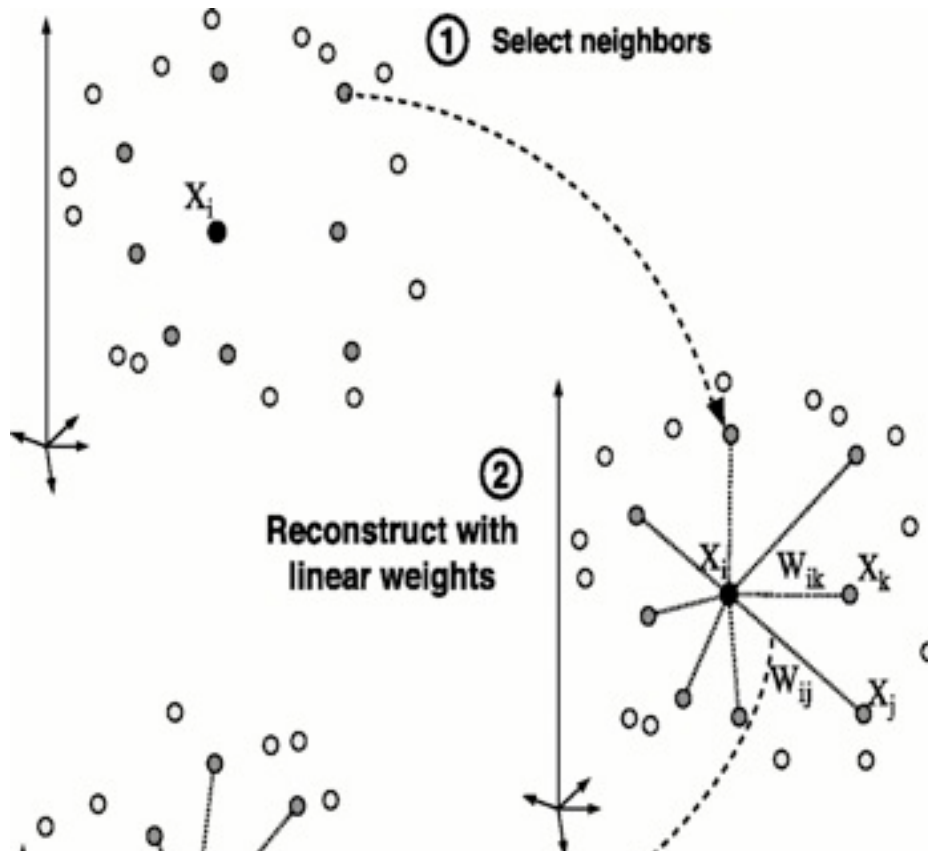
manifold is a topological space which is locally Euclidean."



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 are chosen to minimize the reconstruction Error.

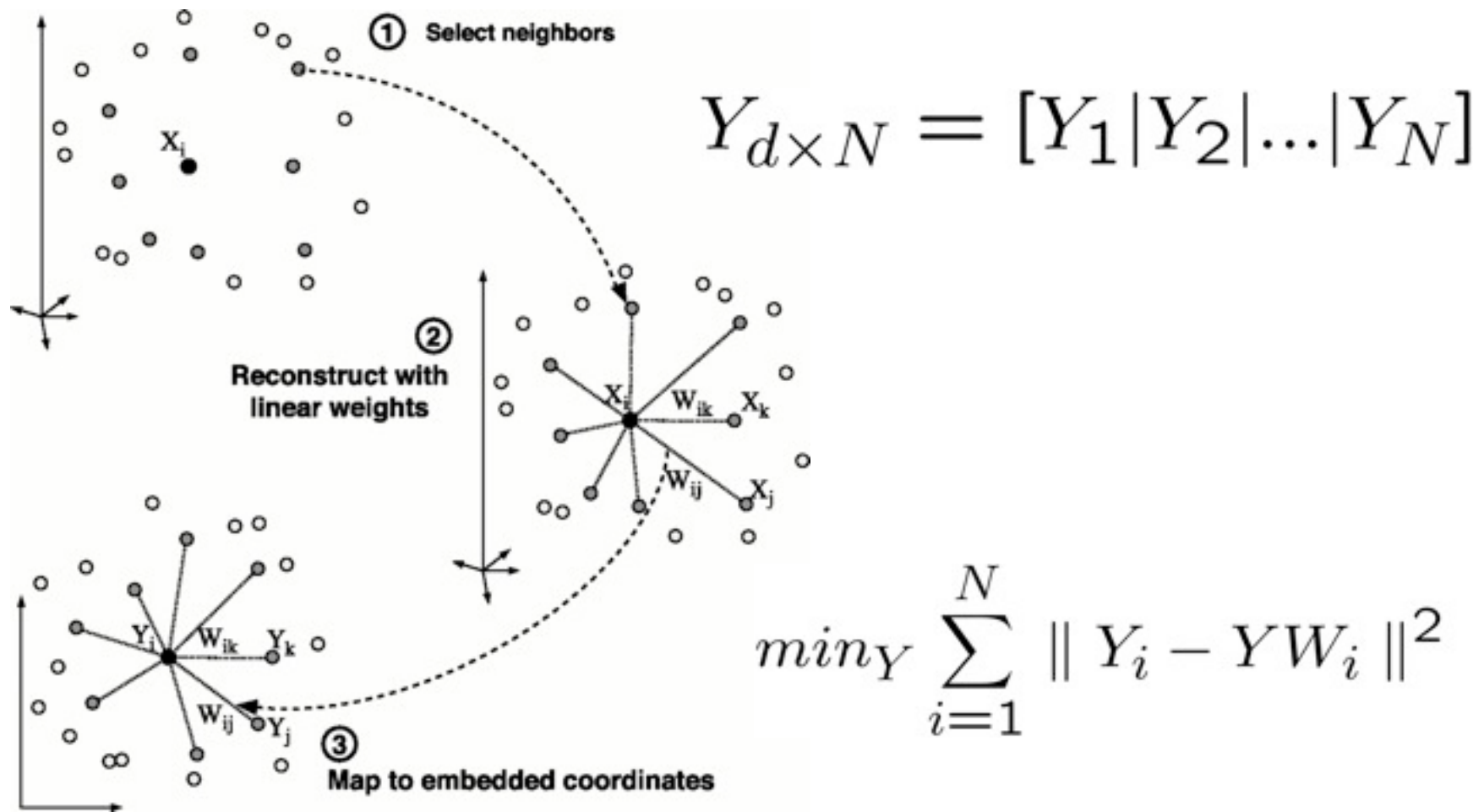
$$\min_W \| X_i - \sum_{j=1}^K W_{ij} X_j \|^2 \quad (1)$$

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...



LLE Algorithm (I)

(1) Construct a neighborhood graph

(2) Local fitting:

Pick up a point x_i and its neighbors \mathbb{N}_i

Compute the local fitting weights

$$\min_{\sum_{j \in \mathbb{N}_i} w_{ij} = 1} \|x_i - \sum_{j \in \mathbb{N}_i} w_{ij}(x_j - x_i)\|^2.$$

This can be done by Lagrange multiplier method, *i.e.* solving

$$\min_{w_{ij}} \frac{1}{2} \|x_i - \sum_{j \in \mathbb{N}_i} w_{ij}(x_j - x_i)\|^2 + \lambda(1 - \sum_{j \in \mathbb{N}_i} w_{ij}).$$

Let $w_i = [w_{ij_1}, \dots, w_{ij_k}]^T \in \mathbb{R}^k$, $\bar{X}_i = [x_{j_1} - x_i, \dots, x_{j_k} - x_i]$, and the local Gram (covariance) matrix $C_{jk}^{(i)} = \langle x_j - x_i, x_k - x_i \rangle$, whence the weights are

$$w_i = C_i^\dagger (\bar{X}_i^T x_i + \lambda \mathbf{1}),$$

where the Lagrange multiplier equals to

$$\lambda = \frac{1}{\mathbf{1}^T C_i^\dagger \mathbf{1}} \left(1 - \mathbf{1}^T C_i^\dagger \bar{X}_i^T x_i \right),$$

and C_i^\dagger is a Moore-Penrose (pseudo) inverse of C_i . Note that C_i is often ill-conditioned and to find its Moore-Penrose inverse one can use regularization method $(C_i + \mu I)^{-1}$ for some $\mu > 0$.

LLE Algorithm (II)

(3) Global alignment

Define a n -by- n weight matrix W :

$$W_{ij} = \begin{cases} w_{ij}, & j \in \mathcal{N}_i \\ 0, & otherwise \end{cases}$$

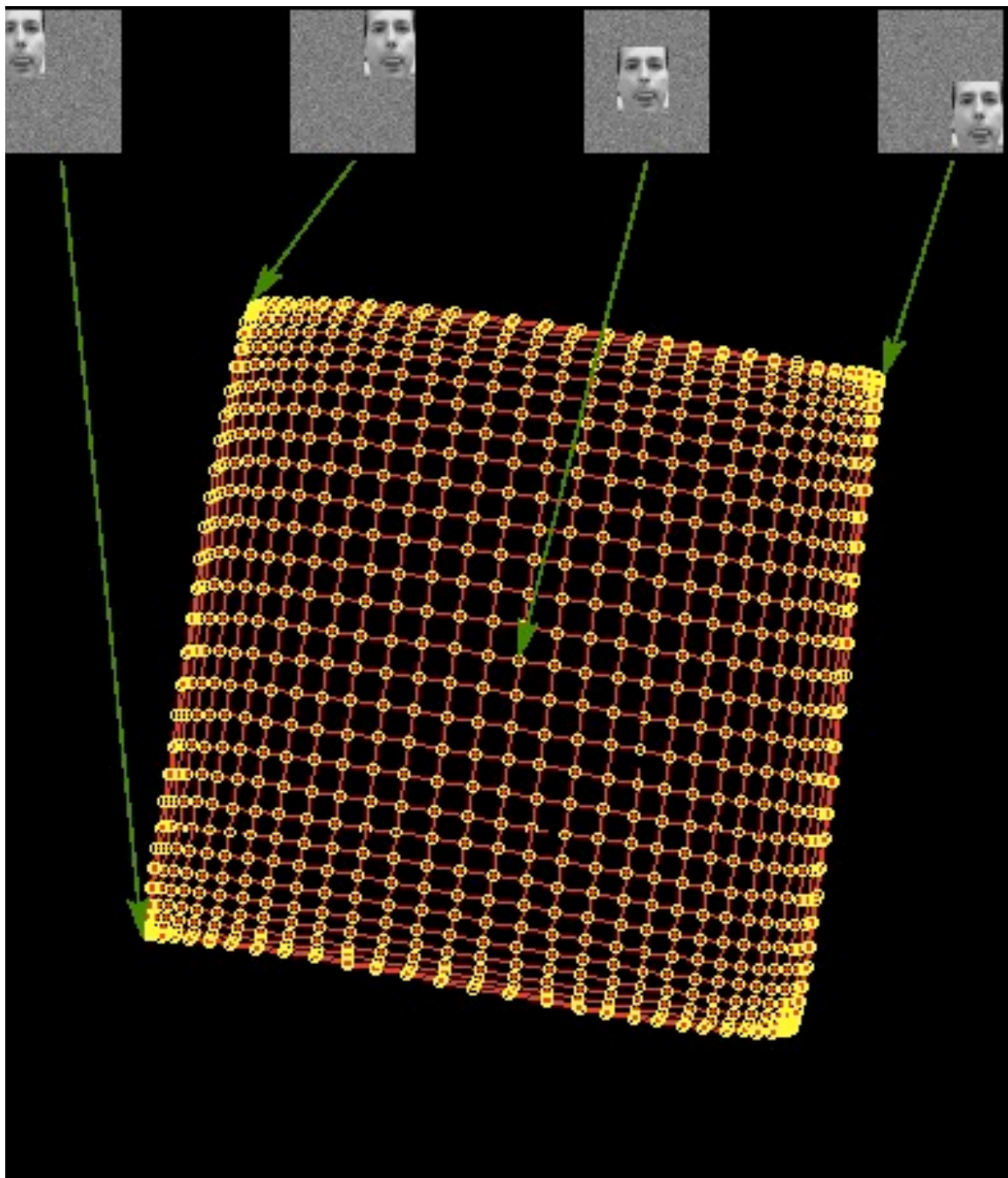
Compute the global embedding d -by- n embedding matrix Y ,

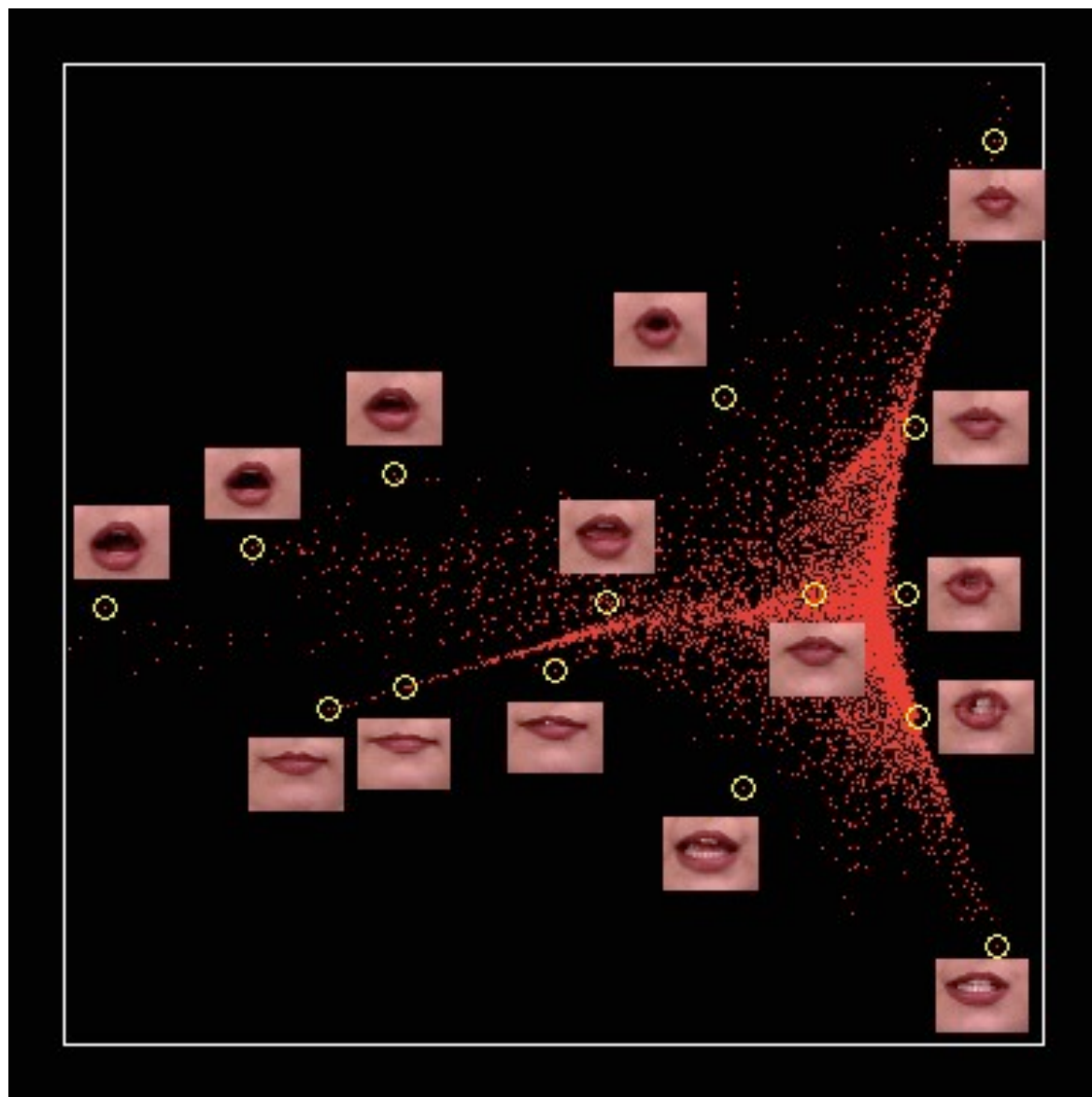
$$\min_Y \sum_i \|y_i - \sum_{j=1}^n W_{ij} y_j\|^2 = \text{trace}(Y(I - W)^T(I - W)Y^T)$$

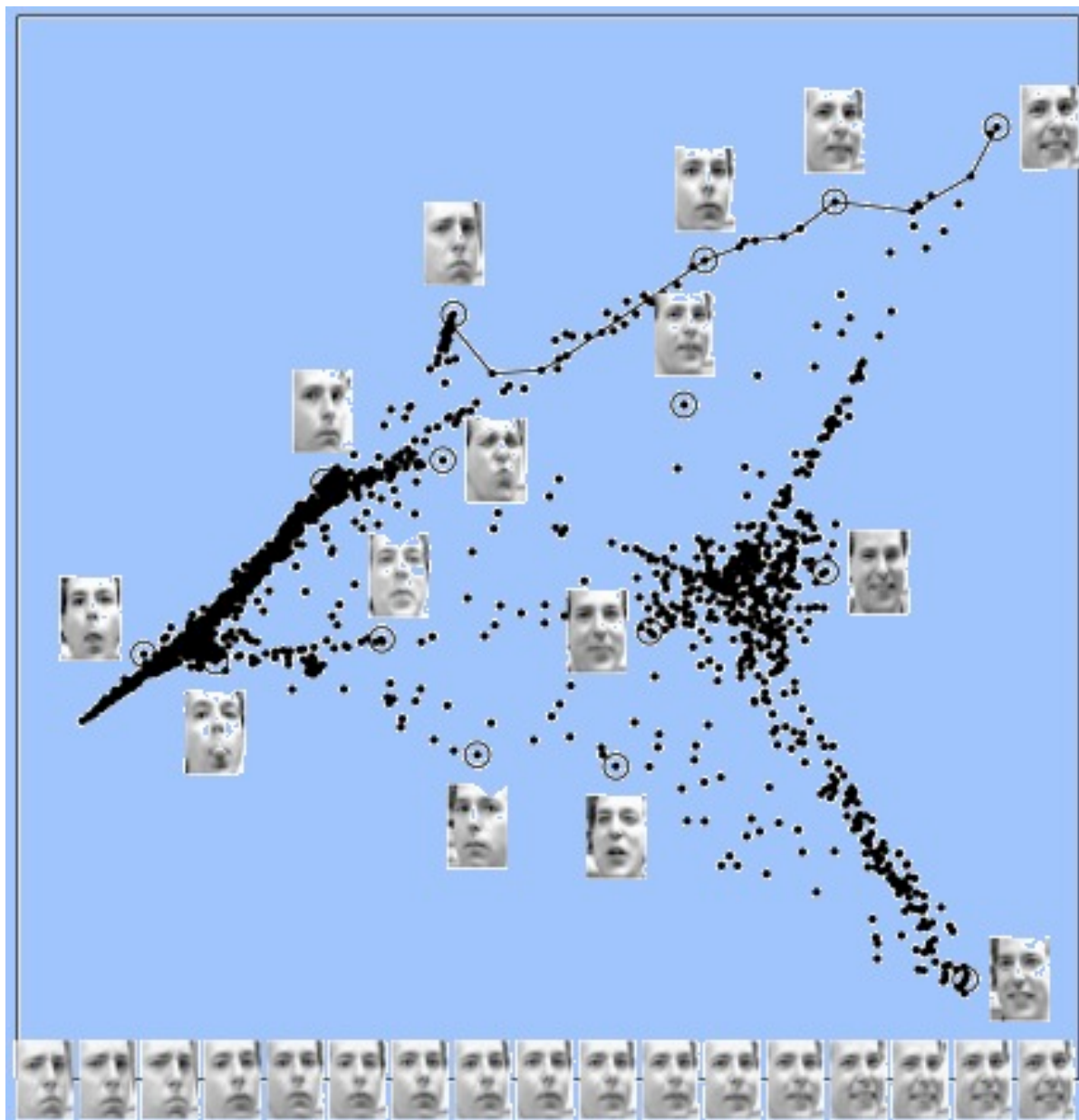
In other words, construct a positive semi-definite matrix $B = (I - W)^T(I - W)$ and find $d+1$ smallest eigenvectors of B , v_0, v_1, \dots, v_d associated smallest eigenvalues $\lambda_0, \dots, \lambda_d$. Drop the smallest eigenvector which is the constant vector explaining the degree of freedom as translation and set $Y = [v_1/\sqrt{\lambda_1}, \dots, v_d/\sqrt{\lambda_d}]^T$.

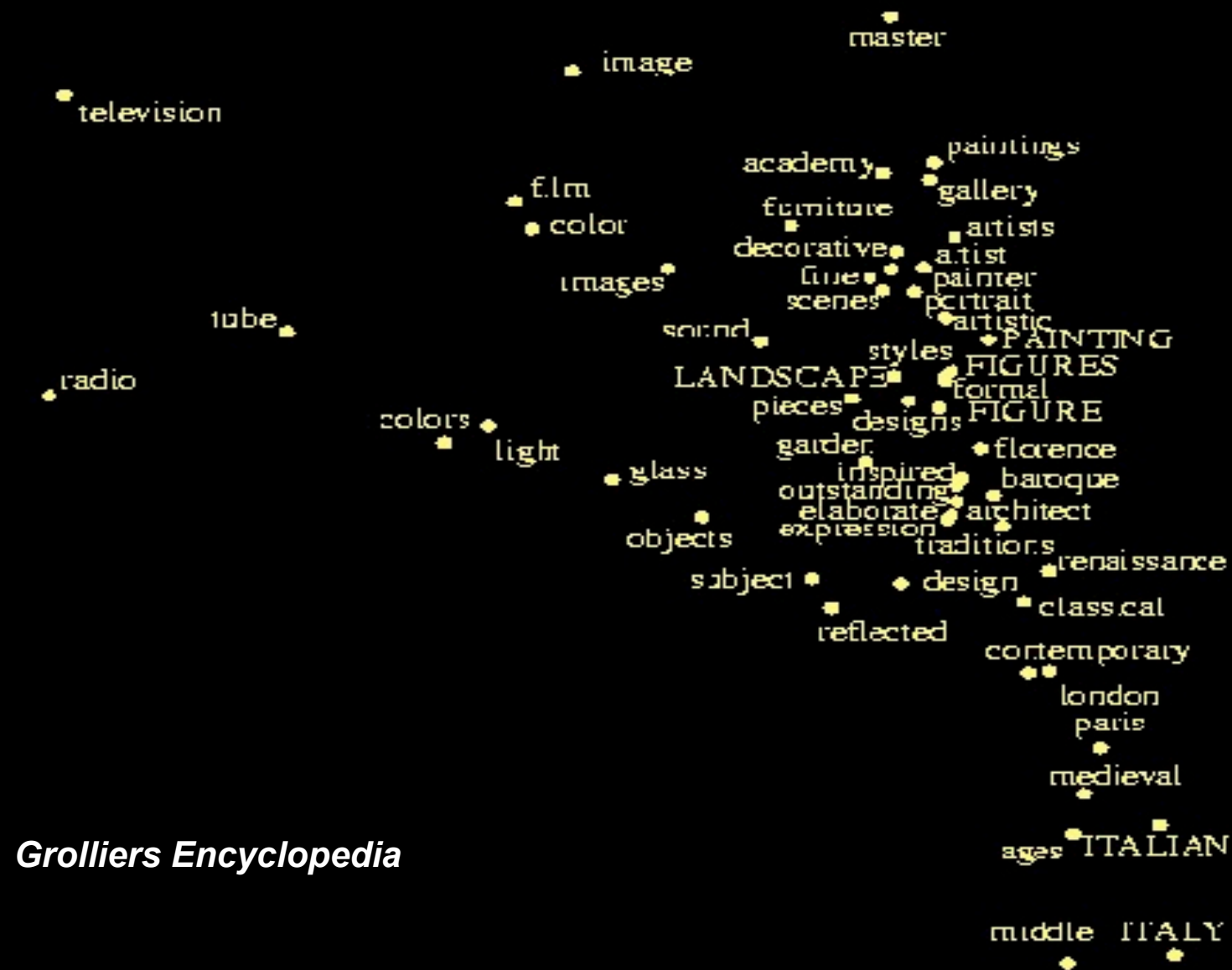
Remarks on LLE

- Searching k-nearest neighbors is of $O(kN)$
- W is **sparse**, $kN/N^2 = k/N$ nonzeros
- W might be **negative**, additional nonnegative constraint can be imposed
- $B = (I - W)^T(I - W)$ is **positive semi-definite** (p.s.d.)
- **Open Problem**: exact reconstruction condition?









Groliers Encyclopedia

Landmark ISOMAP: Nystrom Extension Method

- ▶ ISOMAP out of the box is not scalable. Two bottlenecks:
 - ▶ All pairs shortest path - $O(kN^2 \log N)$.
 - ▶ MDS eigenvalue calculation on a full $N \times N$ matrix - $O(N^3)$.
 - ▶ For contrast, LLE is limited by a sparse eigenvalue computation - $O(dN^2)$.
- ▶ Landmark ISOMAP (L-ISOMAP) Idea:
 - ▶ Use $n \ll N$ *landmark* points from $\{x_i\}$ and compute a $n \times N$ matrix of geodesic distances, D_n , from each data point to the landmark points only.
 - ▶ Use new procedure Landmark-MDS (LMDS) to find a Euclidean embedding of all the data – utilizes idea of triangulation similar to GPS.
- ▶ Savings: L-ISOMAP will have shortest paths calculation of $O(knN \log N)$ and LMDS eigenvalue problem of $O(n^2 N)$.

Landmark Choice

- Random
- MiniMax: k-center
- Hierarchical landmarks: cover-tree
- Nyström extension method

Summary..

ISOMAP	LLE
Do MDS on the geodesic distance matrix.	Model local neighborhoods as linear patches and then embed in a lower dimensional manifold.
Global approach $O(N^3)$, but L-ISOMAP)	Local approach $O(N^2)$
Might not work for nonconvex manifolds with holes	Nonconvex manifolds with holes
Extensions: Landmark, Conformal & Isometric ISOMAP	Extensions: Hessian LLE, Laplacian Eigenmaps etc.

Both needs manifold finely sampled.

Reference

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Acknowledgement

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