

Lecture 8:

Manifold learning (2)

- 1. Laplacian Eigenmaps**
- 2. Log map / Riemannian manifold learning**

Dimensionality Reduction as Sample Embedding problem:

Given an input dataset $\mathbf{X}_n = \{X_1, X_2, \dots, X_n\} \subset \mathbb{R}^p$, find an ' n -point' Embedding mapping

$$h_{(n)}: \mathbf{X}_n \rightarrow \mathbf{Y}_n = h_{(n)}(\mathbf{X}_n) = \{y_1, y_2, \dots, y_n\} \subset \mathbb{R}^q,$$

such that the resulting q -dimensional dataset \mathbf{Y}_n , $q < p$, ***faithfully represents*** the sample \mathbf{X}_n

Embedding: original high-dimensional inputs $\mathbf{X}_n \rightarrow$ low-dimensional features $\mathbf{Y}_n = \{y_1, y_2, \dots, y_n\}$

Laplacian Eigenmaps (LEM)

(Belkin, Niyogi: Laplacian Eigenmaps for Dimensionality Reduction and Data Representation, 2003)

Graph-based algorithms: have 3 basic steps.

1. Find sample points from small neighborhoods of all sample points (ε -ball)

2(a). Constructing the Adjacency graph $\Gamma(\mathbf{X}_n)$ describing local properties of the Data manifold:

- the sample points $\{\mathbf{X}_i\}$ are nodes
- the edges $\mathbf{E} = \{E_{ij}\}$: E_{ij} connect the nodes \mathbf{X}_i and \mathbf{X}_j if and only if $|\mathbf{X}_i - \mathbf{X}_j| < \varepsilon$

2(b). Setting the weights to the Adjacency graph: edge $(\mathbf{X}_i, \mathbf{X}_j) \rightarrow$ weight $\exp\left\{-\frac{1}{t}|\mathbf{X}_i - \mathbf{X}_j|^2\right\}$, $t > 0$

$W = \|W_{ij}\|$ - $n \times n$ weighted adjacent matrix (uses 'heat-transfer' kernel):

- $W_{ij} = \exp \left\{ -\frac{1}{t} |X_i - X_j|^2 \right\}$, if the nodes X_i and X_j are connected ($W_{ij} = 1$ when $t = \infty$)
- $W_{ij} = 0$, otherwise

Weighted adjacency graph $\Gamma(\mathbf{X}_n) = (\mathbf{X}_n, \mathbf{E})$ / weighted matrix W reflect the intrinsic geometric structure of the Data manifold – 'Data manifold is approximated by the adjacency graph'

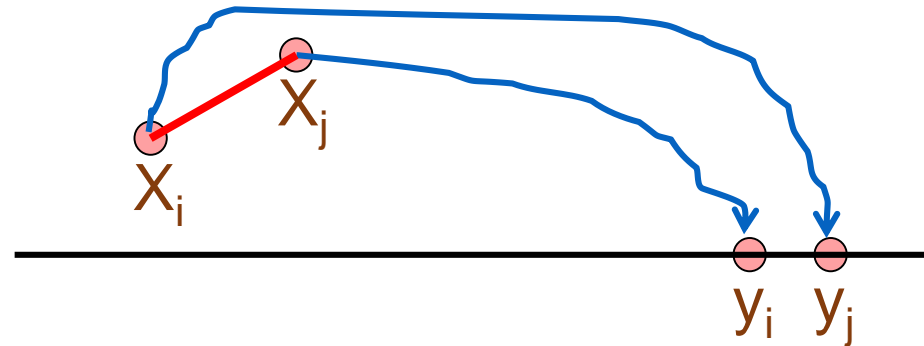
3. Find a global embedding that preserves the local properties:

- choosing a cost function $L(\mathbf{Y}_n) = \sum_{i,j=1}^n W_{ij} \times \|y_i - y_j\|^2$
- minimization of chosen cost function $L(\mathbf{Y}_n)$ over q -dimensional features $\{y_1, y_2, \dots, y_n\}$

$$\text{Cost function } L(\mathbf{Y}_n) = \sum_{i,j=1}^n W_{ij} \times \|y_i - y_j\|^2$$

Features $\{y_1, y_2, \dots, y_n\}$: the images (y_i, y_j) of connected nodes (X_i, X_j) in the weighted graph $\Gamma(\mathbf{X}_n)$ should stay as close together as possible

Example: $q = 1$



Constraints:

- 1) features $\{y_1, y_2, \dots, y_n\}$ may be determined up to a shift: require for definiteness: $\sum_{i=1}^n y_i = 0$
- 2) features $\{y_1, y_2, \dots, y_n\}$ may be determined up to a scale: to avoid trivial degenerate solution, require

$$\sum_{i=1}^n (y_i \times W_i \times y_i^T) = I_q$$

using the weights $W_i = \sum_{j=1}^n W_{ij}$, $i = 1, 2, \dots, n$

This constraint removes an arbitrary scaling factor in the features

Optimization problem: $L(\mathbf{Y}_n) = \sum_{i,j=1}^n W_{ij} \times \|y_i - y_j\|^2 \rightarrow \min$

under constraints: $\sum_{i=1}^n y_i = 0$ and $\sum_{i=1}^n (y_i \times W_i \times y_i^T) = I_q$

$$\begin{aligned}
 L(\mathbf{Y}_n) &= \sum_{i,j=1}^n W_{ij} \times \|y_i - y_j\|^2 = \sum_{i,j=1}^n W_{ij} \times (y_i - y_j)^T \times (y_i - y_j) \\
 &= \sum_{i,j=1}^n W_{ij} \times \{y_i^T \times y_i + y_j^T \times y_j - 2y_i^T \times y_j\} \\
 &= 2 \times \left\{ \sum_{i=1}^n W_i \times (y_i^T \times y_i) - \sum_{i,j=1}^n W_{ij} \times (y_i^T \times y_j) \right\}
 \end{aligned}$$

\mathbf{Y} - $n \times q$ matrix with rows $y_1^T, y_2^T, \dots, y_n^T$

$W = \|W_{ij}\|$ - $n \times n$ **weighted adjacent matrix** $\rightarrow D = \text{Diag}(W_1, W_2, \dots, W_n)$ - $n \times n$ **degree matrix**

$$\sum_{i=1}^n W_i \times (y_i^T \times y_i) - \sum_{i,j=1}^n W_{ij} \times (y_i^T \times y_j) = \text{Tr}(\mathbf{Y}^T \times \mathbf{D} \times \mathbf{Y}) - \text{Tr}(\mathbf{Y}^T \times \mathbf{W} \times \mathbf{Y})$$

$$= \text{Tr}(\mathbf{Y}^T \times \mathbf{L} \times \mathbf{Y}) \quad \mathbf{L} = \mathbf{D} - \mathbf{W} \text{ - } n \times n \text{ **Laplacian matrix**}$$

$$\sum_{i=1}^n y_i = 0 \quad \rightarrow \quad \mathbf{Y}^T \times \mathbf{1}_n = 0 \quad \sum_{i=1}^n (y_i \times W_i \times y_i^T) = I_q \quad \rightarrow \quad \mathbf{Y}^T \times \mathbf{D} \times \mathbf{Y} = I_q$$

Optimization problem: $\text{Tr}(\mathbf{Y}^T \times \mathbf{L} \times \mathbf{Y}) \rightarrow \min$

under constraints: $\mathbf{Y}^T \times \mathbf{1}_n = 0$ and $\mathbf{Y}^T \times \mathbf{D} \times \mathbf{Y} = I_q$

Optimization problem: $\text{Tr}(\mathbf{Y}^T \times \mathbf{L} \times \mathbf{Y}) \rightarrow \min$ under constraint $\mathbf{Y}^T \times \mathbf{D} \times \mathbf{Y} = \mathbf{I}_q$

This problem reduces to finding the ‘minimum eigenvalue solution’ to generalized eigenvalue problem:

$$\mathbf{L}\mathbf{Y} = \lambda\mathbf{D}\mathbf{Y}$$

$(q+1)$ smallest eigenvalues:

$$0 = \lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_q$$

corresponding orthonormal eigenvectors:

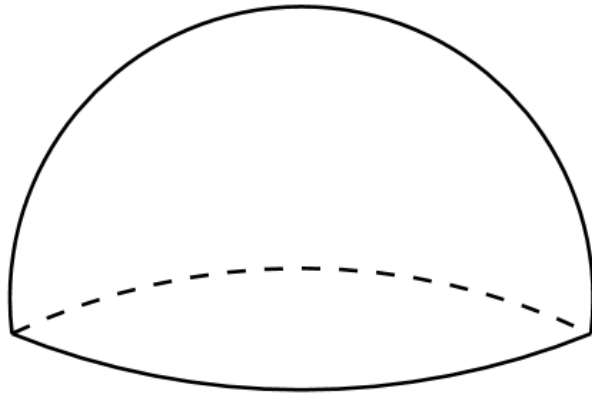
$$\mathbf{Y}_0, \mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_q \in \mathbb{R}^n$$

the eigenvalue $\lambda_0 = 0$ corresponds to the vector $\mathbf{1}_n$ and should be discarded due constraint $\mathbf{Y}^T \times \mathbf{1}_n = 0$

- the eigenvectors $\mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_q \in \mathbb{R}^n$ are taken as columns of desired $n \times q$ matrix \mathbf{Y}
- the columns $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n \in \mathbb{R}^q$ of \mathbf{Y}^T are taken as desired low-dimensional features

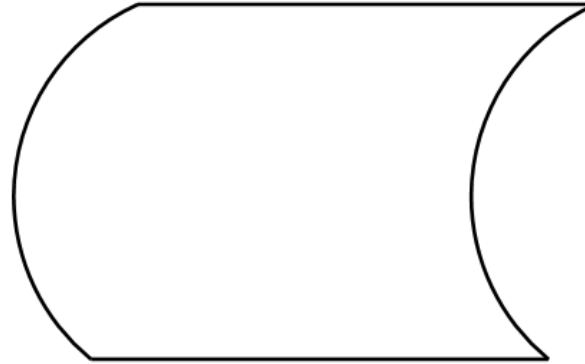
ISOMAP provides a isometric embedding that preserves global geodesic distances

But it works only when **the surface can flatten**



cannot flatten

nonzero curvature



can flatten

zero curvature

No accurate map of Earth exists – Gauss's theorem.

Laplacian eigenmaps tries to preserve the geometric characteristics of the Data manifold
by preserving 'locality properties'

Math: Laplacian Eigenmaps justification – why Laplacian?

$\mathbf{M} \subset \mathbb{R}^p$ – unknown Data manifold

$\mathbf{X}_n = \{X_1, X_2, \dots, X_n\} \subset \mathbf{M}$ – training dataset (sample)

$h: \mathbf{M} \rightarrow \mathbb{R}^q$ - desired Embedding mapping

$\mathbf{X}_n \rightarrow \mathbf{Y}_n = h(\mathbf{X}_n) = \{y_1, y_2, \dots, y_n\} \subset \mathbb{R}^q$ – desired resulting q -dimensional dataset

$$L(\mathbf{Y}_n) = \sum_{i,j=1}^n W_{ij} \times \|y_i - y_j\|^2 = \sum_{i,j=1}^n W_{ij} \times \|h(X_i) - h(X_j)\|^2 = F_n(h) \text{ - functional}$$

Constraint: $D_n(h) = \sum_{i=1}^n (h(X_i) \times W_i \times h^T(X_i)) = I_q$

Let $q = 1$, $\nabla h(X) = \begin{pmatrix} \frac{\partial h}{\partial X_1} \\ \cdots \\ \frac{\partial h}{\partial X_p} \end{pmatrix} \in \mathbb{R}^p$ – gradient $\nabla_{\mathbf{M}} h(X)$ – covariant differentiation is used

$X', X \in \mathbf{M}$ – near points: $h(X') - h(X) = (\nabla_{\mathbf{M}} h(X), X' - X) + o(X' - X)$ - Taylor expansion

$|h(X') - h(X)| \leq |\nabla_{\mathbf{M}} h(X)| \times |X' - X| + o(|X' - X|)$ -

$|\nabla_{\mathbf{M}} h(X)|$ provides us with an estimate of how far apart h maps nearby points.

We look a mapping h that ‘best preserves locality on average’ – minimizes functional

$$F(h) = \int_{\mathbf{M}} |\nabla_{\mathbf{M}} h(X)|^2 \text{mes}(dX)$$

under scale constraint $\|h\|^2 = \int_{\mathbf{M}} |h(X)|^2 \text{mes}(dX) = 1$ to avoid trivial degenerate solution

$$F(h) = \int_{\mathbf{M}} |\nabla_{\mathbf{M}} h(X)|^2 \text{mes}(dX) \approx F_n(h) = \sum_{i,j=1}^n W_{ij} \times \|h(X_i) - h(X_j)\|^2$$

Minimizing $F(h)$ over h defined on the Data manifold \mathbf{M} corresponds to minimizing $F_n(h)$ over $h_{(n)}$ defined on nodes of the graph $\Gamma(\mathbf{X}_n)$

$$\text{Constraint: } \|h\|^2 = \int_{\mathbf{M}} |h(X)|^2 \text{mes}(dX) = 1 \sim D_n(h) = \sum_{i=1}^n (h(X_i) \times (\sum_{j=1}^n W_{ij}) \times h^T(X_i)) = 1$$

- minimization is doing under similar constraints

Stokes theorem: $F(h) = \int_{\mathbf{M}} |\nabla_{\mathbf{M}} h(X)|^2 \text{mes}(dX) = \int_{\mathbf{M}} (h \times \Delta_{\mathbf{M}} h)(X) \text{mes}(dX)$

$\Delta_{\mathbf{M}}(h): h(X) \rightarrow -\text{div}(\nabla_{\mathbf{M}} h(X)) = -\sum_{k=1}^p \frac{\partial^2 h(X)}{\partial X_k^2}$ Laplace operator, if $X \in \mathbb{R}^p$

Laplace-Beltrami operator L_{LB} , if $X \in \mathbf{M}$

$$\int_{\mathbf{M}} (h \times \Delta_{\mathbf{M}} h)(X) \text{mes}(dX) \approx \sum_{i,j=1}^n W_{ij} \times \|h(X_i) - h(X_j)\|^2 = (h(\mathbf{X}_n), L \times h(\mathbf{X}_n)) \quad \mathbf{Y} = h(\mathbf{X}_n)$$

Matrix L - sampling analogous of the Laplace-Beltrami operator – called Laplacian of a graph $\Gamma(\mathbf{X}_n)$

Laplace-Beltrami operator $\Delta_{\mathbf{M}}$: there exists eigensystem $\{f_i(X), i = 0, 1, \dots\}$ consisting of orthonormal eigenfunctions:

$$\Delta_{\mathbf{M}}f_i = \lambda_i \times f_i, \qquad (f_i(X), f_j(X)) = \delta_{ij} \qquad \|f_i\|^2 = \int_{\mathbf{M}} |f_i(X)|^2 \text{mes}(dX) = 1$$

corresponding to eigenvalues $0 = \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \dots$ f_0 - const

The eigenfunctions have properties desirable for embedding

The rows of best Embedding mapping

$$h(X) = \begin{pmatrix} h_1(X) \\ \cdots \\ h_q(X) \end{pmatrix}: X \in \mathbf{M} \rightarrow y = h(X) \in \mathbb{R}^q$$

consists of the eigenvectors $\{f_1(X), f_2(X), \dots, f_q(X)\}$ corresponding smallest eigenvalues $\lambda_1 \leq \dots \leq \lambda_q$

Locally Linear Embedding (LLE): sampling analogous of continuous eigenfunction problem for the squared Laplace-Beltrami operator L_{LB}^2

- has the same eigenfunctions as L_{LB}
- finds the same 'best' embedding

Intrinsic dimension estimation:

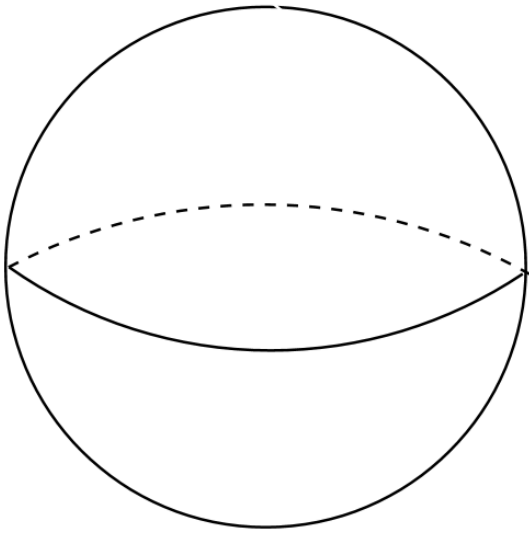
$\lambda_1 \leq \lambda_2 \leq \dots$ - eigenvalues. Then exists the constants A and B :

$$A + \frac{2}{q} \times \log(j) \leq \log(\lambda_j) \leq B + \frac{2}{q} \times \log(j + 1)$$

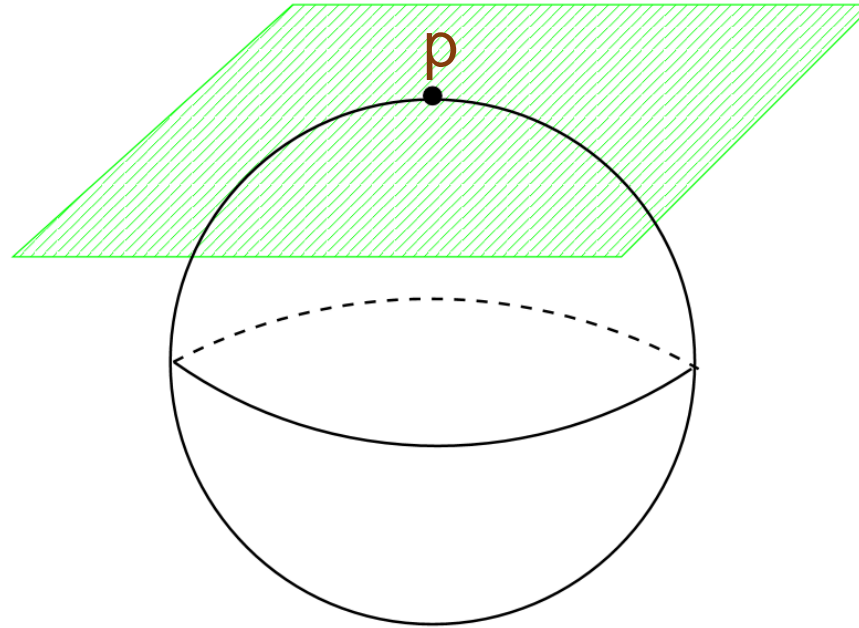
Riemannian manifold learning (RML) – Riemannian Normal Coordinates (RNC)

(Brun et al. Fast Manifold Learning Based on Riemannian Normal Coordinates, 2005;
Lin et al. Riemannian Manifold Learning for Nonlinear dimensionality reduction, 2006)

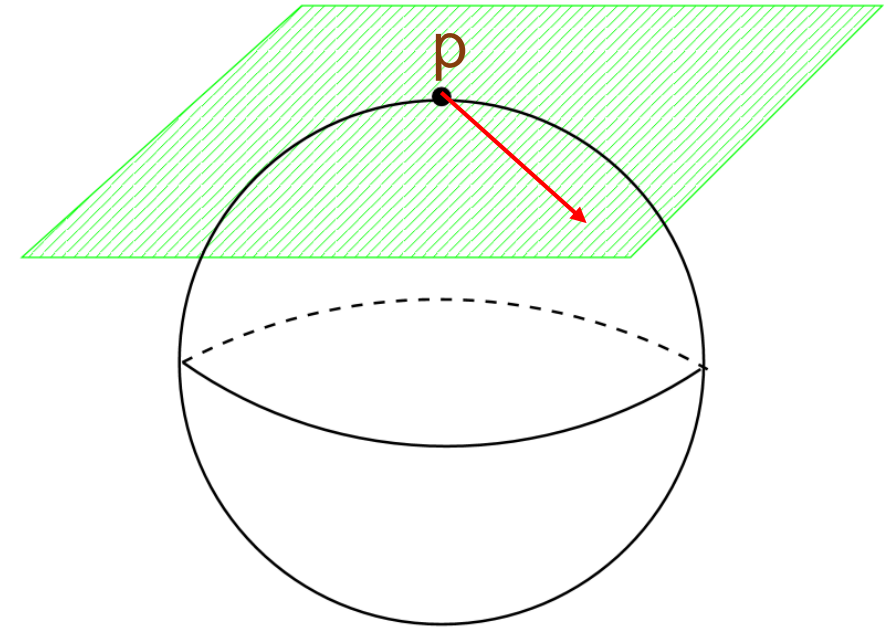
Riemannian Normal Coordinates: B. Riemann (1854)



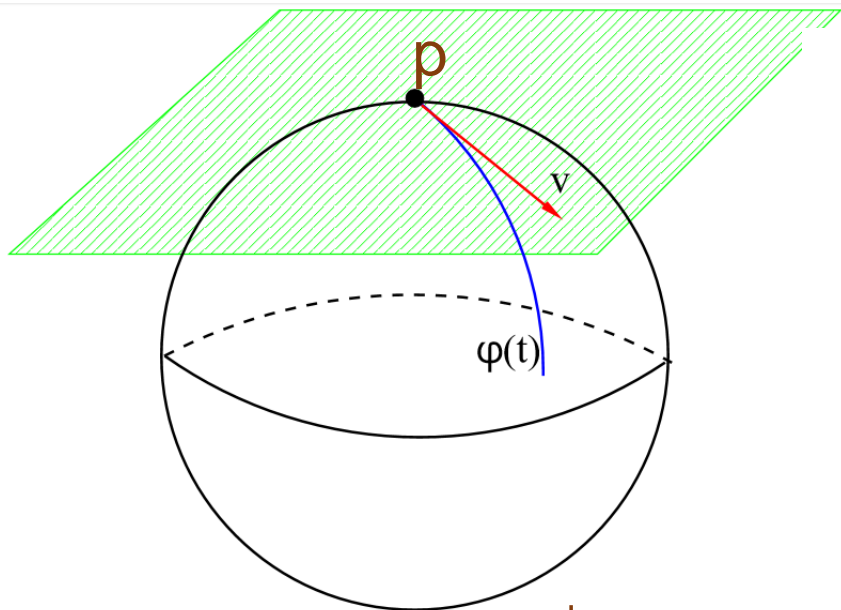
Data manifold \mathbf{M}



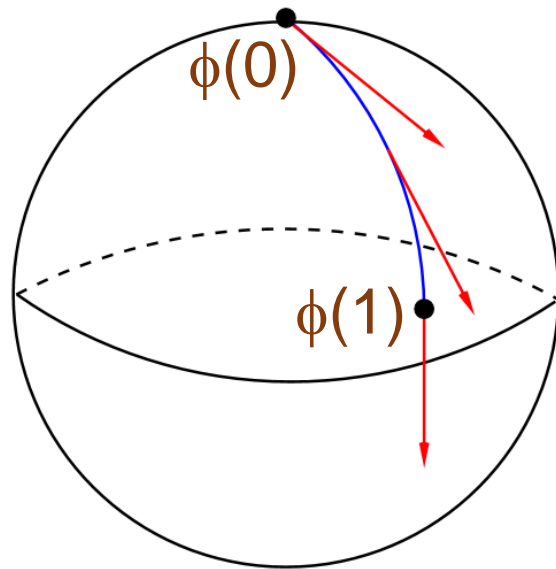
Tangent space $T_p \mathbf{M}$
 $\text{Dim} T_p \mathbf{M} = q$



Tangent vector



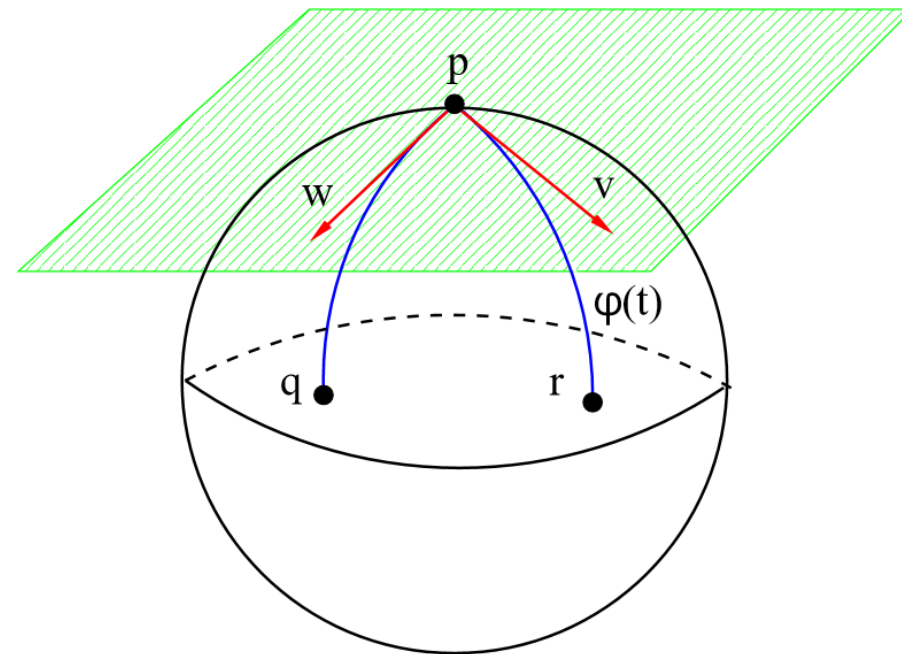
$\phi(t)$ – curve on \mathbf{M} , $\frac{d\phi(t)}{dt} = v$,
 $v \in T_p \mathbf{M}$ – tangent vector



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

$$L(\phi) = \int_0^1 \left| \frac{d\phi(t)}{dt} \right|^2 dt$$

Geodesic – shortest curve
 between two points



Geodesic $\phi(t)$
 $\phi(0) = p, \dot{\phi}(0) = \frac{d\phi(t)}{dt} \Big|_{t=0} = v$
 $\phi(|v|) = r$

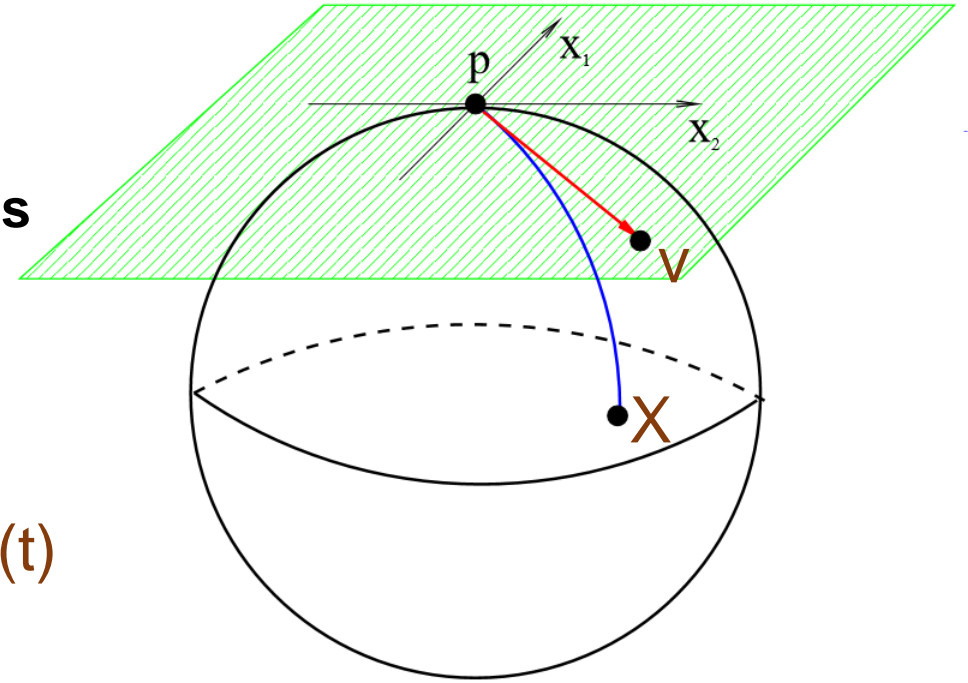
Exponential map $\exp_p: T_p \mathbf{M} \rightarrow \mathbf{M}$
 $\exp_p(v) = r, \exp_p(w) = q$

$\text{dist}_{\mathbf{M}}(p, X)$ – a length of shortest curve (geodesic) between points p and X

Math: For any point $p \in \mathbf{M}$ and any vector $v \in T_p \mathbf{M}$ there exists a **unique geodesic** $\phi(t)$ such that:

$$\phi(0) = p, \dot{\phi}(0) = v$$

All the geodesics passing through p are called **radial geodesics**



Exponential map:

- tangent vector $v \in T_p \mathbf{M}$ determines the unique geodesic $\phi(t)$ traveling through p with the tangent vector v
- geodesic $\phi(t)$ determines a point $X = \phi(1) = \exp_p(v) \in \mathbf{M}$ such that $\text{dist}_{\mathbf{M}}(p, X) = |v|$

Exponential map $v \in T_p \mathbf{M} \rightarrow X = \exp_p(v) \in \mathbf{M}$ is one-to-one in a neighborhood U of p

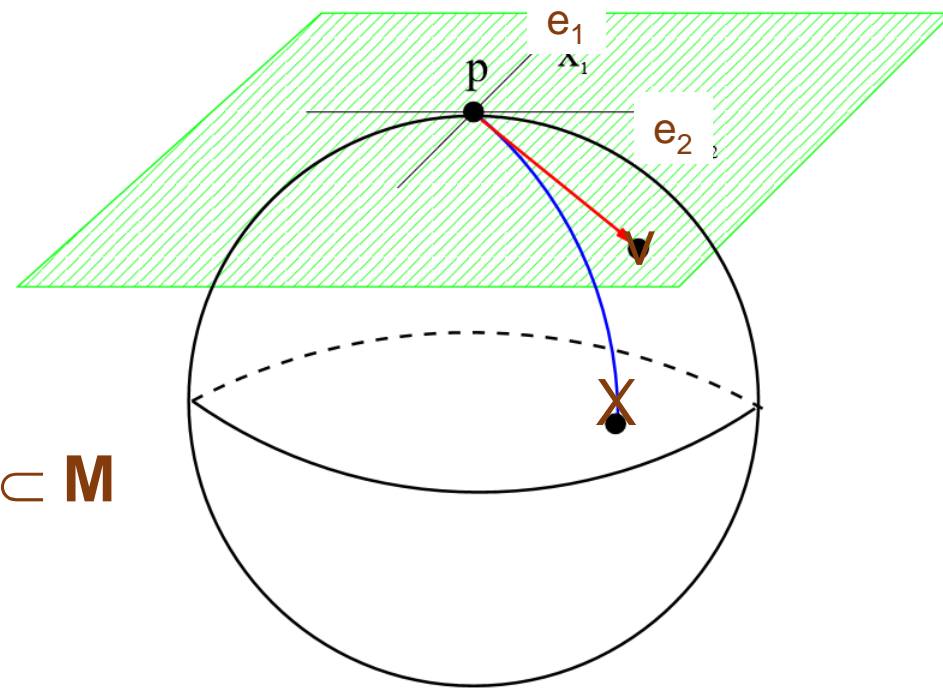
$v = \log_p(X)$ - inverse **logarithmic mapping (log map)** - parameterization of the neighborhood U

$$\log_p: X \in U \subset \mathbf{M} \rightarrow v \in T_p \mathbf{M}$$

Local coordinates defined by the chart (U, \log_p) - **Riemannian Normal Coordinates** with center p

$\{e_1, e_2, \dots, e_q\}$ – basis in $T_p \mathbf{M}$, $v = \sum_{i=1}^q y_i \times e_i$

$\{y_1, y_2, \dots, y_q\}$ – Riemannian Normal Coordinates of $X \in U \subset \mathbf{M}$



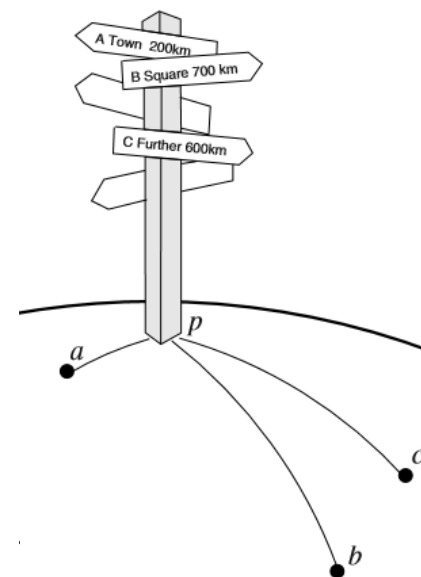
$$\mathbf{v} = \sum_{i=1}^q y_i \times \mathbf{e}_i \in T_p \mathbf{M} \quad \rightarrow \text{polar coordinates: } \mathbf{v} \rightarrow (\mathbf{e} = \frac{\mathbf{v}}{|\mathbf{v}|}, |\mathbf{v}|)$$

Geodesic $\phi(t)$: $\phi(0) = p$, $\dot{\phi}(0) = \mathbf{e} \in S_q(p)$ $S_q(p) = \{\mathbf{v} \in T_p \mathbf{M}: |\mathbf{v}| = 1\}$ – unit sphere

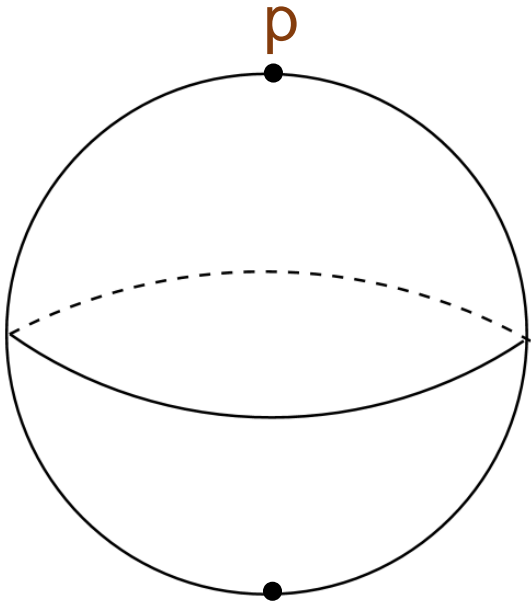
$$\mathbf{X} = \phi(|\mathbf{v}|) = \exp_p(\mathbf{v}) \in \mathbf{M}$$

$(\mathbf{e}, \text{dist}_{\mathbf{M}}(p, \mathbf{X}))$ – Riemannian Normal Coordinates of the point $\mathbf{X} \in \mathbf{M}$:

- the direction \mathbf{e} , $|\mathbf{e}| = 1$, in which you should move to reach the point \mathbf{X} by the shortest way
- the length $\text{dist}_{\mathbf{M}}(p, \mathbf{X})$ which you should move to reach the point \mathbf{X} by the shortest way



The set $CL(p)$ of points on \mathbf{M} for which there exists more than one shortest path from p - **cut locus** of p



$$\mathbf{M}(p) = \mathbf{M} \setminus CL(p)$$

$X \in \mathbf{M}(p) \rightarrow v = \log_p(X)$ - Riemannian Normal Coordinates with center p

Cut locus of p - antipodal point

Manifold embedding via Riemannian Normal Coordinates (RNC)

- input dataset $\mathbf{X}_n = \{X_1, X_2, \dots, X_n\} \subset \mathbb{R}^p$
- desired ' n -point' dataset $\mathbf{Y}_n = \{y_1, y_2, \dots, y_n\} \subset \mathbb{R}^q$

An approach:

- 'ISOMAP' part (start)
- Riemannian Normal Coordinates construction (main content)

ISOMAP part

- find sample points from small neighborhoods (ε -ball, K nearest neighbors) of the sample points
- construct a weighted undirected adjacency graph $\Gamma(\mathbf{X}_n)$ with sample points $\{\mathbf{X}_i\}$ as nodes and edges connecting 'near' nodes \mathbf{X}_i and \mathbf{X}_j with Euclidean distances $\|\mathbf{X}_i - \mathbf{X}_j\|$ as its weight
- compute the shortest-distance paths between all the graph vertices (Dijkstra's algorithm) – $\{D(\mathbf{X}_i, \mathbf{X}_j)\}$
the lengths of the shortest "geodesic paths" between the points

Main algorithm - LOGMAP (Brun et al., 2005)

- choose a base point $\mathbf{p} \in \mathbf{M}$

(1) $\mathbf{p} = \bar{\mathbf{X}}$ - mean vector

(2) \mathbf{p} – a point with minimal geodesic radius (minimal eccentricity): ‘one single chart at this point can represent the entire manifold’

$E(\mathbf{X}) = \max_j D(\mathbf{X}, \mathbf{X}_j)$ – geodesic radius (eccentricity) of a point $\mathbf{X} \in \mathbf{X}_n$

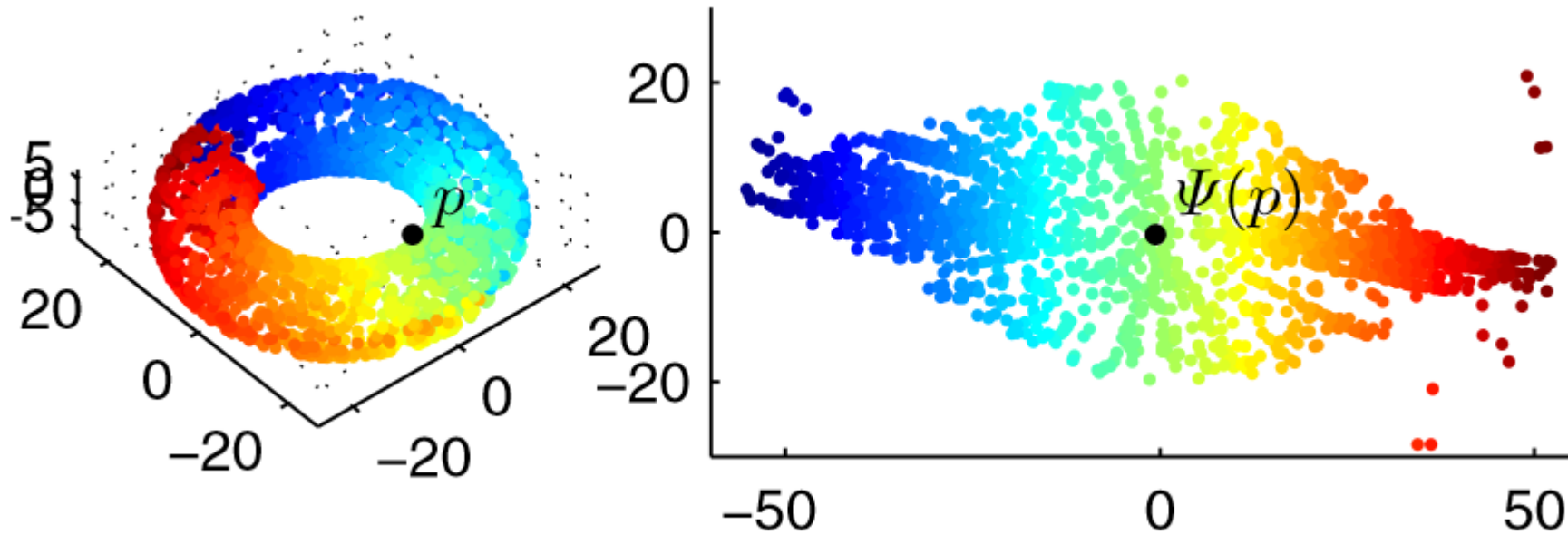
$\mathbf{p} = \arg \min E(\mathbf{X})$ – the point with minimal geodesic radius (eccentricity)

- for selected point $\mathbf{X} \in \mathbf{X}_n$, find the RNC of \mathbf{X} :
 - direction $\mathbf{e} \in \mathbf{S}_q(\mathbf{p})$ of the geodesic curve connecting the points \mathbf{p} and \mathbf{X}
 - the length $\text{dist}_{\mathbf{M}}(\mathbf{p}, \mathbf{X})$ of this geodesic curve – can be estimated by $D(\mathbf{p}, \mathbf{X})$

Estimating the direction $\mathbf{e} \in S_q(\mathbf{p})$

- $f(\mathbf{Z}) = (\text{dist}_{\mathbf{M}}(\mathbf{Z}, \mathbf{X}))^2$ - length of geodesic curve connecting points \mathbf{X} and $\mathbf{Z} \in \mathbf{U}$ (neighborhood of \mathbf{p})
- $f(\mathbf{X}') \approx D^2(\mathbf{X}', \mathbf{X})$ – approximate known values $f(\mathbf{Z})$ at the points $\mathbf{Z} = \mathbf{X}' \in \mathbf{U} \cap \mathbf{X}_n$
- $\varphi(\mathbf{Z})$ - a second order polynomial which approximates the function $f(\mathbf{Z})$ from known values $\{f(\mathbf{X}')\}$
- $\mathbf{g} = \nabla \varphi(\mathbf{Z})|_{\mathbf{Z}=\mathbf{p}} \in \mathbf{R}^q$ – gradient at point \mathbf{p}
- $\mathbf{e} = \mathbf{g} / |\mathbf{g}| \in \mathbf{e} \in S_q(\mathbf{p})$ – normalization \rightarrow desired direction
- $\mathbf{y} = \text{dist}_{\mathbf{M}}(\mathbf{p}, \mathbf{X}) \times \mathbf{e} \in \mathbf{R}^q$ – Riemannian Normal Coordinates of point $\mathbf{X} \in \mathbf{M}(\mathbf{p})$

Example (Torus embedded in 3D)



- training dataset consisting of $n = 2000$ points
- torus embedded in 3D is not flat, the manifold is not mapped to a perfect rectangle
- some outliers are present, due to incorrect estimation of the gradient for points near the cut locus

Main algorithm - Riemannian Manifold Learning (RML)

(Lin, Zha, Lee: Riemannian Manifold Learning for Nonlinear Dimensionality Reduction, 2006)

- choose a base point $\mathbf{p} \in \mathbf{M}$
- estimation of the Tangent space $T_{\mathbf{p}}\mathbf{M}$
 - sample points $\mathbf{X}_0, \mathbf{X}_1, \dots, \mathbf{X}_q$ from the neighborhood \mathbf{U} of base point \mathbf{p} lying in a general position are selected
 - $L(\mathbf{p}) = \mathbf{X}_0 + \text{Span}(\mathbf{X}_1 - \mathbf{X}_0, \mathbf{X}_2 - \mathbf{X}_0, \dots, \mathbf{X}_q - \mathbf{X}_0)$ - estimator of the Tangent space $T_{\mathbf{p}}\mathbf{M}$
 - $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_q\}$ – orthonormal basis in $L(\mathbf{p})$

- constructing the Riemannian Normal Coordinates $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n$ for sample points $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$

1) $\mathbf{X} \in \mathbf{U} \cap \mathbf{X}_n$: $\mathbf{z} = (z_1, z_2, \dots, z_q) = \text{Pr}_{L(p)}\mathbf{X}$ - projection into linear space $L(p)$

the solution to the Least Squares task: $\|\mathbf{X} - (p + \sum_{i=1}^q z_i \times \mathbf{e}_i)\|_{(n)}^2$ $\|\cdot\|_{(k)}$ - Euclidean norm in \mathbf{R}^k

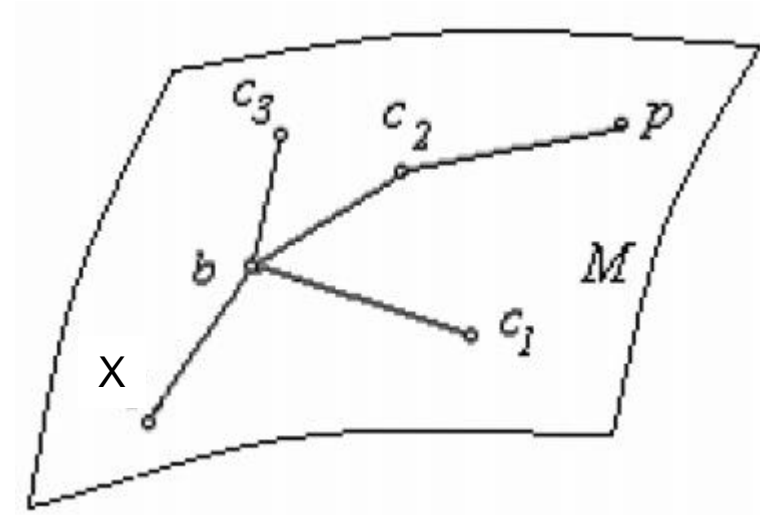
$\mathbf{y} = \frac{\|\mathbf{X}-p\|_{(n)}}{\|\mathbf{X}\|_{(q)}} \times \mathbf{z}$ - Riemannian Normal Coordinates of \mathbf{X}

2) $X \notin U \cap X_n$:

b - the previous point on the shortest path from p to X

point b has $k \geq q$ edge points c_1, c_2, \dots, c_k whose normal coordinates

$y_{(0)}$ and $y_{(1)}, y_{(2)}, \dots, y_{(k)}$ have been computed previously



α_i - an angle between vectors $(X - b)$ and $(c_i - b)$: $\cos(\alpha_i) = \frac{(X - b, c_i - b)}{\|X - b\| \times \|c_i - b\|}$, $i = 1, 2, \dots, k$

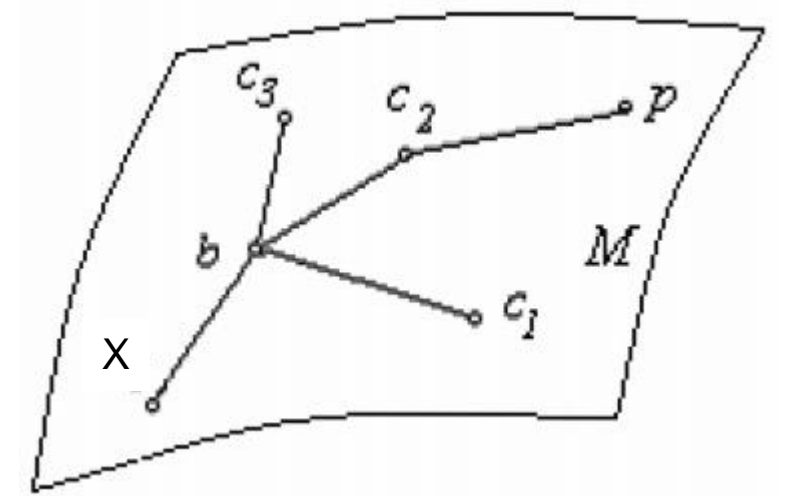
β_i - an angle between their RNC - the vectors $(y - y_{(0)})$ and $(y_{(i)} - y_{(0)})$:

$$\cos(\beta_i) = \frac{(y - y_{(0)}, y_{(i)} - y_{(0)})}{\|y - y_{(0)}\| \times \|y_{(i)} - y_{(0)}\|}, i = 1, 2, \dots, k$$

The desired RNC \mathbf{y} is constructed

- to preserve the angles between the vectors $(\mathbf{X} - \mathbf{b})$ and $(\mathbf{c}_i - \mathbf{b})$ and their RNC: $\cos(\alpha_i) \approx \cos(\beta_i)$, $i = 1, 2, \dots, k$
- to keep the distance between \mathbf{X} and \mathbf{b} unchanged:

$$\|\mathbf{X} - \mathbf{b}\| = \|\mathbf{y} - \mathbf{y}_{(0)}\|$$

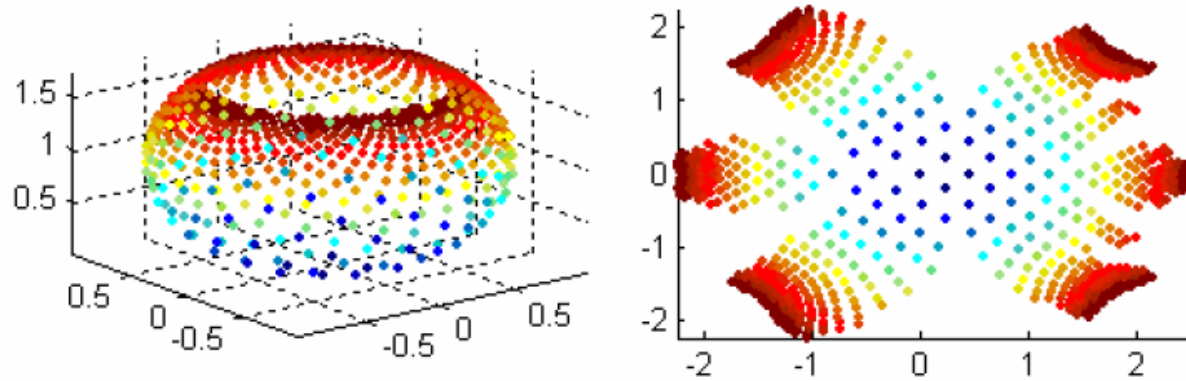


Optimization problem:

$$\|A \times (\mathbf{y} - \mathbf{y}_{(0)}) - \mathbf{h}\|^2 \rightarrow \min \text{ over } \mathbf{y} \text{ under the constraint } \|\mathbf{y} - \mathbf{y}_{(0)}\| = \|\mathbf{X} - \mathbf{b}\|$$

$$\mathbf{h} = \begin{pmatrix} \cos(\alpha_1) \\ \dots \\ \cos(\alpha_k) \end{pmatrix} \in \mathbb{R}^k \quad A - k \times q \text{ matrix with } i\text{-th row } \frac{(\mathbf{y}_{(i)} - \mathbf{y}_{(0)})^T}{\|\mathbf{X} - \mathbf{b}\| \times \|\mathbf{y}_{(i)} - \mathbf{y}_{(0)}\|}, \quad i = 1, 2, \dots, k$$

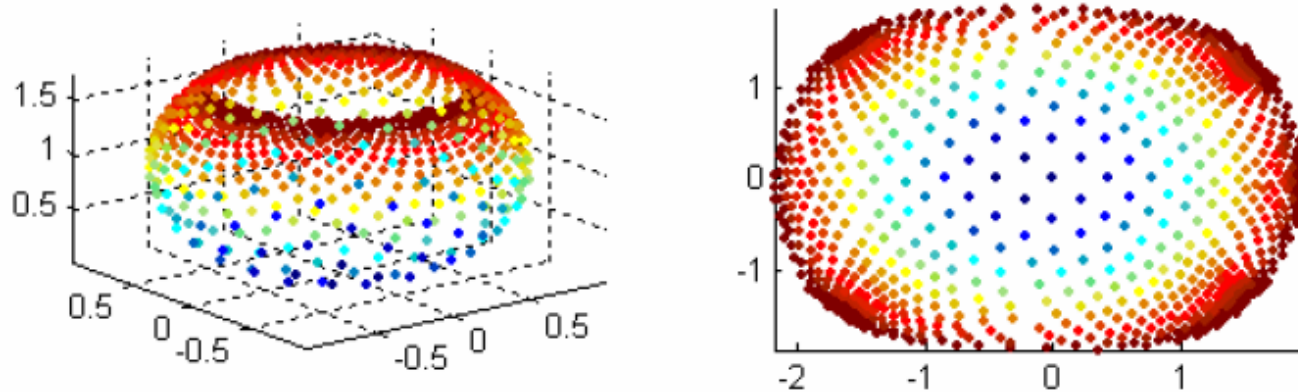
Linear least squares problem with a quadratic constraint: Lagrange multipliers + Newton's method



Improved algorithm - Riemannian Manifold Learning (RML)

(Lin, Zha: Riemannian Manifold Learning, 2008)

- improved procedure for computing the geodesics based on their local quadratic approximation



Locally Linear Embedding - 2000

ISOmetric MAPing (ISOMAP) - 2000

Laplacian Eigenmaps - 2003

Logmap - 2005

Riemannian Manifold Learning - 2006/2008

C-ISOMAP, L-ISOMAP - 2003

Hessian Eigenmaps - 2003

Local Tangent Space Alignment - 2004

Manifold charting - 2003

Semidefinite embedding - 2004

Diffusion maps (2005)/ Vector Diffusion maps (2012)

Grassmann&Stiefel Eigenmaps - 2012

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