MATH466/MATH766
Math of machine learning
03/24 Lecture 17 Laplacian Eigenmap and Spectral Convergence

References:

- Mikhail Belkin, Partha Niyogi, Laplacian eigenmaps for dimensionality reduction and data representation, Neural Computation, (2003)
- Mikhail Belkin, Partha Niyogi, Laplacian eigenmaps and spectral techniques for embedding and clustering, Neurips, 2001
- A. Singer, From graph to manifold Laplacian: the convergence rate, Applied and computational harmonic analysis, 2006
- Yaiza Canzani, Notes for Analysis on Manifolds via the Laplacian

Todays contents:

- Laplacian eigenmap
- spectral convergence

Important concepts:

- manifold hypothesis
- intrinsic

Recommend reading:

- ch1 of Yaiza Canzani, Notes for Analysis on Manifolds via the Laplacian

Review Graph G

affinity / adjacency matrix W $(W_{ij} = W_{ji},\ W_{ii} = 0)$

degree matrix D, $D_{ii} = d_i = \sum_j w_{ij}$, $D_{ij} = 0$ if $i \neq j$

graph Laplacian $L = D - W$

$L_{rw} = I - D^{-1} W$

$L_{sym} = I - D^{-\frac{1}{2}} W D^{-\frac{1}{2}}$

Spectral Clustering: EVD of L: $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$

L_{rw} $\quad \psi_1 \quad \psi_2 \quad \cdots \quad \psi_n$

$$\underbrace{y_i = \begin{bmatrix} \psi_{2i} \\ \psi_{3i} \\ \vdots \\ \psi_{di} \end{bmatrix}}_{\text{Laplacian Eigenmap}} \in \mathbb{R}^d$$

, apply clustering algorithm, e.g. k-means to $\{y_i\}_{i=1}^n$

Laplacian Eigenmap

L_{rw} eigval $\quad 0 = \lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots \le \lambda_n$

eigvec $\quad \underset{\substack{\| \\ 1_n}}{\psi_1} \quad \psi_2 \quad \psi_3 \quad \cdots \quad \psi_n$.

$$y_i = \begin{bmatrix} \psi_{2i} \\ \psi_{3i} \\ \vdots \\ \psi_{di} \end{bmatrix} \in \mathbb{R}^d$$

Laplacian Eigenmap

Understanding LE (p.o.v. 1)

Consider mapping $G = (V, E), (V = \{x_1, \cdots, x_n\})$ to a line

and keep connected points stay close together.

i.e. find $f : V \to \mathbb{R}$, $\quad x_i \mapsto y_i$

s.t. $\sum_{i,j} W_{ij} (y_i - y_j)^2$ is small

Denote $f = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$, then $\sum_{i,j} W_{ij} (y_i - y_j)^2 = \underline{\frac{1}{2} f^T L f}$

need restrictions on f : $\quad f^T D f = 1$

- removes the arbitrary scaling factor in the embedding
- vertex with larger degree is more important.

$$\to \min_{f^T D f = 1} f^T L f$$

By optimization thm, optimality condition $\quad Lf = \lambda D f$

$\Rightarrow$ optimal value $\quad \lambda_{min}(L) = 1 - \lambda_0(P) = 0$

optimizer $\quad f = 1_n = \psi_0$

$f = \frac{1}{\sqrt{n}} 1_n$ is a trivial solution

$$\to \min_{\substack{f^T D f = 1 \\ f^T D 1_n = 0}} f^T L f \qquad \text{optimal value} \quad (1 - \lambda_1) \qquad \text{optimizer} \quad f = \psi_1$$

If we want to map x_i to $y_i \in \mathbb{R}^m$

and keep $\sum_{i,j} \| y_i - y_j \|^2 W_{ij}$ small

we can work with

$$\min_{f} \sum_{k=1}^{m} [(y_1)_k \ (y_2)_k \cdots (y_n)_k] \, L \underbrace{\begin{bmatrix} (y_1)_k \\ (y_2)_k \\ \vdots \\ (y_n)_k \end{bmatrix}}_{=: f_k}$$

s.t. $f_k^T D f_k = 1$,

$f_k^T D 1_n = 0$,

$f_k^T D f_{k'} = 0$, $k \neq k'$

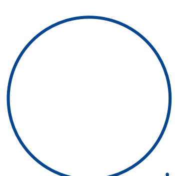
Understanding LE (p.o.v. 2)

- Manifold $M \subseteq \mathbb{R}^D$

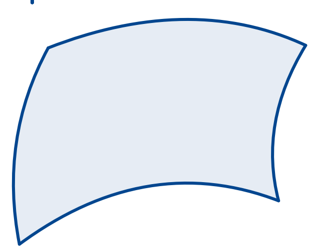
  " every point has a nbhd homeomorphic to an open subset of $\mathbb{R}^d$ "

  homeomorphism : a cts, invertible func with cts inversion

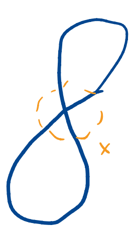
e.g.



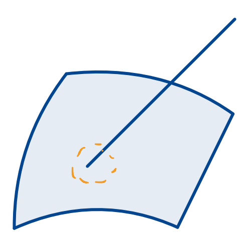
1d manifold in 2d space



2d manifold in 3d space



not a manifold



not a manifold

- Manifold hypothesis :

  many high-dim data sets that occurs in the real world

  actually lie along low-dim latent manifolds inside that high-dim space

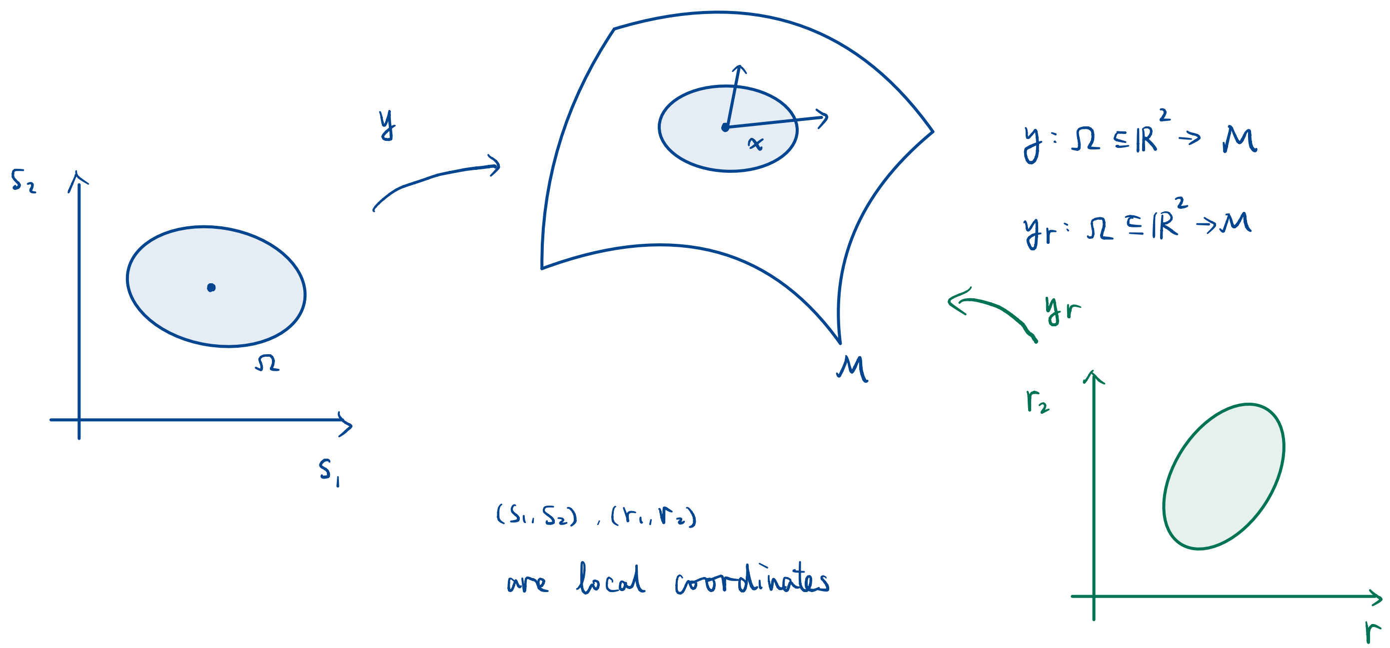
- differential operators on manifold

"intrinsic" v.s. "extrinsic"

Similar to Euclidean space,

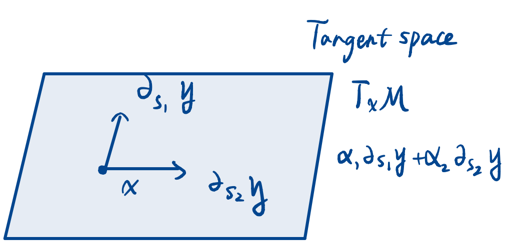
we can define Laplacian operator Δ_M on a manifold M

Δ_M is intrinsic



(s_1, s_2), (r_1, r_2)

are local coordinates



metric $g_x : T_x M \times T_x M \to \mathbb{R}$

$$(\alpha_1 \partial_{s_1} + \alpha_2 \partial_{s_2},\ \beta_1 \partial_{s_1} + \beta \partial_{s_2})$$

$$\mapsto (\alpha_1\ \alpha_2) \begin{pmatrix} \partial_{s_1}^T \\ \partial_{s_2}^T \end{pmatrix} (\partial_{s_1}\ \partial_{s_2}) \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}$$

① metric is intrinsic to the manifold geometry

② differential operators on a manifold depends on metric

③ If s are local normal coordinates

i.e. $\partial s_i^T \partial s_j = \delta_{ij} = \begin{cases} 1, & i=j \\ 0, & i \neq j \end{cases}$

then $$\Delta_M f(x) = -\sum_{i=1}^{d} \frac{\partial^2}{\partial s_i^2} f(y(s)) \Big|_{y=x}$$

$$= -\mathrm{div}_M \nabla_M f(x)$$

$$M \underset{?}{\overset{\longrightarrow}{\longleftarrow}} \Delta_M$$

"can you hear the shape of a drum"

eigen-problem : $\Delta \varphi = \lambda \varphi$

① full sequence of eigenvalues of Ω

$\Downarrow$

area, perimeter and # of holes in Ω

dim, volume and total scalar curvature

② Sturm-Liouville's decomposition

(M, g) compact Riemannian manifold

w/. o.n. basis $\varphi_1, \varphi_2, \dots, \varphi_j$

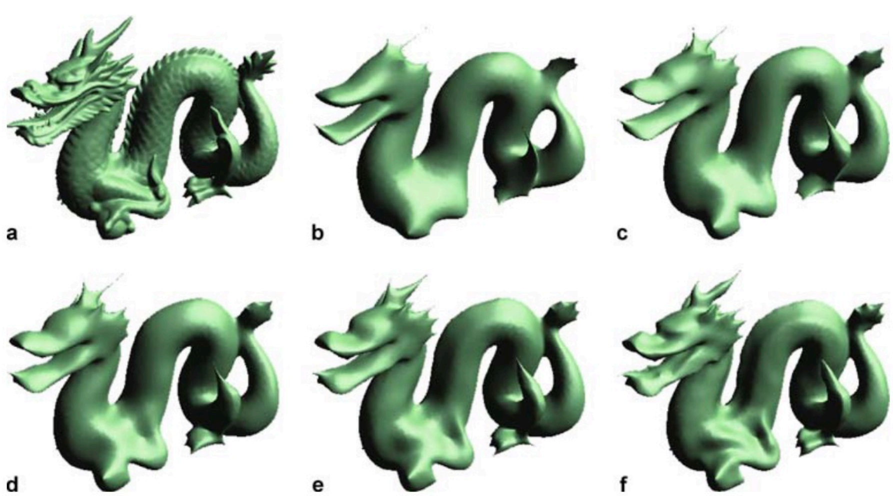
(eig-funcs of Δ_g)

Any function $f \in L^2(M)$ can be written as

a convergent series in $L^2(M)$

$$f = \sum_{j=1}^{\infty} a_j \varphi_j \quad \text{for some } a_j \in \mathbb{R}$$

e.g. Euclidean space, Fourier sequence



a. M =Dragon. **b-f.** reconstructed manifold using $N = 100, 200, 300, 500$ and 900 eigenfunctions respectively. Picture from paper *Spectral mesh deformation.*

$$\begin{tikzcd}
\text{graph} \arrow[r, rightsquigarrow] \arrow[d, dash] & \text{point cloud } \{x_i\}_{i=1}^{n} \arrow[r, rightsquigarrow] & \text{manifold } (M, g) \arrow[d, dash] \\
\text{graph Laplacian } L \arrow[rr, "? \text{ as } n \to +\infty"] \arrow[d, dash] & & \text{Laplacian } \Delta_M \arrow[d, dash] \\
\text{spectral of } L & & \text{spectral of } \Delta_M
\end{tikzcd}$$

- Convergence [Singer 06]

$$W_{ij} = k\left(\frac{\|x_i - x_j\|^2}{2\varepsilon}\right), \quad k \text{ p.s.d. e.g. } k(x) = e^{-x}$$

$$L = I - D^{-1}W. \qquad x_i \sim_{i.i.d} U(M), \; i = 1, \cdots, n$$

then

$$\frac{1}{\varepsilon}\sum_{j=1}^{n} L_{ij} f(x_j) = \frac{1}{2}\Delta_M f(x_i) + \underbrace{O\left(\frac{1}{n^{1/2}\varepsilon^{1/2+d/4}}, \varepsilon\right)}_{\leq C_1 \frac{1}{n^{1/2}\varepsilon^{1/2+d/4}} + C_2\varepsilon, \; n \to +\infty, \; \varepsilon \to 0}$$

- Demo