Lecture Note for Laplacian Eigenmaps

I. Notations and Assumptions.

$\mathcal{X} = \{x_1, \dots x_n\} \subset \mathbb{R}^D$ Data Set on manifold $\mathcal{M}$.

$\mathcal{M}$ yields a parametrization, $g: \mathbb{R}^d \to \mathcal{M}$

$h := g^{-1}$ denots the coordinate mapping, such that for each $x \in \mathcal{M}$, $y = h(x) \in \mathbb{R}^d$ provides coordinate for x in $\mathbb{R}^d$

Then Data set $\mathcal{Y} := \{y_1 \dots y_n\}$, with $y_i := h(x_i)$ will be the DR set.

Still, $G = [\mathcal{X}, E]$ is the graph defined using $\underline{\underline{\varepsilon\text{-ball}}}$

$\underset{\substack{\uparrow \\ \text{adjacent indices of } x_i}}{N(i)} = \{i_1, \dots i_k\}$, $\underset{\substack{\uparrow \\ \text{neighborhood of } x_i}}{O(i)} = \{x_{i_1}, \dots x_{i_k}\}$

Note: $s \in N(i) \iff i \in N(s)$

II. Laplace - Beltrami Operator.

Recall: Riemannian Manifold (M, g)

Define $g_{ij} = \langle \partial_i, \partial_j \rangle$, g^{ij}, satisfy $\dfrac{(g^{ij}) = (g_{ij})^{-1}}{G = (g_{ij})}$

For $f \in C^2(\mathcal{M})$

One can define $\operatorname{grad} f := (g^{ij} \partial_j f)_{i=1 \dots d}$

For vector field $X = X^i \partial_i$

One can define $\operatorname{div} X := \dfrac{1}{\sqrt{|G|}} \partial_i (\sqrt{|G|} X^i)$ $\quad |G| := \det(G)$

$\Rightarrow$ Laplace - Beltrami $\Delta f := \operatorname{div}(\operatorname{grad} f) = \dfrac{1}{\sqrt{|G|}} \partial_i (\sqrt{|G|}\, g^{ij} \partial_j f)$

Roughly speaking $\sqrt{|G|}$ provides a way to define volume on M, which allows us to discuss intergation on M.

$\Rightarrow$ inner product $\langle f, g \rangle = \int_M fg$ for $f, g \in L^2(M)$

For $g, f \in C_0^2(M)$ ($g, f = 0$ on ∂M)

$$\begin{cases} \int_M f \Delta g = \int_M \Delta f g \\ \int_M |\text{grad} f|^2 = - \int_M f \Delta f \end{cases}$$

Proof: Notice $\begin{cases} \int_M \text{div} fX = 0 \\ \text{div} fX = \langle \text{grad} f, X \rangle + f \,\text{div} X \end{cases}$

$\Rightarrow \int_M \langle \text{grad} f, X \rangle = - \int_M f \,\text{div} X$ take $X = \text{grad}\, g$

$\Rightarrow - \int_M f \Delta g = \int_M \langle \text{grad} f, \text{grad} g \rangle = - \int_M g \Delta f$

II. Hilbert - Schmidt

image of bounded set is pre-compact

If A is a compact, self-adjoint operator on a Hilbert space then

possible

1° $\{0\}$ is the only accumulate point of $\sigma(A)$

2° Eigen-function $\{\varphi_i\}$ form an orthonormal basis for $R(A)$.

Rk: Δ^{-1} is a compact, self-adjoint operator.

$X = L^2(M)$, $R(\Delta^{-1}) = H_0^2(M)$

Result ~~of~~ from Maximum principle + Sobolev Embedding.

III. Semi-Group.

D(A) dense in X.

Let A be a closed densely defined linear operator on Banach space X.

consider the ODE

$$\begin{cases} u'(t) = Au(t) \\ u(0) = u. \end{cases} \quad u \in X, \qquad (*)$$

We will write $S(t)u := u(t)$ to display explicitly the dependence of $u(t)$ on the initial value of u. ($S(t) = e^{tA}$)

$$Au := \lim \frac{S(t)u - u}{t} \qquad (u \in D(A)) \qquad (**)$$

A (infinitesimal) generator of semigroup $\{S(t)\}_{t\geq 0}$.

Rk: A in $(*)$ & $(**)$ corresponds on D(A) if $\{S(t)\}_{t\geq 0}$ is ω-contraction, that is $\|S(t)\| \leq e^{\omega t}$ $(t \geq 0)$ $(\omega \in \mathbb{R})$

Theorem (Hille-Yosida) Operator A generate an ω-contractive semigroup

$\Leftrightarrow$

$(\omega, \infty) \subset \rho(A)$ and $\|R_\lambda\| \leq \frac{1}{\lambda - \omega}$, for $\forall \lambda > \omega$.

where $\rho(A)$ resolvent set of A

($\lambda I - A : D(A) \to X$ is one-to-one and onto)

$R_\lambda u := (\lambda I - A)^{-1} u$. resolvent operator.

Rk: 1° $R_\lambda - R_\mu = (\mu - \lambda) R_\lambda R_\mu$

2° $R_\lambda R_\mu = R_\mu R_\lambda$

3° $R_\lambda u = \underbrace{\int_0^\infty e^{-\lambda t} S(t) u \, dt}_{\text{Laplace transform of semigroup}}$, ~~and so $\|R_\lambda\| \leq \frac{1}{\lambda}$~~

$$Lu = -\sum_{i,j=1}^{n} (a^{ij}(x,t) u_{x_i})_{x_j} + \sum_{i=1}^{n} b^i(x) u_{x_i} + c(x)u.$$

Application:

Second-order parabolic PDE

$$\begin{cases} u_t + Lu = 0 & \text{in } U_T \\ u = 0 & \text{on } \partial U \times [0, T] \\ u = g & \text{on } U \times \{t = 0\} \end{cases}$$

L satisfies strong ellipticity condition. $\sum_{i,j=1}^{n} a^{ij}(x) \xi_i \xi_j \geq \theta |\xi|^2$

Define $A = -L$, $D(A) := H_0^1(U) \cap H^2(U)$ dense in $L^2(U)$

Energy estimates $\exists\ \beta > 0,\ \gamma \geq 0$ s.t.

$$\beta \|u\|^2_{H_0^1(\Omega)} \leq B[u,u] + \gamma \|u\|^2_{L^2(U)}, \quad \theta \qquad u \in H_0^1(\Omega).$$

$$B[u,v] := \int_U \sum_{i,j=1}^{n} a^{ij}(\cdot) u_{x_i} v_{x_j} + \sum_{i=1}^{n} b^i(x) u_{x_i} v + c(x) uv \, dx.$$

$\Rightarrow$ Operator A generates a γ-contraction semigroup.

V Basic Idea of Laplacian Eigenmap

Approximate the coordinate map $h = [h^1, \cdots h^d]$, by a linear combination of $\{\varphi_j\}$.

$\{\varphi_j\}$ are eigenfunctions of Δ, such that $\Delta\varphi_j = \lambda_j \varphi_j$.

In general, consider

$$h^i \approx \hat{h}^i = \sum_{j=1}^{m} \alpha_j^i \varphi_j \quad (*), \qquad \alpha_j^i := \frac{\langle h^i, \varphi_j \rangle}{\langle \varphi_j, \varphi_j \rangle}$$

Problem: We have no access to $\{\varphi_j\}$.

Rewrite $(*)$ $\Rightarrow$ $\min \int_M \| \mathrm{grad}(h^i - \hat{h}^i) \|^2 \Leftrightarrow \min \int \hat{h}^i \Delta \hat{h}^i$ under certain constraints.

VI Approximation of Laplace-Beltrami Operator

Let $\mathcal{L} = -\Delta$, and consider the ODE problem.

$$\begin{cases} \dot{u} + Lu = 0 \\ u(0) = u_0 \end{cases} \Rightarrow \text{Semi-group } S_t u_0 \to u(t), \quad S_t = e^{-t\mathcal{L}}$$

$$\underbrace{u \in H^2(M)}$$

$$\Rightarrow \quad \mathcal{L} = \lim_{t \to 0^+} \frac{S_t - Id}{t} \quad \Rightarrow \quad \Delta f \approx \frac{1}{t}(f - S_t f)$$

for some t small.

Recall the heat kernel in $\mathbb{R}^d$ (to approximate S_t)

$$G_t(x, y) = \begin{cases} (4\pi t)^{-\frac{d}{2}} e^{-\frac{|x-y|^2}{4t}} & t > 0 \\ 0 & t < 0 \end{cases}$$

then $S_t f(x) \approx (4\pi t)^{-\frac{d}{2}} \int_M e^{-|x-y|^2/4t} f(y)$

$\Rightarrow \Delta f \approx \lim_{t \to 0^+} \frac{1}{t} \left(f - (4\pi t)^{-d/2} \int_M e^{-|x-y|^2/4t} f(y) \right)$

The discrete form is given by,

$$\Delta f(x_i) \approx \frac{1}{t} \left(f(x_i) - d_i^{-1} \sum_{x_j \in O(i)} e^{-\frac{|x_i - x_j|^2}{4t}} f(x_j) \right) \qquad (t \ll 1)$$

where $d_i = \sum_{x_j \in O(i)} e^{-|x_i - x_j|^2/4t}$ (normalizing constant).

Introduce the notation.

$$w_{ij} := \begin{cases} \exp\left(-\frac{|x_i - x_j|^2}{4t}\right), & \text{if } x_j \in O(i). \\ 0 & \text{else}. \end{cases} \qquad (*)$$

Rk : $w_{ij} = w_{ji}$ matrix $W = (w_{ij})$ is symmetric.

then ~~Δf~~ let $F = [f(x_1) \cdots f(x_n)]^T$,

then $[\Delta f(x_1) \cdots \Delta f(x_n)]^T \approx \frac{1}{t} [Id - D^{-1} W] F$, where

$D = \mathrm{diag}(d_1 \cdots d_n)$

Notice $\cancel{(Id - D^{-1} W) F = (Id - D^{-1/2} W D^{-1/2})} F$

we take the symmetric matrix $L := Id - D^{-1/2} W D^{-1/2}$

as our discrete form of Δ. $= D^{\frac{1}{2}} [Id - D^{-1} W] D^{-1/2}$

$D^{\frac{1}{2}}$ – pre-condition

VII. DR Data Set

Let $Y = [y_1 \cdots y_n] \in \mathbb{R}^{d \times n}$ be our DR Data set.

Take it i^{th} row $Y_i = [h^i(x_1), \cdots h^i(x_n)]$

then

$$\int_M \hat{h}^i \Delta \hat{h}^i \approx Y_i \cdot L Y_i^T$$

$\Rightarrow$ We obtain Y by solving

$$\min \ tr(Y L Y^T) \quad s.t \quad Y \mathbb{1} = 0 \ , \ Y Y^T = I_d .$$

Rk 1° this is an eigenvalue problem of L.
L is symmetric - semi-positive-definite and sparse.
In particular, $D^{1/2} \mathbb{1}$ is a 0-eigenvector.

2° this ~~justify~~ justifies the "weight-methods" introduces in the ~~big~~ previous meetings.

~~We are~~

All these methods are minimizing certain energy.