Heat kernel for Dirichlet Laplacian

We next discuss a construction of $P_t = e^{t\Delta}$ via Dirichlet Laplacians.

Let D be a finite connected subgraph of G.

$\mathrm{bdy}\, D = \{ x \in V_D : \exists\, y \notin \text{ s.t. } x \sim y \}$

$\mathrm{int}\, D = V_D \setminus \mathrm{bdy}\, D$.

Consider the function space

$$C(D, \mathrm{bdy} D) := \{ f : V_D \to \mathbb{R} \mid f|_{\mathrm{bdy} D} = 0 \}$$

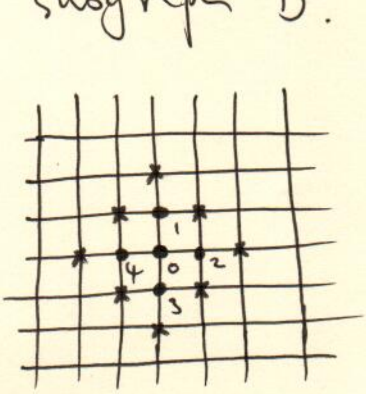
Then we define the Dirichlet Laplacian Δ_D as

$$\Delta_D : C(D, \mathrm{bdy} D) \to C(D, \mathrm{bdy} D)$$

s.t. $$\Delta_D f(x) = \begin{cases} \Delta f(x) \xrightarrow{\text{only need the values of } f \text{ on } D}, & x \in \mathrm{int}\, D \\ 0, & \text{otherwise}. \end{cases}$$

If we extend each $f \in C(D, \mathrm{bdy} D)$ as $f : V \to \mathbb{R}$ s.t. $f|_{V \setminus D} \equiv 0$, then $\Delta_D f = (\Delta f)|_{\mathrm{int} D}$.

Rmk: Δ_D is different from the Laplacian on the induced subgraph D. However, Δ_D can be represent by a square matrix.



× bdy D

• int D

Laplacian on the subgraph:

$$\begin{array}{c|c} & \begin{matrix} 0 & 1 & 2 & 3 & 4 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{matrix} & \begin{pmatrix} -1 & \frac14 & \frac14 & \frac14 & \frac14 \\ 1 & -1 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & -1 \end{pmatrix} \end{array}$$

while

$$\Delta_D = \begin{array}{c|c} & \begin{matrix} 0 & 1 & 2 & 3 & 4 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{matrix} & \begin{pmatrix} -1 & \frac14 & \frac14 & \frac14 & \frac14 \\ \frac14 & -1 & 0 & 0 & 0 \\ \frac14 & 0 & -1 & 0 & 0 \\ \frac14 & 0 & 0 & -1 & 0 \\ \frac14 & 0 & 0 & 0 & -1 \end{pmatrix} \end{array}$$

<u>Lemma III.2.5</u>: Δ_D is a self-adjoint, non-positive operator on $C(D, \text{bdy} D)$.

<u>Proof</u>: By the Green's thm Lemma III.2.3, we have

$$\langle \Delta_D f, g \rangle_D = \sum_{x \in D} \Delta_D f(x) g(x) d_x = \langle f, \Delta_D g \rangle_D$$

for any $f \in C(D, \text{bdy} D)$. Therefore Δ_D is self-adj.

Moreover $\langle \Delta_D f, g \rangle_D = - \sum_{\{x,y\} \in E_D} (f(y) - f(x))(g(y) - g(x))$

Then Δ_D is non-positive. $\square$

That is, the matrix Δ_D is similar to a symmetric matrix.

We say λ an eigenvalue of Δ_D, if $\exists f \in C(D, \text{bdy} D)$, $f \not\equiv 0$, s.t. $\Delta_D f + \lambda f = 0$. We list all eigenvalues as

$$\lambda_1^D \le \lambda_2^D \le \cdots \le \lambda_{|\text{int} D|}^D$$

Similar to previous discussion on heat kernel of finite graphs, we have $P_t^D := e^{t \Delta_D}$ is a self-adjoint operator on $C(D, \text{bdy} D)$. We define the kernel

$$p_t^D(x,y) = \left\langle P_t^D \left(\frac{\delta_y}{d_y} \right), \frac{\delta_x}{d_x} \right\rangle, \quad \forall x, y \in D, \ t \ge 0.$$

Let $\phi_1^D, \ldots, \phi_{|\text{int} D|}^D$ be eigenfunctions corresponding to $\lambda_1^D, \ldots, \lambda_{|\text{int} D|}^D$ ~~such that~~ which are an orthonormal basis for $C(D, \text{bdy} D)$ w.r.t. the $\ell^2_{\mu = d_x}$ inner product.

Similar as in Prop II.10.10 (Spectral decomposition) on p.p. 154, we derive

$$p_t^D(x,y) = \langle P_t^D(\tfrac{\delta_y}{d_y}), \tfrac{\delta_x}{d_x} \rangle = \sum_{n=1}^{|\mathrm{int} D|} e^{-\lambda_n t} \phi_n^D(x) \phi_n^D(y).$$

Theorem III.2.6: Let D be a finite connected subgraph of $G=(V,E)$. Then $p_t^D(x,y)$ has the following properties:

(1) $p_t^D(x,y) = p_t^D(y,x)$, $p_t^D(x,y) = 0$ if ~~and only if~~ $x \in \mathrm{bdy} D$ or $y \in \mathrm{bdy} D$.

(2). $\frac{\partial}{\partial t} p_t^D(x,y) = \Delta_D p_t(x,y)$, where Δ_D denotes the Dirichlet Laplacian in either x or y.

(3). $p_{s+t}^D(x,y) = \sum_{z \in D} p_s^D(x,z) p_t^D(z,y)\, d_z$

(4) $p_0^D(x,y) = \frac{\delta_y}{d_y}(x)$, for $x,y \in \mathrm{int} D$.

(5) $p_t^D(x,y) > 0$ for all $t>0$, all $x,y \in \mathrm{int} D$

(6) $\sum_{y \in D} p_t^D(x,y) d_y < 1$ for all $t>0$, all $x \in D$.

Proof: The symmetry in (1) and (2), (4) follows directly from definition. If $x \in \mathrm{bdy} D$, or $y \in \mathrm{bdy} D$, we have

$$\phi_n^D(x)\phi_n^D(y) = 0, \ \forall\ n=1,\dots,|\mathrm{int} D|.$$

Therefore, $p_t^D(x,y) = 0$.

(3) Follows from the semigroup property of P_t^D. Indeed, we have

$$p^D_{s+t}(x,y) = \left\langle P^D_{s+t}\left(\frac{\delta_y}{dy}\right), \frac{\delta_x}{dx}\right\rangle = \left\langle P^D_s P^D_t\left(\frac{\delta_y}{dy}\right), \frac{\delta_x}{dx}\right\rangle$$

$$= \left\langle P^D_t\left(\frac{\delta_y}{dy}\right), P^D_s\left(\frac{\delta_x}{dx}\right)\right\rangle$$

$$= \sum_{z\in D} P^D_t\left(\frac{\delta_y}{dy}\right)(z)\, P^D_s\left(\frac{\delta_x}{dx}\right)(z)\, dz$$

$$= \sum_{z\in D} \left\langle P^D_t\left(\frac{\delta_y}{dy}\right), \frac{\delta_z}{dz}\right\rangle \left\langle P^D_s\left(\frac{\delta_x}{dx}\right), \frac{\delta_z}{dz}\right\rangle dz$$

$$= \sum_{z\in D} p^D_t(z,y)\, p^D_s(z,x)\, dz.$$

(5). This follows from the ~~maximal~~ principle. $p^D_t(x,y)$ is a solution of the heat equation in either x or y on $\text{int}\, D$; At $t=0$, $p^D_0(x,y) \geq 0$, $\forall x,y \in D$

When $x \in \text{bdy}\, D$ or $y \in \text{bdy}\, D$, $p^D_t(x,y) = 0$, $\forall t \geq 0$.

Therefore, we have $p^D_t(x,y) \geq 0$, $\forall t \geq 0$. $\forall x,y \in D$ by maximum principle.

Suppose that there exists a $t_0 > 0$, and $\hat{x}, \hat{y} \in \text{int}\, D$ s.t. $p^D_{t_0}(\hat{x},\hat{y}) = 0$. Then ~~$p^D_{t_0}$ attains its minimum~~ $(t_0, \hat{x}, \hat{y})$ is a minimum of p^D_t on $D \times D \times [0, t_0+1]$.

Since D is connected, and $p^D_t(x,y)$ satisfies the heat equ. in either x or y, we derive from the maximum principle that

$$p^D_{t_0}(x,y) = p^D_{t_0}(\hat{x},\hat{y}), \quad \forall x,y \in \text{int}\, D.$$

In particular, $p^D_{t_0}(x,x) = \sum_{n=1}^{|\text{int}\, D|} e^{-\lambda_n t} \left(\phi^D_n(x)\right)^2 = 0$, $\forall x \in \text{int}\, D$

That is, $\phi_n^D(x) = 0$, $\forall\, x \in \text{int}\, D$, $\forall\, n$

This is a contradiction.

(6). Since when $x \in \text{bdy}\, D$, $\sum_{y\in D} p_t^D(x,y) = 0$.

That is, we only need consider the case that $x \in \text{int}\, D$.

For any $x \in \text{int}\, D$, we first observe that

$$\sum_{y\in D} p_t^D(x,y) d_y \Big|_{t=0} = \sum_{y\in \text{int} D} p_t^D(x,y) d_y \Big|_{t=0} = 1.$$

Moreover, we calculate

$$\frac{\partial}{\partial t}\left(\sum_{y\in \text{int} D} p_t^D(x,y)\, d_y\right) = \sum_{y\in \text{int} D} \frac{\partial}{\partial t} p_t^D(x,y)\, d_y$$

$$= \sum_{y\in \text{int} D} \underset{\substack{\uparrow \\ \text{in } y}}{\Delta_D} p_t^D(x,y)\, d_y$$

$$= \langle \Delta_D p_t^D(x,\cdot),\, 1 \rangle \quad \text{where } 1(y) = \begin{cases} 1 & \text{if } y \in \text{int} D \\ 0 & \text{otherwise.} \end{cases}$$

$$= \langle p_t^D(x,\cdot),\, \Delta_D 1(\cdot) \rangle \quad \Delta_D 1(y) = \begin{cases} 0, & \text{if } y \in \text{int} D, \text{ and } S_1(y) \subset \text{int} D. \\ \frac{1}{d_y}\sum_{\substack{z\sim y \\ z\in \text{bdy} D}} (-1) & \text{if } y \in \text{int} D, \exists\, z\sim y,\, z \in \text{bdy} D. \end{cases}$$

$$= \sum_{\substack{y\in \text{int} D \\ \exists z\sim y \\ z\in \text{bdy} D}} p_t^D(x,y)\cdot \frac{1}{d_y} \sum_{\substack{z\sim y \\ z\in \text{bdy} D}} (-1) \cdot d_y$$

$$= \sum_{\substack{y\in \text{int} D \\ \exists z\sim y,\, z\in \text{bdy} D}} \sum_{\substack{z\sim y \\ z\in \text{bdy} D}} \left(- p_t^D(x,y)\right) < 0.$$

Therefore, we have

$$\sum_{y\in D} p_t^D(x,y) < 1 \quad \text{for } t > 1, \text{ and all } x \in D. \qquad \square$$

<u>Rmk</u>: Property (6) implies that a finite graph with Dirichlet boundary is <u>not</u> stochastically complete.

<u>Exhaustion by finite connected graphs</u>:

On a locally finite infinite graph $G=(V,E)$, we're going to construct a ~~fun~~ solution to the heat equation:

$$\begin{cases} \frac{\partial}{\partial t} u(x,t) = \Delta u(x,t), & \forall x \in V, \forall t > 0 \\ u(x,0) = \frac{\delta_y}{d_y}(x)., & \forall x \in V. \end{cases}$$

We start with an exhaustion sequence of the graph and its associated ~~Dir~~ heat kernels with Dirichlet boundary. This procedure was first ~~intro~~ introduced on manifold setting by Józef Dodziuk (1983). ~~and~~

Let us exhaust the graph G by balls $B_r(x_0)$ of increasing radii: $V_{B_r} = \{ x \in V : d(x, x_0) \leq r \}$

$$E_{B_r} = \{ \{x,y\} \in E : x, y \in V_{B_r} \}$$

Then we have a sequence of heat kernels

$$p_t^r := p_t^{B_r} : B_r \times B_r \times [0, \infty) \to \mathbb{R}.$$

<u>Lemma III.2.7</u>: $p_t^r(x,y) \leq p_t^{r+1}(x,y)$, $\forall t \geq 0$, $x,y \in B_r$.

<u>Proof</u>: If $y \in \operatorname{bdy} B_r$ or $x \in \operatorname{bdy} B_r$, we have

$$p_t^r(x,y) = 0 \leq p_t^{r+1}(x,y), \forall t \geq 0, \cancel{x,y \in}$$

For $y \in \operatorname{int} B_r$, consider the function

$$u(x,t) := p_t^{r+1}(x,y) - p_t^r(x,y)$$

Then it holds that

$$\frac{\partial}{\partial t} u(x,t) = \Delta u(x,t) \quad \text{for } x \in \operatorname{int} B_r,\ t \geq 0$$

Therefore, the minimum of u on $B_r \times [0,T]$, $T>0$ is attained on the set

$$B_r \times \{0\} \cup \operatorname{bdy} B_r \times [0,T].$$

On $B_r \times \{0\}$, we have $u = 0$.

On $\operatorname{bdy} B_r \times [0,T]$, we have $u(x,t) = p_t^{r+1}(x,y) - \overset{\overset{0}{\shortparallel}}{p_t^r(x,y)}$

$$= p_t^{r+1}(x,y) > 0.$$

In conclusion,

$$\min_{B_r \times [0,T]} u \geq 0.$$

That is $p_t^{r+1}(x,y) \geq p_t^r(x,y)$, $\forall x,y \in B_r$ and all $t \geq 0$. □

We extend $p_t^r(x,y)$ to be zero outside of B_r.

Then for given x,y, the sequence of functions

$$\Big\{ t \longmapsto \underset{\underset{f_r(t)}{\shortparallel}}{p_t^r(x,y)} \Big\}_{r=1}^{\infty}$$

is monotonic nondecreasing. Moreover, $0 \leq p_t^r(x,y) \leq 1$.

Therefore, they converge ~~to a finite number~~ pointwisely (in t).

Observe that for each r, and given x,y,

$$f_r(t) = p_t^r(x,y) \text{ is } C^\infty \text{ on } [0, \infty)$$

~~For any~~ Let us denote by

$$f(t) := p_t(x,y) = \lim_{r \to \infty} p_t^r(x,y)$$