Estimates for the Heat Kernel on Weighted Graphs

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Why study Laplacians on Graphs?

- Heat transport in structured solids — integrated circuits.
- Quantum Mechanics — The Schrödinger operator on graphs.
- Non-commutative geometry — graphs are an instructive model.

References

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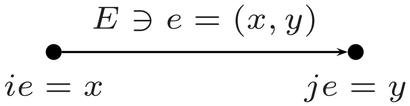
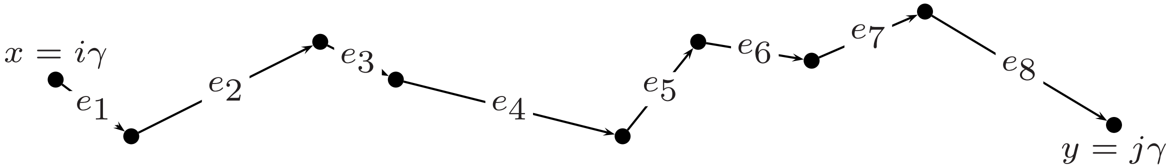
The Graph-Theoretic Setting

Graph : A countable set X of vertices $\{x, y, \dots\}$.

Edges : $E \subset X \times X \setminus \text{Diag}$.



Paths : $\Gamma(x, y) \stackrel{\text{def}}{=} \left\{ \gamma = (e_1, \dots, e_m) \subset E \;\middle|\; ie_1 = x,\ je_m = y,\ ie_{k+1} = je_k \right\}.$



$|\gamma| \stackrel{\text{def}}{=} m$ is the **length** of γ. The **combinatorial distance** between x and y is

$$d_0(x, y) \stackrel{\text{def}}{=} \min\{\, |\gamma| \mid \gamma \in \Gamma(x, y)\}\,.$$

X is assumed to be **connected**, that is, $\Gamma(x, y) \neq \varnothing$, for all $x, y \in X$.

Weights : A mapping $b\colon E \longrightarrow (0, \infty)$. We assume that X is **symmetric**, that is,

$$e = (x, y) \in E \Rightarrow \overline{e} = (y, x) \in E \text{ and } b(\overline{e}) = b(e).$$

The Laplacian and Heat Kernel on X

The discrete Laplacian on X is the operator $\Delta\colon l^2(X) \longrightarrow l^2(X)$ defined by

$$\Delta f(x) \stackrel{\text{def}}{=} \sum_{e\in E, ie=x} b(e)\big(f(je) - f(x)\big).$$

It is **bounded** and **nonnegative**. It generates a strongly continuous **semigroup**, and thus gives rise to a continuous-time **Markov process** with transition probabilities

$$p_t(x,y) = \left(\mathrm{e}^{\Delta t}\delta_x\right)(y), \quad x, y \in X,$$

where $\delta_x \in l^2(X)$ is the unit mass concentrated at the site $x \in X$. The function $p_t(x,y)$ is called the **heat kernel** on X. The Markov chain $(X_t \mid t \geq 0)$ 'jumps' from site x to a neighbouring site y with probability

$$\frac{b\big((x,y)\big)}{\sum_{\substack{e\in E,\\ ie=x}} b(e)}.$$

That means, the weight b measures the 'conductance' of edges.

The Result of Metzger and Stollmann [MS00]

Assume that

$$b_{\max} \stackrel{\text{def}}{=} \sup_{e \in E} b(e) < \infty, \quad \text{and} \quad M \stackrel{\text{def}}{=} \sup_{x \in X} \big| \{ e \in E \mid ie = x \} \big| < \infty.$$

Then holds for $x, y \in X$, $t \geq 0$:

$$\frac{\mathrm{e}^{-b_{\max} M t}}{\sqrt{2\pi}} \sup_{\gamma \in \Gamma(x,y)} \left(\prod_{e \in \gamma} \frac{t b(e)}{|\gamma|} \right)$$

$$\leq$$

$$p_t(x, y)$$

$$\leq$$

$$\mathrm{e}^{b_{\max} M t + 1} \sup_{\gamma \in \Gamma(x,y)} \left(\prod_{e \in \gamma} \frac{b(e)}{b_{\max}} \right) \left(\frac{\mathrm{e} M b_{\max} t}{d_0(x, y)} \right)^{d_0(x,y)} .$$

Stochastic Interpretation of the Estimates

For the **holding time** of X_t at site x we have the probability distribution

$$\mathbb{P}\Big[\inf\{\, s > t \mid X_s(\omega) \neq X_t(\omega)\} > t + h \;\Big|\; X_t(\omega) = x\Big] = \exp\left[-h \sum_{ie=x} b(e)\right] .$$

That is, the probability of jumping from x to a neighbour in less than h time-units is

$$1 - \exp\left[-h \sum_{ie=x} b(e)\right] \sim \left(h \sum_{ie=x} b(e)\right) .$$

In the upper estimate, we must make $d_0(x, y)$ jumps in the time-interval $[0, t]$, thus $h \sim \dfrac{t}{d_0(x, y)}$. Now $\sum_{ie=x} b(e) \leq M b_{\max}$. This gives a probability for making a way of length $d_0(x, y)$ in time t:

$$\left(\frac{M b_{\max} t}{d_0(x, y)}\right)^{d_0(x,y)} .$$

A Special Lower Estimate

Assume further

$$b_{\min} \stackrel{\text{def}}{=} \inf_{e \in E} b(e) \geq 0 \text{ and } N \stackrel{\text{def}}{=} \inf_{x \in X} \left| \{ e \in E \mid ie = x \} \right| \geq 1.$$

Inserting into the lower estimate one obtains

$$p_t(x,y) \geq \frac{\mathrm{e}^{-b_{\max} M t}}{\sqrt{2\pi}} \sup_{\gamma \in \Gamma(x,y)} \left(\frac{t b_{\min}}{|\gamma|} \right)^{|\gamma|} = \frac{\mathrm{e}^{-b_{\max} M t}}{\sqrt{2\pi}} \sup_{k \geq d_0(x,y)} \left(\frac{t b_{\min}}{k} \right)^{k}.$$

Now, $(t b_{\min}/x)^x$ is maximal at $x = t b_{\min}/\mathrm{e}$ and monotonuously decreasing for $k \geq d_0(x,y) > t b_{\min}/\mathrm{e}$ with supremum at $k = d_0(x,y)$. This yields the two cases:

$$p_t(x,y) \geq \begin{cases} (1-E) \cdot \dfrac{\mathrm{e}^{t(b_{\min}/\mathrm{e} - b_{\max} M)}}{\sqrt{2\pi}}, & \text{if } d_0(x,y) \leq t b_{\min}/\mathrm{e}; \\[2ex] \dfrac{\mathrm{e}^{-b_{\max} M t}}{\sqrt{2\pi}} \left(\dfrac{t b_{\min}}{d_0(x,y)} \right)^{d_0(x,y)}, & \text{otherwise.} \end{cases}$$

The cut-off error $E \geq 0$ depends on $t/b_{\min}$.

A Physical Interpretation of the Estimates

The estimates represent a balance between diffusion and conductance:

$$\frac{\mathrm{e}^{-b_{\max}Mt}}{\sqrt{2\pi}} \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma} \frac{tb(e)}{|\gamma|} \right)$$

$$\leq$$

$$p_t(x,y)$$

$$\leq$$

$$\mathrm{e}^{b_{\max}Mt+1} \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma} \frac{b(e)}{b_{\max}} \right) \left(\frac{\mathrm{e}Mb_{\max}t}{d_0(x,y)} \right)^{d_0(x,y)} .$$

But a diffusive term is missing in the upper estimate.

Derivation of the (New) Upper Estimate: Basic Principles

We represent the heat kernel as

$$p_t(x,y) = \lim_{n\to\infty} \left[\left(I + \frac{t}{n}\Delta \right)^n \delta_x \right](y).$$

Define operators on $l^2(X)$ by

$$Sf(x) \overset{\text{def}}{=} \sum_{ie=x} b(e) f(je),$$ that is, the ‘off-diagonal’ part of Δ, and

$$D \overset{\text{def}}{=} \Big(-\sum_{ie=x} b(e) \Big) \mathbb{I}, \quad D_{\min} \overset{\text{def}}{=} -N b_{\min} \mathbb{I}, \quad D_{\max} \overset{\text{def}}{=} -M b_{\max} \mathbb{I}.$$

Then $\Delta = D + S$ and the estimates $D_{\max} \le D \le D_{\min} \le 0$ entail by induction:

Lemma: For $f \in l^2(X)$, $f \ge 0$, $n \in \mathbb{N}$, and $s > 0$ small enough holds

$$0 \le \big(\mathbb{I} + s(D_{\max} + S) \big)^n f \;\le\; (\mathbb{I} + s\Delta)^n f \;\le\; \big(\mathbb{I} + s(D_{\min} + S) \big)^n f.$$

Derivation of the Upper Estimate: Calculation 1

$$\left[\left(\mathbb{I} + \frac{t}{n}\Delta\right)^n \delta_x\right](y) \leq \left[\left(\mathbb{I} - \frac{tNb_{\min}}{n}\mathbb{I} + \frac{t}{n}S\right)^n \delta_x\right](y)$$

$$= \sum_{k=0}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \cdot \left[\left(\frac{t}{n}S\right)^k \delta_x\right](y)$$

$$b(\gamma) \stackrel{\text{def}}{=} \prod_{e\in\gamma} b(e) \Longrightarrow S^k\delta_x = \sum_{\substack{i\gamma=x,\\ |\gamma|=k}} b(\gamma)\delta_{j\gamma} \Longrightarrow \left(S^k\delta_x\right)(y) = \sum_{\substack{\gamma\in\Gamma(x,y),\\ |\gamma|=k}} b(\gamma).$$

$$= \sum_{k=0}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \cdot \left(\frac{t}{n}\right)^k \sum_{\substack{\gamma\in\Gamma(x,y),\\ |\gamma|=k}} b(\gamma).$$

Derivation of the Upper Estimate: Calculation 2

$$= \sum_{k=0}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \cdot \left(\frac{t}{n}\right)^{k} \sum_{\substack{\gamma\in\Gamma(x,y),\\ |\gamma|=k}} b(\gamma)$$

We use:

- Only terms with $k \geq d_0(x,y)$ contribute to the overall sum.
- $\#\{\gamma \in \Gamma(x,y) \mid |\gamma| = k\} \leq M^k$. Therefore $\Longrightarrow$
- $\displaystyle\sum_{\substack{\gamma\in\Gamma(x,y)\\ |\gamma|=k}} b(\gamma) \leq M^k \sup_{\substack{\gamma\in\Gamma(x,y)\\ |\gamma|=k}} b(\gamma) = M^k \sup_{\substack{\gamma\in\Gamma(x,y)\\ |\gamma|=k}} \prod_{e\in\gamma} b(e).$

$$\leq \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma} \frac{b(e)}{b_{\max}}\right) \sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k}.$$

Derivation of Upper Estimate: Application of Stirling's Formula

The sum has the structure

$$\sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k} = \sum_{k=m}^{n} \binom{n}{k} \left(1 - \frac{d}{n}\right)^{n-k} \left(\frac{c}{n}\right)^{k}$$

$$= \left(1 - \frac{d}{n}\right)^{n} \sum_{k=m}^{n} \binom{n}{k} \left(\frac{c}{n-d}\right)^{k} = \left(1 - \frac{d}{n}\right)^{n} \sum_{k=m}^{n} \binom{n}{k} \left(\frac{c'}{n}\right)^{k},$$

with $c' = \dfrac{c}{1 - d/n}$. Stirling's formula: $\Gamma(z) = z^z \mathrm{e}^{-z} \mathrm{e}^{\vartheta/(12z)} \sqrt{2\pi/z}$, with $\vartheta \in (0, 1)$, entails (see [MS00, Lemma 3(b)]):

$$\leq \left(1 - \frac{d}{n}\right)^{n} \left(\frac{c'}{m}\right)^{m} \left(1 + \frac{m}{n-m}\right)^{n-m} \mathrm{e} \sqrt{1 + \frac{m}{n-m}}\, \mathrm{e}^{\frac{1}{12(n-1)}} \left(1 + \frac{c'}{n}\right)^{n-m}$$

Derivation of Upper Estimate: The Limit $n \to \infty$

$$
\begin{array}{ccccccccccc}
=\left(1-\frac{d}{n}\right)^{n} & & \left(\frac{cn}{m(n-d)}\right)^{m} & & \left(1+\frac{m}{n-m}\right)^{n-m} & & \mathrm{e}\sqrt{1+\frac{m}{n-m}} & & \mathrm{e}^{\frac{1}{12(n-1)}} & & \left(1+\frac{c}{n-d}\right)^{n-m} \\
\downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow \\
\mathrm{e}^{d} & \cdot & \left(\frac{c}{m}\right)^{m} & \cdot & \mathrm{e}^{m} & \cdot & \mathrm{e} & \cdot\ 1 & \cdot & 1 & \cdot\ \mathrm{e}^{c}
\end{array}
$$

Re-inserting $m = d_0(x, y)$, $d = tNb_{\min}$, and $c = tMb_{\max}$ we obtain

$$
\lim_{n\to\infty} \sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k}
$$

$$
\leq \mathrm{e}^{-tNb_{\min}} \left(\frac{\mathrm{e}tMb_{\max}}{d_0(x, y)}\right)^{d_0(x,y)} \mathrm{e}^{tMb_{\max}+1}.
$$

The Upper Estimate

Collecting all results we finally get

$$p_t(x, y) \leq \mathrm{e}^{-tNb_{\min}} \mathrm{e}^{tMb_{\max}+1} \sup_{\gamma \in \Gamma(x,y)} \left(\prod_{e \in \gamma} \frac{b(e)}{b_{\max}} \right) \left(\frac{\mathrm{e} t M b_{\max}}{d_0(x, y)} \right)^{d_0(x,y)} .$$

The **diffusive term** $\mathrm{e}^{-tNb_{\min}}$ tends to 1 for $b_{\min} \longrightarrow 0$, reproducing the upper estimate of [MS00] in this case. Thus we obtained a proper generalization.