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A Note on Heat Kernel Estimates on Weighted Graphs with Two-Sided Bounds on the Weights [*†]

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Abstract

We reconsider estimates for the heat kernel on weighted graphs recently found by Metzger and Stollmann. In the case that the weights satisfy a positive lower bound as well as a finite upper bound, we obtain a specialized lower estimate and a proper generalization of a previous upper estimate.

Estimates for the heat kernels on graphs have recently attracted the interest of mathematical physicists [1, 2, 5]. In [6], Metzger and Stollmann derived physically significant upper and lower bounds for the heat kernel on a weighted graph which also give rise to a probabilistic interpretation in terms of stochastic processes. They considered the case that the 'heat conductance', that is, the weight function on the edges of the graph, is bounded from above. Here, we follow their lucent method of proof under the additional assumption that there is also a strictly positive lower bound on the weights. This case seems to be of physical relevance, for example, in the modeling of heat transport in structured media. It turns out that, while the lower estimate takes on a special form under this assumption, the upper estimate becomes properly generalized and tends to the upper estimate of [6] when the lower bound on the weights tends to zero. Our refinement of the upper estimate amounts physically to the appearance of a 'diffusive' term governed by the minimal conductance and limiting the transition probability. We may note, that the results of Davies [4, 3] are now completely rendered as special cases of the estimates that can be derived by the method of Metzger and Stollmann.

We first fix notation as in [6]: We consider a countable set of vertices X and edges $E \subset X \times X$ of a directed graph. For $E \ni e = (x, y)$ we write $x = ie$, $y = je$. The weight $b : E \to (0, \infty)$ is assumed to be symmetric, that is, for $e = (x, y) \in E$ we have $\overline{e} = (y, x) \in E$ and $b(\overline{e}) = b(e)$. Further $(x, x) \notin E$ for all $x \in X$. We denote by $b_{\max}$ the upper bound on the weight: $b_{\max} = \sup_{e \in E} b(e)$, and assume that $b_{\max} < \infty$.

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There shall be an uniform upper bound $M = \sup_{x\in X} |\{e \in E|\ ie = x\}|$ on the number of edges emanating from a vertex.

In addition to the assumptions of [6] just stated, we assume that the weights on the graph also satisfy a lower bound $b_{\min} = \inf_{e\in E} b(e) \geq 0$ (this is a stronger assumption than in [6], of course, only if $b_{\min} > 0$, see below). We denote by $N = \inf_{x\in X} |\{e \in E|\ ie = x\}|$ the minimum number of edges connecting to a vertex.

The Laplacian on this graph is the bounded and non-negative operator $\Delta : l^2(X) \to l^2(X)$ given by

$$\Delta f(x) = \sum_{e\in E, ie=x} b(e)\left(f(je) - f(x)\right).$$

The heat kernel then is the transition probability $p_t(x,y) = \left(e^{\Delta t}\delta_x\right)(y)$ of the continuous-time Markov process generated by Δ, where δ_x is the unit mass concentrated at x.

The estimates for $p_t(x,y)$ involve the notion of paths from x to y. By this we mean finite sequences $\gamma = (e_1, \ldots, e_m)$ with $ie_1 = x$, $je_m = y$, $je_k = ie_{k+1}$. The number $|\gamma| = m$ is called the length of γ. The set $\Gamma(x,y)$ of paths from x to y is nonempty since we assume the graph to be connected. Therefore we also have $N \geq 1$. The function $d_0(x,y) = \min\{|\gamma|\mid \gamma \in \Gamma(x,y)\}$ on $X \times X$ is called the combinatorial distance from x to y and defines a metric on the graph.

The above assumptions lead in a straightforward manner to the special case for the lower bound in [6, Theorem 1]:

$$\begin{aligned} p_t(x,y) &\geq \frac{e^{-b_{\max}Mt}}{\sqrt{2\pi}} \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma} \frac{tb(e)}{|\gamma|}\right) \\ &\geq \frac{e^{-b_{\max}Mt}}{\sqrt{2\pi}} \sup_{\gamma\in\Gamma(x,y)} \left(\frac{tb_{\min}}{|\gamma|}\right)^{|\gamma|} = \frac{e^{-b_{\max}Mt}}{\sqrt{2\pi}} \sup_{k\geq d_0(x,y)} \left(\frac{tb_{\min}}{k}\right)^{k}. \end{aligned}$$

The function $(tb_{\min}/x)^x$ takes its maximum at $x = tb_{\min}/e$, thus we find for $d_0(x,y) \leq tb_{\min}/e$ that

$$p_t(x,y) \geq (1-E) \cdot \frac{e^{t(b_{\min}/e - b_{\max}M)}}{\sqrt{2\pi}},$$

with a relative cut-off error $E \geq 0$ caused by the fact that $k \in \mathbb{N}$ and depending on $t/b_{\min}$ (E can be estimated by looking at the Taylor expansion of $(tb_{\min}/x)^x$ around the maximum). In the other case $k \geq d_0(x,y) > tb_{\min}/e$, the function $(tb_{\min}/k)^k$ is decreasing and thus the supremum is attained at $k = d_0(x,y)$, yielding

$$p_t(x,y) \geq \frac{e^{-b_{\max}Mt}}{\sqrt{2\pi}} \left(\frac{tb_{\min}}{d_0(x,y)}\right)^{d_0(x,y)}.$$

More interesting is the new upper bound we obtain under the assumption $b_{\min} \geq 0$. We first note that the basic upper estimate for the Laplacian in [6, Lemma 2] becomes in our case:

$$(I + s\Delta)^n f \leq (I + s(D_{\min} + S))^n f,$$

for sufficiently small positive s, $n \in \mathbb{N}$, and every positive $f \in l^2(X)$. Here, $D_{\min}$ is the operator of multiplication by $-Nb_{\min}$ and S is the off-diagonal part

$$Sf(x) = \sum_{ie=x} b(e) f(je).$$

We essentially repeat the derivation of the upper bound in [6], and approximate the heat kernel as follows:

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

Using the basic estimate above, we can estimate the n-th order approximation by

$$\begin{aligned} \left[\left(I + \frac{t}{n}\Delta \right)^n \delta_x \right](y) &\leq \left[\left(I - \frac{tNb_{\min}}{n} I + \frac{t}{n} S \right)^n \delta_x \right](y) \\ &= \sum_{k=0}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n} \right)^{n-k} \cdot \left[\left(\frac{t}{n} S \right)^k \delta_x \right](y) \\ &\leq \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma} \frac{b(e)}{b_{\max}} \right) \cdot \Sigma, \end{aligned}$$

where

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

Now

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

with $c' = c/(1-d/n)$. Thus we can apply [6, Lemma 3(b)] to yield the estimate

$$\begin{aligned} \sum_{k=m}^{n} \binom{n}{k} \left(1 - \frac{d}{n} \right)^{n-k} \left(\frac{c}{n} \right)^k &\leq \left(\frac{cn}{m(n-d)} \right)^m e \left(1 + \frac{m}{n-m} \right)^{n-m} \\ &\quad \cdot \sqrt{1 + \frac{m}{n-m}} e^{\frac{1}{12(n-1)}} \left(1 + \frac{c}{n-d} \right)^{n-m}. \end{aligned}$$

Putting it all together and performing the limit $n \to \infty$ we get the final result

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

For $b_{\min} \to 0$ this degenerates to the upper estimate of [6] and thus represents a proper generalization of it.

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