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], Bernd Metzger and Peter 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', *i.e.*, 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, *e.g.*, in the modelling 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 $b\colon E \to (0,\infty)$ is assumed to be symmetric, *i.e.*, 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 $b_{\max} < \infty$. There shall be an uniform upper

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bound $M = \sup_{x\in X} \left|\{e \in E \mid ie = x\}\right|$ 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 $N = \inf_{x\in X} \left|\{e \in E \mid ie = x\}\right|$ the minimum number of edges connecting to a vertex.

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

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

The heat kernel then is the transition probability $p_t(x,y) = \big(\mathrm{e}^{\Delta t}\delta_x\big)(y)$ 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 $\gamma = (e_1,\dots,e_m)$ 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 straightforwardly lead to special case for the lower bound in [6, Theorem 1]:

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

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

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

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 $k \geq d_0(x,y) > tb_{\min}/\mathrm{e}$, the function $(tb_{\min}/k)^k$ is monotonuously decreasing and thus the supremum is attained at $k = d_0(x,y)$, yielding

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

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:

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

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

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

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

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

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

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

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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