Pointwise upper estimates for transition probability of continuous time random walks on graphs

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Continuous Time Random Walk

Let $\Gamma = (\mathbb{V}, \mathbb{E})$ be a connected, locally finite graph without double edges.

Let $\mu = (\mu_{xy})$ be an edge weight function on $\mathbb{E}$, such that $\mu_{xy} = \mu_{yx} > 0$ for each $(x, y) \in \mathbb{E}$, while $\mu_{xy} = 0$ for each $(x, y) \notin \mathbb{E}$.

Let $\nu = (\nu_x)$ be a positive vertex weights on $\mathbb{V}$.

Denote by $X = \{X_t : t \geq 0\}$ a continuous time random walk on $\Gamma$ with generator

$$\mathcal{L} f(x) = \frac{1}{\nu_x} \sum_{y \in \mathbb{V}} (f(y) - f(x))\mu_{xy}.$$
If $\nu_x = \sum \mu_{xy}$ and $\mu_{xy} \in \{0, 1\}$ for all $x, y$, then the process $X$ is called continuous time simple random walk on $\mathbb{V}$. It is a process that waits an exponential time mean 1 at each vertex and then jumps along one of its neighbor uniformly.

If $\nu_x \equiv 1$, then the expected waiting time of each jump may vary greatly. Moreover, such a process may explode in finite time. For example, $\Gamma = \mathbb{Z}^+$, $\mu_{x-1,x} = 2^x$. 
Fix vertices \( x_1, x_2 \) and functions \( f_1, f_2 \) such that

\[
\mathbb{P}_{x_i}(X_t = x_i) \leq \frac{1}{f_i(t)}.
\]

Our interest is, under what circumstance \( \mathbb{P}_{x_1}(X_t = x_2) \) will have Gaussian upper bounds. For example, Let \( X \) be a continuous time simple random walk on \( \mathbb{Z}^d \). We have

\[
\mathbb{P}_x(X_t = x) \leq \frac{C}{t^{d/2}};
\]

and

\[
\mathbb{P}_x(X_t = y) \leq \frac{c}{t^{d/2}} \exp \left( -\frac{C \|x - y\|^2}{t} \right).
\]

for any \( t \geq \|x - y\| \).
The problem of getting a Gaussian upper bound from two point estimates was introduced in the manifold case by Grigor’yan (1997). In the subsequent researches, Coulhon, Grigor’yan & Zucca (2005) studied the problem for discrete time random walks on graphs, while Folz (2011) studied in the continuous time random walks. The current paper considers the same problem, however, it improves the result of Folz(2011) by · · ·.

Barlow and Chen, Gaussian bounds and Parabolic Harnack inequality on locally irregular graphs, In preparation.


Grigor’yan and Yau (2003), Isoperimetric properties of higher eigenvalues of elliptic operators, Amer. J. Math.

Chung and Yau (1999), Coverings, heat kernels and spanning trees, The electronic journal of combinatorics.
Let $d_\nu(\cdot, \cdot)$ be a metric of $\Gamma$ such that

\[
\begin{align*}
\frac{1}{\nu_x} \sum_y d_\nu(x, y)^2 \mu_{xy} &\leq 1 \quad \text{for all } x \in \mathbb{V}, \\
d_\nu(x, y) &\leq 1 \quad \text{whenever } x, y \in \mathbb{V} \text{ and } x \sim y.
\end{align*}
\] (1)

Metrics satisfying (1) are called adapted metrics. Such metrics were initiated by Davies (1993), and are closely related to the intrinsic metric associated with a given Dirichlet form. Intuition: If $\mu_{xy}$ is larger, then more quickly for a particle transfers from $x$ to $y$ and so $d_\nu(x, y)$ should be smaller.
Let $f : \mathbb{R}_+ \to \mathbb{R}_+$. Let $A \geq 1$ and $\gamma > 1$. We say that $f$ is $(A, \gamma)$-regular if the function $f$ is increasing and satisfies that

$$\frac{f(\gamma s)}{f(s)} \leq A \frac{f(\gamma t)}{f(t)} \quad \text{for all } t \geq s \geq 0,$$

which was introduced by Grigor’yan (1997).

For example, $t^n, e^{t^{1/2}}, e^t$;

$$f(t) = \begin{cases} 
ct & \text{if } t \leq T_1, \\
Ct^2 & \text{if } t > T_1;
\end{cases}$$

In particular, if Volume Doubling holds, that is, $V(x, 2r) \leq CV(x, r)$ then

$$f(t) = V(x, \sqrt{t}).$$

is regular.
Theorem (Grigor’yan) Let $x_1, x_2$ be distinct points on a smooth Riemannian manifold $M$, and suppose that there exist $(A, \gamma)$–regular functions $g_1, g_2$ such that, for all $t > 0$ and $i \in \{1, 2\}$,

$$q_t(x_i, x_i) \leq \frac{1}{g_i(t)}$$

Then for any $D > 2$ and all $t > 0$, the Gaussian upper bound

$$q_t(x_1, x_2) \leq \frac{4A}{g_1(\delta t)g_2(\delta t)} \exp \left( -\frac{d(x_1, x_2)^2}{2Dt} \right)$$

holds, where $\delta = \delta(D, \gamma)$. 
Theorem (Coulhon, Grigor’yan and Zucca) Let $(\Gamma, \mu)$ be a weighted graph satisfying condition $\inf_{x \in V} P_x(X_1 = x) \geq \alpha > 0$. Let $x_1, x_2$ be two fixed vertices in $\Gamma$, and assume that there are two $(A, \gamma)$–regular functions $g_1, g_2$ such that, for all $k \in \mathbb{N}$,

$$h_{2k}(x_i, x_i) \leq \frac{1}{g_i(k)}.$$

Then, for all $k \in \mathbb{N}$,

$$h_k(x_1, x_2) \leq \frac{C_0}{g_1(\eta k)g_2(\eta k)} \exp \left( -\frac{d(x_1, x_2)^2}{2D_0k} \right),$$

where $\eta = \eta(\gamma) > 0$, $D_0 = D_0(\alpha, \gamma) > 0$ and $C_0 = C_0(A, \alpha, \gamma)$. 
Let $p_t(x, y) = \frac{P_x(X_t = y)}{\nu_y}$.

**Theorem A (Folz 2011)**

Suppose there exists $C_\nu > 0$ such that $\nu_x \geq C_\nu$ for all $x$. Let $g_1, g_2$ be $(A, \gamma)$-regular functions satisfying

$$g_i(t) \leq Ae^{t^{1/2}}. \quad (3)$$

Suppose that

$$p_t(x_i, x_i) \leq \frac{1}{g_i(t)}. \quad (4)$$

Then there exists $C_1(A, \gamma, C_\nu), C_2(\gamma)$ and $\alpha(\gamma) > 0$, such that for all $t \geq d_\nu(x_1, x_2),

$$p_t(x_1, x_2) \leq \frac{C_1}{\sqrt{g_1(\alpha t)g_2(\alpha t)}} \exp \left( -\frac{C_2 d_\nu(x_1, x_2)^2}{t} \right). \quad (5)$$
However, our work improves the result of Folz (2011) by no longer requiring a lower bound on $\nu_x$. The improvement comes from imposing conditions on the transition probabilities $P_x(X_t = x)$ instead of the heat kernels $p_t(x, x)$. Note that the transition probabilities are invariant under the transformation from $(\mu, \nu)$ to $(c\mu, c\nu)$, where $(c\mu)_{xy} = c\mu_{xy}$ and $(c\nu)_x = c\nu_x$. 
Theorem 1

Suppose

\[ P_{x_i}(X_t = x_i) \leq \frac{1}{f_i(t)}. \]  \hspace{1cm} (6)

Let \( \delta \geq 1 \). If each \( f_i \) is \((A, \gamma)\)-regular and satisfies

\[ f_i(t) \leq Ae^{\delta t} \text{ for all } t \in \mathbb{R}_+, \]  \hspace{1cm} (7)

then there exist universal positive constants \( C_1 \) and \( \theta \), such that for any \( t \geq d_\nu(x_1, x_2) \) we have

\[ P_{x_1}(X_t = x_2) \leq \frac{C_1A^\beta(\nu_{x_2}/\nu_{x_1})^{1/2}}{\sqrt{f_1(\alpha t)f_2(\alpha t)}} \exp \left( -\theta \frac{d_\nu(x_1, x_2)^2}{t} \right), \]  \hspace{1cm} (8)

where \( \alpha = \min\{(2\gamma)^{-1}, (64\delta)^{-1}\} \) and \( \beta = \left\lceil \frac{\log \gamma}{\log 2} \right\rceil \).
Remark 1. The condition (7) is quite natural. Note that $\mathbf{P}_x(X_t = x) \geq \exp\left(-\frac{\mu_x}{\nu_x} t\right)$, where $\mu_x = \sum_y \mu_{xy}$. It implies that (7) holds if $A = 1$ and $\delta = \max\{\frac{\mu_{x_1}}{\nu_{x_1}}, \frac{\mu_{x_2}}{\nu_{x_2}}\}$. In particular, for CSRW one can take $\delta = 1$.

Remark 2. One can also trace the values of $C_1$ and $\theta$. Indeed, we select $\theta = 10^{-7}$ in our proof.

Remark 3. It is potentially very useful for random walks in random environments where one may lack global regularity.

**Lemma.** There exist random variables $T_x(\omega) < \infty$ and non-random constants $c_1, c_2$ such that almost surely, for all $x \in G(\omega)$ and $t > 0$,

$$q^\omega_t(x, x) \leq \begin{cases} 
c_1 t^{-1/2} & \text{if } 0 < t \leq T_x(\omega) \\
c_2 t^{-d/2} & \text{if } t > T_x(\omega).
\end{cases}$$

The theorem above shows that if $t \geq C_1(T_x \lor T_y) \lor d(x, y)$ then we have the Gaussian upper bound

$$q_t(x, y) \leq C_2 t^{-d/2} \exp \left( -C_3 \frac{d(x, y)^2}{t} \right).$$
Let $I$ be an interval of $\mathbb{R}_+$. We say that $u : I \times \mathbb{V} \mapsto \mathbb{R}_+$ is a positive subsolution on $I \times \mathbb{V}$ if

$$\frac{\partial}{\partial t} u \leq Lu \quad \text{on} \quad I \times \mathbb{V}.$$ 

Furthermore, we define a set of functions:

$$\mathcal{H}(I) = \{ u : \text{$u$ is a positive subsolution on $I \times \mathbb{V}$ and} \}
|\{z \in \mathbb{V} : u(t, z) \neq 0, t \in I\}| < \infty\}.$$ 

Let $o \in B \subseteq \mathbb{V}$ with $|B| < \infty$. Set

$$u_B(t, z) = \frac{\nu_0^{1/2}}{\nu_z} P_o(X_t = z, \inf\{s \geq 0 : X_s \notin B\} > t). \quad (9)$$

Then $u_B \in \mathcal{H}(\mathbb{R}_+)$. 
Question: Let $u$ be a positive subsolution. Does there exist a sequence of positive subsolutions $u_n, n = 1, 2, \cdots$, such that, each $u_n$ has finite support and $(u_n)$ converges to $u$ in some sense?
For any functions $f, g$ on $\mathbb{V}$, define
\[
\langle f, g \rangle = \sum_{x \in \mathbb{V}} f(x)g(x)\nu_x.
\]

**Integral Maximum Principle**

Let $h$ be a positive function on $\mathbb{I} \times \mathbb{V}$ and $u \in \mathcal{H}(\mathbb{I})$. If for each $t \in \mathbb{I}$ one has
\[
\frac{1}{\nu_y} \sum_x \frac{|h(t, x) - h(t, y)|^2}{4h(t, x)h(t, y)} \mu_{xy} \leq -\frac{\partial}{\partial t} \log h(t, y) \quad \text{for all} \quad y \in \mathbb{V},
\]
then $J(t) = \langle u^2(t, \cdot), h(t, \cdot) \rangle$ is decreasing on $\mathbb{I}$. 
Owing to the Adapted metric $d_\nu$, it leads immediately to Corollary as follows. Define a set of functions:

\[ \mathcal{F}(\mathbb{I}) = \{ h : h \text{ is a positive function on } \mathbb{I} \times \mathbb{V} \text{ and for each } t \in \mathbb{I}, x \sim y, \frac{|h(t, x) - h(t, y)|^2}{4h(t, x)h(t, y)} \leq -d_\nu(x, y)^2 \frac{\partial}{\partial t} \log h(t, y) \}. \]

**Corollary**

Let $u \in \mathcal{H}(\mathbb{I})$ and $h \in \mathcal{F}(\mathbb{I})$. Then $J(t) = \langle u^2(t, \cdot), h(t, \cdot) \rangle$ is decreasing on $\mathbb{I}$. 
Let $\rho(\cdot) = d_\nu(o, \cdot) \land R$ for some $o \in \mathbb{V}$ and $R \geq 0$.

**Example 2**

*Fix $a \in [0, \frac{1}{4}]$. Let $h_1(t, x) = e^{a \rho(x) - \frac{a^2}{2} t}$. Then $h_1 \in \mathcal{F}(\mathbb{R}_+)$.***

**Example 3**

*Fix $\tau > 0$. For each $t \geq 0$ and $z \in \mathbb{V}$, set

$$h(t, z) = \exp \left\{ \left( \rho(z) - 4^{-1} e^{(t + \tau)} \right) \log \left( 1 \lor \frac{\rho(z)}{4^{-1} e^{(t + \tau)}} \right) - \frac{t}{\tau} \right\}.$$

*Then $h(t, z) \in \mathcal{F}(\mathbb{R}_+)$.***
Set $\mathcal{H}_o = \{u \in \mathcal{H}(\mathbb{R}_+) : u(0, z) = \nu_o^{-1/2} 1_{\{o\}}(z) \text{ for each } z \in \mathbb{V} \}$.

**Proposition 4**

Let $u \in \mathcal{H}_o$. For any $t, R > 0$, we have

$$\langle u(t, \cdot)^2, 1 - 1_{B_R} \rangle \leq \exp \left( -\frac{R^2}{8t} \right) \text{ if } t \geq R.$$  

Proof. Let $a = \frac{4R}{t}$. Then $a \in [0, \frac{1}{4}]$. Obviously,

$$\langle u(t, \cdot)^2, 1 - 1_{B_R} \rangle \leq \langle u(t, \cdot)^2, e^{a\rho(x) - \frac{a^2}{2}t} \rangle e^{-aR + \frac{a^2}{2}t}.$$  

By the Integer Maximum Principle,

$$\langle u(t, \cdot)^2, e^{a\rho(x) - \frac{a^2}{2}t} \rangle \leq \langle u(0, \cdot)^2, e^{a\rho(x)} \rangle = 1.$$
Corollary 5

For any \( z \in \mathbb{V} \),

\[
\mathbb{P}_o(X_t = z) \leq (\nu_z/\nu_o)^{1/2} \exp \left\{ -\frac{r^2}{16t} \right\} \text{ if } t \geq r > 0,
\]

where \( r = d_\nu(o, z) \).

The intuition of our main theorem can be seen from Corollary 5, if \( f_1 = f_2 \equiv 1 \) are selected as the trivial upper bounds.
Corollary

For any $z \in \mathbb{V}$,

$$P_o(X_t = z) \leq (\nu_z/\nu_o)^{1/2} \exp \left( -\frac{r}{2} \log \left( \frac{1.01r}{t} \right) + 60 \right) \text{ if } r \geq t > 0,$$

where $r = d_\nu(o, z)$. 
Compared with Theorems B and C, Corollaries 5 and 6 work more efficiently when \( t \in [0.9r, 1.1r] \) and \( r = d_\nu(o, z) \) is large.

**Theorem B (Folz 2011)**

*If \( x, y \in \mathcal{V} \), then for all \( t > 0 \),*

\[
p_t(x, y) \leq (\nu_x \nu_y)^{-1/2} \exp \left( -\frac{r^2}{2t} \left( 1 - \frac{r}{t} \right) - \Lambda t \right),
\]

*where \( r = d_\nu(x, y) \) and \( \Lambda \geq 0 \) is the bottom of the \( L^2 \) spectrum of the operator \( L_\nu \).*

**Theorem C (Folz 2011)**

*If \( x, y \in \mathcal{V} \), then for all \( t > 0 \),*

\[
p_t(x, y) \leq (\nu_x \nu_y)^{-1/2} \exp \left( -\frac{r}{2} \log \left( \frac{r}{2et} \right) - \Lambda t \right).
\]
Let $f : \mathbb{R}_+ \rightarrow \mathbb{R}_+$. Let $A \geq 1$ and $\gamma > 1$. We say that $f$ is $(A, \gamma)$–regular on $[a, b)$ if the function $f$ is increasing on $\mathbb{R}_+$ and satisfies that

$$\frac{f(\gamma s)}{f(s)} \leq A \frac{f(\gamma t)}{f(t)} \quad \text{for all } a \leq s < t < \gamma^{-1} b. \quad (11)$$
Theorem 7

If each $f_i$ is $(A, \gamma)$-regular on $[T_1, T_2)$ and satisfies

$$f_i(t) \leq Ae^{\delta t} \text{ for all } t \in [T_1, T_2)$$

(12)

then there exist universal positive constants $C_1$ and $\theta$, such that for any $t \in [\tilde{T}_1, T_2)$ we have

$$P_{x_1}(X_t = x_2) \leq \frac{C_1 A^\beta (\nu_{x_2}/\nu_{x_1})^{1/2}}{\sqrt{f_1(\alpha t) f_2(\alpha t)}} \exp \left( -\theta \frac{d_\nu(x_1, x_2)^2}{t} \right), \quad (13)$$

where $\tilde{T}_1 = (8\alpha^{-2}T_1^2) \lor d_\nu(x_1, x_2)$. 
Thank you!