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On the precision of the spectral profile

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Abstract. We examine the spectral profile bound of Goel, Montenegro and Tetali for the L^∞ mixing time of continuous-time random walk in reversible settings. We find that it is precise up to a $\log\log$ factor, and that this $\log\log$ factor cannot be improved.

1. Introduction

Of all the formulas suggested in the literature as bounds for the mixing time of a finite graph (see e.g. Lovász and Kannan (1999); Morris and Peres (2005); Fountoulakis and Reed (2007)), possibly the most promising, from a geometric point of view, is the spectral profile formula. Introduced by Goel, Montenegro and Tetali (Goel et al., 2006), it brings into the realm of finite graphs the idea of *Faber-Krahn inequalities*. A Faber-Krahn inequality is an inequality relating the volume of a set A and the first eigenvalue of the Laplacian with Dirichlet boundary conditions on A — we will give all definitions in the discrete settings below, but for the history of the topic, mainly in continuous settings, one should consult Grigor'yan (1994), Chavel (2001, §VIII.6) or Benguria (2001), which has a somewhat different take on this topic and an excellent historical survey. This approach is promising because, as Grigory'an discovered (Grigor'yan, 1994), on a general complete manifold it gives sharp estimates on the decay of the heat kernel, *even in cases where the manifold does not have polynomial volume growth.* The requirement of polynomial growth was essential in previous approaches to this problem, using Sobolev (Varopoulos, 1985) or Nash (Carlen et al., 1987) inequalities.

Let us describe Faber-Krahn inequalities in the discrete settings. We will work with weighted, undirected, finite graphs. Let G be such a graph and $\omega : G \times G \to$

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$[0, \infty)$ the weight function. The *heat kernel* is defined by

$$K(x, y) := \frac{\omega(x, y)}{\omega(x)} \quad \omega(x) := \sum_z \omega(x, z).$$

The heat kernel is a stochastic matrix (i.e. $\sum_y K(x, y) = 1$) and hence describes a Markov chain on G. The symmetry $\omega(x, y) = \omega(y, x)$ gives that it is self-adjoint with respect to the stationary measure π defined by

$$\pi(x) := \frac{\omega(x)}{\sum_y \omega(y)}$$

and therefore the associated Markov chain is *reversible.* It is important to note that the results of Goel et al. (2006) are not restricted to the reversible case, and apply to any finite Markov chain, but in this paper we will restrict our attention to the reversible case. The Laplacian, which is an operator on $L^2(G, \omega)$ is defined simply as $\Delta := I - K$ and is self-adjoint and positive.

When $A \subset G$ is some subset, we will introduce the restricted Laplacian with Dirichlet boundary conditions

$$(\Delta_A f)(x) = \begin{cases} \Delta f(x) & x \in A \\ 0 & \text{otherwise.} \end{cases} \tag{1.1}$$

The smallest eigenvalue for Δ_A will be denoted by $\lambda_0(A)$. It is easy to see that $\lambda_0(A)$ may also be defined as

$$\lambda_0(A) = \inf_{\substack{\operatorname{supp} f \subset A \\ f \not\equiv 0}} \frac{\langle \Delta f, f \rangle}{||f||_2^2} \tag{1.2}$$

where $\langle f, g \rangle = \sum_x f(x) g(x) \pi(x)$ and $||f||_p^p = \sum_x f(x)^p \pi(x)$. It is somewhat more elegant to describe the results of Goel et al. (2006) with the following quantity instead,

$$\lambda(A) = \inf_{\substack{\operatorname{supp} f \subset A \\ f \geq 0, f \not\equiv \text{const}}} \frac{\langle \Delta f, f \rangle}{||f||_2^2 - ||f||_1^2} \tag{1.3}$$

and we will adhere to this convention. Note that as long as $\pi(A) \leq 1 - \epsilon$ the quatities λ_0 and λ are comparable, Goel et al. (2006, eq. (1.4)). A Faber-Krahn inequality is an inequality of the form $\lambda(A) \leq \Lambda(\pi(A))$ for some function Λ, so the minimal function Λ satisfying this is defined by

$$\Lambda(r) := \inf_{0 < \pi(A) \leq r} \lambda(A).$$

$\Lambda(r)$ is the *spectral profile.* It is defined for all $r \geq \pi_* := \min_{\emptyset \neq A \subset G} \pi(A)$.

The main result of Goel et al. (2006) is a bound for the L^∞ mixing time of the continuous-time random walk in terms of the spectral profile. Let us give the necessary definitions. The continuous-time random walk on G is defined using $-\Delta$ as the infinitesimal generator. Explicitly, we define

$$H_t = e^{-t\Delta} = e^{-t} \sum_{n=0}^{\infty} \frac{t^n}{n!} K^n(x, y)$$

and think about $H_t(x, y)$ as the probability that a particle doing continuous-time random walk on G, starting from x will be at y at time t. Hence we define the mixing time using

$$\tau_\infty(\epsilon) := \inf\left\{t>0 : \sup_{x,y\in G}\left|\frac{H_t(x,y)-\pi(y)}{\pi(y)}\right| \le \epsilon\right\}.$$

We may now state the main result of Goel et al. (2006),

$$\tau_\infty(\epsilon) \le \int_{4\pi_*}^{4/\epsilon} \frac{2\,dr}{r\Lambda(r)}. \tag{1.4}$$

In the rest of the discussion we will fix $\epsilon = \frac{1}{2}$ and denote the left hand side by τ_∞ and the right hand side by ρ.

1.1. The starting point of this short note was the hope that in fact (1.4) is precise in the sense that $\rho < C\tau_\infty$ ([1]). This was motivated by the fact that Faber-Krahn inequalities give sharp bounds in many interesting manifolds, and by the fact that (1.4) is in fact sharp under a certain δ-regularity condition (see Goel et al. (2006, §3)). And in fact, the techniques there give quite easily (and with no regularity assumption), the following:

Theorem 1.1. *For any finite graph G,*

$$\rho < C\tau_\infty \log\log 1/\pi_*(G).$$

Unfortunately, it turns out that this cannot be improved. Indeed we have

Theorem 1.2. *There exist a sequence $n_k \to \infty$ and graphs G_k of size n_k and $\pi_* = \frac{1}{n_k}$ such that*

$$\rho \ge c\tau_\infty \log\log n_k.$$

The proof of theorem 1.2 is also not difficult — the graphs G_k will be (details in section 2) composed of $\log\log n_k$ pieces H_i where each H_i corresponds to a distinct range of r-s in the integral defining ρ (1.4). On the other hand, a random walker starting at H_i will see only H_i — when it finally leaves H_i it will already be too mixed to notice any effects from the other H_j-s. Thus, perhaps the most natural question to ask is

Question 1.3. *Is it possible to have the graphs G_k transitive?*

A graph G is transitive if for all $x, y \in G$ there exists an automorphism of the graph taking x to y. It would be extremely exciting if the answer to the question were to be no. A less exciting, but nonetheless very natural question is as follows.

Question 1.4. *Is it possible to have the graphs G_k unweighted and of uniformly bounded degrees?*

Here the rationale for the question is geometric. The analogy between graphs and manifolds works best for manifolds with bounded geometry and graphs with bounded degrees. Hence there is a certain discord in the fact that the examples constructed in theorem 1.2 are weighted. One would be tempted to solve the question by constructing the graphs (call them G_k^{simple}) randomly, namely put an edge between x and y in G_k^{simple} with probability $\omega(x, y)$ where ω is the weight

[1]Here and below we use C and c to denote absolute positive constants that may be different from place to place. C will be used for constants which are "large enough" and c for constants which are "small enough". The notation $f \approx g$ will stand for $cf \le g \le Cf$.

function of G_k. However, more care is needed — applying the recipe above naively would immediately create logarithmic tails that would dominate the mixing time.

Finally, we remark that in non-reversible settings existing bounds are quite weak. For example, it is possible to have $\rho \geq c|G|^2$ while $\tau_\infty \leq C|G|\log|G|$. A careful discussion of this phenomenon can be found in Montenegro and Tetali (2006, examples 5.3-5.5).

1.2. Another relevant set of problems revolves around the following: is the mixing time a geometric property? This is particularly interesting since many results in mixing have been achieved using representation theory (Bayer and Diaconis (1992) is probably the most famous) or using coupling (e.g. Luby et al. (2001)), techniques which are better described as "algebraic" rather than "geometric". To make the question formal let us define the notion of a rough isometry.

Definition 1.5. Let X and Y be metric spaces and let $f : X \to Y$ be a function and let $K \in (0, \infty)$. We say that f is a K-rough isometry if the following two properties hold:

(1) For any $a, b \in X$,

$$\frac{1}{K}d(a,b) - K \leq d(f(a), f(b)) \leq Kd(a,b) + K.$$

(2) For any $y \in Y$ there exists an $x \in X$ such that

$$d(f(x), y) \leq K.$$

To use this for Markov chains we will restrict ourselves to the simplest settings, that of random walk on a (unweighted) graph with bounded degree. In this case the graph has a natural metric structure given by the path metric, i.e. the distance $d(v, w)$ is defined to be the length of the shortest path between v and w. And we ask: is the mixing time invariant to rough isometries? Formally:

Conjecture 1.6. *Let G, H be two graphs with $\deg G, \deg H \leq d$. Let $f : G \to H$ be a K-rough isometry in the path metrics on G and H. Then*

$$\tau(G) \leq C(K, d)\tau(H). \tag{1.5}$$

Since a rough isometry is reversible, this would in fact imply that $\tau(G) \approx \tau(H)$.

It is an interesting observation that all approximations for the mixing time I am aware of are rough isometry invariants. It is easy to see that isoperimetric inequalities are rough-isometry invariants, and hence both the Lovász-Kannan integral (Lovász and Kannan, 1999) and the Fountoulakis-Reed integral (Fountoulakis and Reed, 2007, which bounds the L^1 mixing time rather than our τ_∞, but the conjecture is just as relevant for τ_1) are rough-isometry invariants. To see that, for example, the spectral gap is a rough isometry invariants one has to define it using functional inequalities i.e. (1.3) — note that the spectral gap is exactly $\lambda(G)$ — and then it becomes easy to check that the spectral gap and the spectral profile are both rough isometry invariants. Thus a *precise* bound of this style for the spectral gap would probably imply the conjecture.

In particular, combining Goel et al. (2006, theorem 1.1) with theorem 1.1 gives a weaker form of (1.5):

$$\tau_\infty(G) \leq C(K, d)(\log\log|G|)\tau_\infty(H). \tag{1.6}$$

This result, however, is not new. Indeed, τ_∞ is comparable to the best constant in the logarithmic Sobolev inequality α defined by

$$\alpha = \inf_{\mathrm{Ent}_\pi f^2 \neq 0} \frac{\langle \Delta f, f\rangle}{\mathrm{Ent}_\pi f^2}$$

in the sense that

$$\frac{c}{\alpha} \le \tau_\infty \le \frac{C \log\log 1/\pi_*}{\alpha}.$$

See Montenegro and Tetali (2006) for historical background, the definition of the entropy Ent_π and for the equivalence (theorem 4.13 ibid). It is easy to see that α is a rough isometry invariant hence this gives another derivation of (1.6).

We end this discussion with an observation of Itai Benjamini, that the mixing time *from a given point* is not a rough isometry invariant. Thus, for example, the mixing time from the root of a binary tree of height h is $\approx h$. However, the mixing time from a neighbor of the root is $\approx 2^h$ (see Aldous and Fill (2007, chapter 5) for both). Since there is a rough isometry of a tree on itself carrying the root to a neighbor, this demonstrates the claim.

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2. Proofs

Proof of theorem 1.1. Denote by A_k a Rayleigh set of measure 2^{-k} i.e. $\pi(A_k) \le 2^{-k}$ and

$$\lambda(A_k) = \min\{\lambda(S) : \pi(S) \le 2^{-k}\}.$$

Where λ is from (1.3). It is easy to see that

$$\rho \approx \sum_{k=1}^{\lfloor \log_2 1/\pi_* \rfloor} \frac{1}{\lambda(A_k)}.$$

On the other hand, by Goel et al. (2006, lemma 3.1), for any $k \ge 2$

$$\tau_\infty \ge c\frac{-\log(\pi(A_k))}{\lambda(A_k)} \ge \frac{ck}{\lambda(A_k)}. \tag{2.1}$$

As for $k = 1$, we have $1/\lambda(A_1) \le 1/\lambda(G)$ but $\lambda(G)$ is just the spectral gap and hence $1/\lambda(G) \le C\tau_\infty$ Montenegro and Tetali (2006, theorem 4.9). Hence (2.1) holds for $k = 1$ as well. Therefore

$$\rho \le \sum_{k=1}^{\lfloor \log_2 1/\pi_* \rfloor} \frac{C\tau}{k} \approx \tau \log\log 1/\pi_*. \qquad \square$$

Proof of theorem 1.2. We may assume w.l.o.g. that k is sufficiently large. We define simply

$$n_k = (k - \lceil \log k \rceil + 1)2^{2^k}$$

where log, here and below, is to base 2. The graph will consist of $k-\lceil\log k\rceil+1$ pieces, which we denote by $H_{\lceil\log k\rceil},\dots,H_k$, each with 2^{2^k} vertices. We can already define the weight function between the H_ls: for every v_1,v_2 in different H_ls we set

$$\omega(v_1,v_2)=\frac{k2^{-k}}{|G|}.$$

Let A_l be a set of vertices of size $2^{2^k-2^l}$ and B_l a set of size 2^{2^l}. Setwise we define $H_l=A_l\times B_l$ and then define the weight function ω as follows:

$$\omega((a_1,b_1),(a_2,b_2))=\begin{cases}\frac{1}{|H_l|}2^{l-k}+\frac{1}{|G|}k2^{-k} & b_1\neq b_2\\ \frac{1}{|A_l|}+\frac{1}{|H_l|}2^{l-k}+\frac{1}{|G|}k2^{-k} & b_1=b_2.\end{cases}$$

With this definition of ω we would have that $\omega(v)=1+2^{l-k}+k2^{-k}$ for every $v\in H_l$. The inhomogeneity of ω is somewhat bothersome so we modify $\omega(v,v)$ to fix this, writing

$$\omega(v,v)=(1-2^{l-k})+\frac{1}{|A_l|}+\frac{1}{|H_l|}2^{l-k}+\frac{1}{|G|}k2^{-k}\quad\forall v\in H_l$$

with the result being that $\omega(v)=2+k2^{-k}$ for all v.

With our graph G defined we can start investigating its properties. We first estimate the spectral profile ρ. By the discrete inverse Cheeger inequality (Alon and Milman (1985, lemma 2.1)), for any set S,

$$\lambda(S)\le C\frac{\pi(\partial S)}{\pi(S)}=C\frac{\omega(\partial S)}{\omega(S)}.$$

where we consider the weight function ω as a measure which is a constant multiple of π. We use it for the set $A_l\times\{\mathrm{pt}\}$ which we confusingly call $\tilde A_l$. Now, $\omega(\tilde A_l)\approx|A_l|=2^{2^k-2^l}$. There are two types of edges coming out of $\tilde A_l$, edges to H_l and edges to the other H_is. The first type has weight

$$\frac{1}{|H_l|}2^{l-k}+\frac{1}{|G|}k2^{-k}=\frac{1}{|H_l|}2^{l-k}(1+o(1))$$

where the o notation above and also below means "as $k\to\infty$, uniformly in $l\in[\log k,k]$". So, after summing over all couples (v_1,v_2), $v_1\in\tilde A_l$ and $v_2\in H_l\setminus\tilde A_l$ gives a total contribution $\le|A_l|2^{l-k}(1+o(1))$. The second type has weight $\frac{1}{|G|}k2^{-k}$ so after summing over all (v_1,v_2), $v_1\in\tilde A_l$ and $v_2\in G\setminus H_l$ gives a total contribution $\le|A_l|k2^{-k}$. Since $l>\log k$ we get

$$\lambda(\tilde A_l)\le C\frac{\omega(\partial\tilde A_l)}{\omega(\tilde A_l)}\le C2^{l-k}. \tag{2.2}$$

Now, $\pi(\tilde A_l)=|A_l|/|G|=1/(k-\lceil\log k\rceil+1)2^{2^l}$. For brevity denote $\epsilon=1/(k-\lceil\log k\rceil+1)$. We get that,

$$\int_{\epsilon/2^{2^l}}^{\epsilon/2^{2^{l-1}}}\frac{dv}{v\Lambda(v)}\ge\frac{1}{\Lambda(\epsilon/2^{2^l})}\int_{\epsilon/2^{2^l}}^{\epsilon/2^{2^{l-1}}}\frac{dv}{v}\ge\frac{1}{\lambda(\tilde A_l)}\cdot c2^l\overset{(2.2)}{\ge}c2^k.$$

Summing we get

$$\rho=\int_{4\pi_*}^{8}\frac{dv}{v\Lambda(v)}\ge c2^k(k-\lceil\log k\rceil+1)\ge ck2^k.$$

The proof will be finished once we show that $\tau\le C2^k$.

Let us therefore investigate the random walk on G. It will be convinient to represent it as follows. Assume the walker is at a vertex $v \in H_l$. We first throw a coin which has probability $k/2^k\omega(v)$ of success. Call the event that this throw succeeded ξ_1 and in this case choose one of the vertices of G randomly with equal probability and move there. If ξ_1 did not occur, throw a second coin which has probability

$$\frac{2^{l-k}}{\omega(v) - k2^{-k}} = 2^{l-k-1}$$

to succeed. Call the event that this throw succeeded ξ_2 and in this case choose one of the vertices of H_l randomly with equal probability and move there. Finally, throw a coin with probability

$$\frac{1}{\omega(v) - k2^{-k} - 2^{l-k}} = \frac{1}{2 - 2^{l-k}}$$

to succeed (if $l = k$ it always does). Call the event that this throw succeeded ξ_3 and in this case choose one of the vertices of the copy of A_l containing v randomly with equal probability and move there. If none of ξ_1, ξ_2 and ξ_3 succeeded, stay at v. It is easy to see that this is equivalent to the walk on the graph (in fact, we defined the weights on the graph with this representation in mind).

Examine a random walk of length 2^{k+1}, starting from some $v \in H_l$. Let $w \in G$ and examine $\mathbb{P}(R(2^{k+1}) = w)$ (that starting point will always be v — we will not remind this fact in the notation). We first note that after an event of type ξ_1 the walk is completly mixed. Define τ_1 to be the first time when ξ_1 occurred, which is a stopping time. Using the strong Markov property we get, for every $t \leq 2^{k+1}$,

$$\mathbb{P}(\{\tau_1 = t\} \cap \{R(2^{k+1}) = w\}) = \mathbb{P}(\tau_1 = t)\frac{1}{|G|}$$

and summing over t gives

$$\mathbb{P}(\{\tau_1 \leq 2^{k+1}\} \cap \{R(2^{k+1}) = w\}) = \mathbb{P}(\tau_1 \leq 2^{k+1})\frac{1}{|G|} \leq \frac{1}{|G|}. \tag{2.3}$$

Now, the event $\tau_1 > 2^{k+1}$ can be estimated simply using

$$\mathbb{P}(\tau_1 > 2^{k+1}) = \left(1 - \frac{k2^{-k}}{2 + k2^{-k}}\right)^{2^{k+1}} \leq \left(1 - \frac{k2^{-k}}{3}\right)^{2^{k+1}} \leq e^{-2k/3} \tag{2.4}$$

which immediately gives a lower bound $\mathbb{P}(R(2^{k+1}) = w) \geq (1 - o(1))/|G|$ valid for all w. Further, if $w \notin H_l$ then (2.3) gives an upper bound, since one cannot reach from v to w without a ξ_1 event. Hence we will henceforth assume $w \in H_l$ and $\tau_1 > 2^{k+1}$. The estimate (2.4) is nice, but far from our goal of $\frac{3}{2|G|}$.

After an event of type ξ_2 the walk is totally mixed in H_l. Therefore if we define τ_2 to be the first time when ξ_2 occurred then a similar calculation to the above shows that

$$\begin{aligned}\mathbb{P}(\{\tau_1 > 2^{k+1}\} \cap \{\tau_2 \leq 2^{k+1}\} \cap \{R(2^{k+1}) = w\}) = \\ \mathbb{P}(\tau_1 > 2^{k+1})\mathbb{P}(\tau_2 \leq 2^{k+1} \mid \tau_1 > 2^{k+1})\frac{1}{|H_l|} \overset{(2.4)}{\leq} e^{-2k/3}\frac{1}{|H_l|} = o\left(\frac{1}{|G|}\right).\end{aligned}$$

With (2.3) we have

$$\mathbb{P}(\{\min\{\tau_1, \tau_2\} \leq 2^{k+1}\} \cap \{R(2^{k+1}) = w\}) \leq \frac{1}{|G|}(1 + o(1)). \tag{2.5}$$

Again we note the probability that $\tau_2 > 2^{k+1}$:

$$\mathbb{P}(\min\{\tau_1,\tau_2\} > 2^{k+1}) \le \left(1-2^{l-k-1}\right)^{2^{k+1}} \le e^{-2^l} \tag{2.6}$$

For the last part we assume $w \in \tilde{A}_l$ where here $\tilde{A}_l$ is the copy of A_l containing v. We define τ_3 as the first time ξ_3 occurred and get

$$\begin{aligned}&\mathbb{P}(\{\min\{\tau_1,\tau_2\} > 2^{k+1}\} \cap \{\tau_3 \le 2^{k+1}\} \cap \{R(2^{k+1}) = w\}) = \\ &\qquad \mathbb{P}(\{\min\{\tau_1,\tau_2\} > 2^{k+1}\})\mathbb{P}(\tau_3 \le 2^{k+1} \mid \min\{\tau_1,\tau_2\} > 2^{k+1})\frac{1}{|A_l|} \stackrel{(2.6)}{\le} \\ &\qquad\qquad \le e^{-2^l}\cdot 2^{2^l-2^k} = o\left(\frac{1}{|G_k|}\right).\end{aligned} \tag{2.7}$$

Finally, in the case that $\tau_1,\tau_2,\tau_3 > 2^{k+1}$ (so w must be v) we definitely have

$$\mathbb{P}(\min\{\tau_1,\tau_2,\tau_3\} > 2^{k+1}) \le \left(1-\frac{1}{2-2^{l-k}}\right)^{2^{k+1}} \le 2^{-2^{k+1}} = o\left(\frac{1}{|G_k|}\right). \tag{2.8}$$

Summing up (2.3), (2.5), (2.7) and (2.8) we finally get

$$\mathbb{P}^v(R(2^{k+1}) = w) \le \frac{1}{|G|}(1+o(1))$$

and hence for k sufficiently large, $\tau \le 2^{k+1}$. This ends the theorem. □

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