Coverings, heat kernels and spanning trees

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Abstract

We consider a graph G and a covering $\tilde{G}$ of G and we study the relations of their eigenvalues and heat kernels. We evaluate the heat kernel for an infinite k-regular tree and we examine the heat kernels for general k-regular graphs. In particular, we show that a k-regular graph on n vertices has at most

$$(1+o(1))\frac{2\log n}{kn\log k}\left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}}\right)^n$$

spanning trees, which is best possible within a constant factor.

1 Introduction

We consider a weighted undirected graph G (possibly with loops) which has a vertex set $V = V(G)$ and a weight function $w : V \times V \to \mathbb{R}$ satisfying

$$w(u,v) = w(v,u) \text{ and } w(u,v) \geq 0.$$

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If $w(u,v) > 0$, then we say $\{u,v\}$ is an edge and u is adjacent to v. A simple graph is the special case where all the weights are 0 or 1 and $w(v,v) = 0$ for all v. In this paper, by a graph we mean a weighted graph unless specified.

The degree d_v of a vertex v is defined to be:

$$d_v = \sum_u w(u,v).$$

A graph is regular if all its degrees are the same. For a vertex v in G, the neighborhood $N(v)$ of v consists of all vertices adjacent to v.

This paper is organized as follows: In Section 2, we define a covering of a graph and give several examples. In Section 3, we give the definitions for the Laplacian, eigenvalues and the heat kernel of a graph. In Section 4, we consider the relations between the eigenvalues of a graph and the eigenvalues of its covering. In particular, we give a proof for determining the eigenvalues and their multiplicities of a strongly cover-regular graph G from the eigenfunctions of the (smaller) graph covered by G. In Section 5, we derive the heat kernel of an infinite k-regular tree. Then in Section 6, we consider heat kernels of some k-regular graphs. In Section 7, we consider the relations between the trace of the heat kernel and the number of spanning trees in a graph. In Section 8, we focus on an old problem of determining the maximum number of spanning trees in a k-regular graph. We consider the zeta function of a graph and we improve the upper and lower bounds for the maximum number of spanning trees in a k-regular graph on n vertices.

2 The coverings of graphs

Suppose we have two graphs $\tilde{G}$ and G. We say $\tilde{G}$ is a *covering* of G (or G is covered by $\tilde{G}$) if there is a mapping $\pi : V(\tilde{G}) \to V(G)$ satisfying the following two properties:

(i) There is an $m \in \mathbb{R}^+ \cup \{\infty\}$, called the *index* of π, such that for $u, v \in V(G)$, we have

$$\sum_{\substack{x \in \pi^{-1}(u) \\ y \in \pi^{-1}(v)}} w(x,y) = m \; w(u,v).$$

(ii) For $x, y \in V(\tilde{G})$ with $\pi(x) = \pi(y)$ and $v \in V(G)$, we have

$$\sum_{z \in \pi^{-1}(v)} w(z,x) = \sum_{z' \in \pi^{-1}(v)} w(z',y).$$

Remark 1: For simple graphs G and $\tilde{G}$, (i) is equivalent to
(i') For every $\{u,v\} \in E(G)$, we have

$$|\{\{x,y\} \in E(\tilde{G}) : \pi(x) = u, \pi(y) = v\}| = m.$$

And (ii) is equivalent to
(ii') For $x, y \in V(\tilde{G})$ with $\pi(x) = \pi(y)$, and v adjacent to $\pi(x)$ in G, we have

$$|N(x) \cap \pi^{-1}(v)| = |N(y) \cap \pi^{-1}(v)|.$$

In other words, π^{-1} defines a so-called *equitable* partition of $V(\tilde{G})$ which has been studied extensively in the literature. The reader is referred to Cvetković, Doob and Sachs [5], McKay [14], Godsil and McKay [12].

Example 1: Suppose $\tilde{G} = C_{2n}$, the cycle on $2n$ vertices and $G = P_{n+1}$, the path on $n+1$ vertices. The covering has index 2 since each edge of P_{n+1} is covered by two edges of C_{2n}.

Example 2: A graph $\tilde{G}$ is said to be a *regular covering* of G if for a fixed vertex v in $V(G)$ and for any vertex x of $V(\tilde{G})$, $\tilde{G}$ is a covering of G under a mapping π_x which maps x into v. In addition, if π_x^{-1} is just x, we say $\tilde{G}$ is a *strong regular covering* of G. A graph G is said to be *distance regular* if G is a strong regular covering of a (weighted) path P (with possible non-zero $w(v, v)$). For example, for a vertex x in $V(G)$, we can consider a mapping π_x so that all vertices y at distance i from x are mapped to the i-th vertex of P. This definition is equivalent to the definition of distance regular graphs, given by Biggs [2].

Example 3: Let T_k denote an infinite k-tree. It is not hard to check that T_k is a covering of a k-regular graph G. More on this will be discussed in Sections 5 and 6.

We note that in a covering $\tilde{G}$ of G, the vertices v in G can have preimages $\pi^{-1}(v)$ of different sizes (as in Example 2). In addition, the degrees of vertices in $\tilde{G}$ or G are not necessarily the same. Nevertheless, there is a certain uniformity in the preimage of a vertex as illustrated in the following facts:

Fact 1 *Suppose $\tilde{G}$ is a covering of G under π with index m. Then for $x \in \pi^{-1}(v)$, we have*

$$|\pi^{-1}(v)| \sum_{z \in \pi^{-1}(u)} w(z, x) = m w(u, v).$$

The proof follows from (i) and (ii). For a simple graph, Fact 1 implies

$$|\pi^{-1}(v)| \cdot |N(x) \cap \pi^{-1}(u)| = m.$$

As an immediate consequence, we have

Fact 2 *Suppose $\tilde{G}$ is a covering of G under π with edge multiplicity m. Then for $x, y \in \pi^{-1}(v)$, we have*

$$d_x = d_y.$$

3 The Laplacian and the heat kernel of a graph

For a weighted graph G on n vertices associated with a weight function w, we consider the combinatorial Laplacian L of G.

$$L(u,v) = \begin{cases} d_v - w(v,v) & \text{if } u = v, \\ -w(u,v) & \text{if } u \text{ and } v \text{ are adjacent,} \\ 0 & \text{otherwise.} \end{cases}$$

In particular, for a function $f : V \to \mathbb{R}$, we have

$$Lf(v) = \sum_y (f(v) - f(u))w(u,v).$$

Let T denote the diagonal matrix with the (v,v)-th entry having value d_v. The (normalized) *Laplacian* of G is defined to be

$$\mathcal{L}(u,v) = \begin{cases} 1 - \dfrac{w(v,v)}{d_v} & \text{if } u = v, \text{ and } d_v \neq 0, \\ -\dfrac{w(u,v)}{\sqrt{d_u d_v}} & \text{if } u \text{ and } v \text{ are adjacent,} \\ 0 & \text{otherwise.} \end{cases}$$

In other words, we have

$$\mathcal{L} = T^{-1/2} L T^{-1/2}.$$

For a k-regular graph, we have

$$\mathcal{L} = I - \frac{1}{k} A$$

where A is the adjacency matrix.

We denote the eigenvalues of $\mathcal{L}$ by $0 = \lambda_0 \leq \lambda_1 \cdots \leq \lambda_{n-1}$ (which are sometimes called the eigenvalues of G). If G is connected, we have $0 < \lambda_1$. The reader is referred to [7] for various properties of eigenvalues of a graph.

In this paper, we mainly deal with connected graphs. Let g denote an eigenfunction of $\mathcal{L}$ associated with eigenvalue λ. It is sometimes convenient to consider $f = T^{-1/2} g$, called the *harmonic eigenfunction*, which satisfies, for every vertex v of G,

$$\sum_u (f(v) - f(u))w(u,v) = \lambda d_v f(v).$$

For a graph G, we consider the heat kernel h_t, which is defined for $t \geq 0$ as follows:

$$\begin{aligned} h_t &= \sum_i e^{-\lambda_i t} P_i \\ &= e^{-t\mathcal{L}} \\ &= I - t\mathcal{L} + \frac{t^2}{2}\mathcal{L}^2 - \ldots \end{aligned} \tag{1}$$

where P_i denotes the projection into the eigenspace associated with eigenvalue λ_i. In particular,

$$h_0 = I.$$

and h_t satisfies the heat equation

$$\frac{\partial h_t}{\partial t} = -\mathcal{L} h_t.$$

For any two vertices $x, y \in V$, we have

$$h_t(x, y) = \sum_i e^{-\lambda_i t} \phi_i(x)\phi_i(y)$$

where ϕ_i's are orthonormal eigenfunctions of the Laplacian $\mathcal{L}$.

In particular, the trace of h_t satisfies

$$\begin{aligned} Trh_t &= \sum_x h_t(x, x) \\ &= \sum_i e^{-\lambda_i t}. \end{aligned}$$

4 Eigenvalues of a graph and its covering

If $\tilde{G}$ is a covering of G, their eigenvalues are intimately related. Namely, the spectrum of a large (covering) graph can often be determined from a small (covered) graph. This provides a simple method for determining the spectrum of certain families of graphs. Such approaches have long been studied in the literature. Here we will list several facts which will be used later. The proofs of some of these facts can be found in Godsil and McKay [12] (in which the definitions involve $(0, 1)$ matrices but the proofs often can be adapted for general weighted graphs). We will sketch the proofs here for the sake of completeness.

If $\tilde{G}$ is a covering of G, we can "lift" the harmonic eigenfunction f of G to $\tilde{G}$ by defining, for each vertex x in $\tilde{G}$, $f(x) = f(u)$ where $u = \pi(x)$. From definition (ii) of covering, we have

$$\begin{aligned} \sum_y (f(x) - f(y))w(x, y) &= \sum_v (f(u) - f(v))w(u, v) \\ &= \lambda d_x. \end{aligned}$$

Therefore we have

Lemma 1 *If $\tilde{G}$ is a covering of G, then an eigenvalue of G is an eigenvalue of $\tilde{G}$.*

For each $x \in \pi^{-1}(v)$,

$$\sum_y (f(x) - f(y))w(x,y) = \lambda f(x) d_x.$$

By summing over x in $\pi^{-1}(v)$, we have

$$\sum_{x \in \pi^{-1}(v)} \sum_y (f(x) - f(y))w(x,y) = \lambda \sum_{x \in \pi^{-1}(v)} f(x) d_x.$$

We define the induced mapping of f in G, denoted by $\pi f : V(G) \to \mathbb{R}$ by

$$(\pi f)(v) = \sum_{x \in \pi^{-1}(v)} \frac{f(x) d_x}{d_v}.$$

Then, for $g = \pi f$, we have

$$\sum_u (g(v) - g(u))w(u,v) = \lambda g(v) d_v.$$

If g is nontrivial, λ is an eigenvalues of $\tilde{G}$. Thus we have shown the following:

Lemma 2 *Suppose $\tilde{G}$ is a covering of G and. If a harmonic eigenfunction f of $\tilde{G}$, associated with an eigenvalue λ, has a nontrivial image in G, then λ is also an eigenvalue for G.*

Lemma 3 *Suppose $\tilde{G}$ is a strong regular covering of G. Then, $\tilde{G}$ and G have the same eigenvalues.*

Proof: For any nontrivial harmonic eigenfunction f of $\tilde{G}$ we can choose v to be a vertex with nonzero value of f. The induced mapping of f in G has a nonzero value at v and therefore is a nontrivial harmonic eigenfunction for G. From Lemma 2, we see that any eigenvalue of $\tilde{G}$ is an eigenvalue of G. By Lemma 1, we conclude that $\tilde{G}$ and G have the same eigenvalues. □

Therefore the eigenvalues of a covering graph $\tilde{G}$ can be determined by computing the eigenvalues of a smaller graph G. However, the multiplicities for the eigenvalues in $\tilde{G}$ are, in general, different from those in G since, for example, $\tilde{G}$ and G can have different numbers of vertices. Nevertheless, the multiplicities of eigenvalues of $\tilde{G}$ and G are related through the relations of their heat kernels.

Lemma 4 *Suppose $\tilde{G}$ is a covering of G. Let $\tilde{h}_t$ and h_t denote the heat kernels of $\tilde{G}$ and G, respectively. Then we have*

$$\sum_{x \in \pi^{-1}(u)} \sum_{y \in \pi^{-1}(v)} \tilde{h}_t(x,y) = \sqrt{|\pi^{-1}(u)| \cdot |\pi^{-1}(v)|}\, h_t(u,v).$$

Proof: We note that the heat kernel $h_t(u,v)$ satisfies

$$h_t(u,v) = e^{-t}\sum_r S_r(u,v)\frac{t^r}{r!}$$

where S_r is the sum of weights of all walks of length r joining u and v. (Here a walk p_r is a sequence of vertices $u_0,\ldots,u_r$ such that $u_i = u_{i+1}$ or $\{u_i,u_{i+1}\}$ is an edge. The weight of a walk is the product of $w(u_i,u_{i+1})/\sqrt{d(u_i)d(u_{i+1})}$, for $i=0,\ldots,r-1$.) We want to show that the total weights of the paths in $\tilde{G}$ lifted from p_r (i.e., whose image in G is p_r) is exactly the weight of p_r in G multiplied by $\sqrt{|\pi^{-1}(u_0)|\cdot|\pi^{-1}(u_r)|}$. Let p_{r-1} denote the walk $u_0,\ldots,u_{r-1}$. Suppose $u_{r-1}\neq u_r$ (The other case is easy). For each path $\tilde{p}_{r-1}$ lifted from p_{r-1}, its extensions to paths lifted from p_r has total weights

$$\begin{aligned}
& w(\tilde{p}_{r-1})\cdot\sum_{z\in\pi^{-1}(u_r)}\frac{-w(u_{r-1},z)}{\sqrt{d(u_{r-1})d(z)}}\\
= \quad & w(\tilde{p}_{r-1})\frac{-mw(u_{r-1},u_r)/|\pi^{-1}(u_{r-1})|}{\sqrt{md(u_{r-1})md(u_r)/(|\pi^{-1}(u_{r-1})|\ \ |\pi^{-1}(u_r)|)}}\\
= \quad & w(\tilde{p}_{r-1})\frac{-w(u_{r-1},u_r)}{\sqrt{d(u_{r-1})d(u_r)}}\sqrt{\frac{|\pi^{-1}(u_r)|}{|\pi^{-1}(u_{r-1})|}}.
\end{aligned}$$

By summing over all $\tilde{p}_{r-1}$, we have

$$\sum_{x\in\pi^{-1}(u)}\sum_{y\in\pi^{-1}(v)} S_r(x,y) = \sqrt{|\pi^{-1}(u)|\cdot|\pi^{-1}(v)|}S_r(u,v).$$

Therefore, we complete the proof of Lemma 4. □

As a consequence of Lemma 4, we have

Corollary 1 *Suppose $\tilde{G}$ is a strong regular covering of G. Let $\tilde{h}_t$ and h_t denote the heat kernels of $\tilde{G}$ and G, respectively. For $x\in\pi^{-1}(u)$, we have*

$$\sum_{y\in\pi^{-1}(v)}\tilde{h}_t(x,y) = \sqrt{\frac{|\pi^{-1}(v)|}{|\pi^{-1}(u)|}}h_t(u,v).$$

Corollary 2 *Suppose G is a distance regular graph which is a covering of a path P with vertices $v_0,\ldots,v_p$ where $p = D(G)$. Suppose G and P have heat kernels $\tilde{h}_t$ and h_t, respectively. For any two vertices x and y in G with distance $d(x,y)=r$, we have*

$$\tilde{h}_t(x,y) = \sqrt{|\pi^{-1}(u_r)|}h_t(v_0,v_r).$$

Theorem 1 *Suppose $\tilde{G}$ is a strong regular covering of G. Let v denote the vertex of G with preimage in $\tilde{G}$ consisting of one vertex. Then any eigenvalue λ of $\tilde{G}$ has multiplicity*

$$n \sum_i \frac{\phi_i^2(v)}{||\phi_i||^2},$$

where $n = |V(\tilde{G})|$ and ϕ_i 's span the eigenspace of λ in G. If the eigenvalue λ has multiplicity 1 in G with eigenfunction ϕ, then the multiplicity of λ in $\tilde{G}$ is

$$\frac{n\phi^2(v)}{||\phi||^2}.$$

Proof: Suppose $\tilde{G}$ has heat kernel H_t and G has heat kernel h_t. Since $\tilde{G}$ is a strong regular covering of G, we have

$$\begin{aligned} Tr(\tilde{h}_t) &= \sum_{x \in V(\tilde{G})} H_t(x,x) \\ &= nh_t(v,v) \\ &= n \sum_j e^{-t\lambda_j} \frac{\phi_j^2(v)}{||\phi_j||^2}. \end{aligned}$$

Therefore, the multiplicity of λ_j in $\tilde{G}$ is exactly

$$\frac{n\ \phi_j^2(v)}{||\phi_j||^2}$$

if the multiplicity of λ in G is 1 and . In general, the multiplicity of λ in $\tilde{G}$ is

$$n \sum_i \frac{\phi_i^2(v)}{||\phi_i||^2}$$

where ϕ_i 's span the eigenspace of λ in G. □

As an immediate consequence of Theorem 1, we have the following:

Corollary 3 *A distance regular graph G with diameter D has $D+1$ distinct eigenvalues λ's which are the eigenvalues of a weighted path P of length D. (The weight of edge $\{v_i, v_{i+1}\}$ in P is the number of edges joining a vertex at distance i from x to a vertex at distance $i+1$ from x for a fixed number x. The weight of the loop $\{v_i, v_i\}$ is twice the number of edges with both endpoints at distance i from x.) The multiplicity of λ in G is*

$$\frac{n\phi^2(x)}{||\phi||^2}$$

where n is the number of vertices in G and ϕ is the eigenfunction of λ of the Laplacian of P.

Example 4: The Petersen graph G is a covering for a path P of 3 vertices. It is easy to check that P has three eigenvalues $0, 2/3, 5/3$ with eigenfunctions $\phi_0 = (\sqrt{3}, \sqrt{6}, \sqrt{18})$, $\phi_1 = (\sqrt{3}, 1, -\sqrt{2})$ and $\phi_2 = (\sqrt{6}, -2\sqrt{2}, 1)$, respectively. Using Lemma 8, we see that eigenvalues $0, 2/3, 5/3$ have multiplicities $1, 5, 4$ in G, respectively.

5 The heat kernel of $k-$trees

Let T_k (or k-tree, in short) denote an infinite $k-$regular tree. Let $T_{k,l}$ denote an $l-$level tree with a root at the $0-$th level. The $l-$th level consists of the $k(k-1)^{l-1}$ vertices at distance l from the root. The infinite tree can be viewed as taking the limit of $T_{k,l}$ as l approaches infinity.

The heat kernel of T_k plays a central role in examining the spectrum of any k-regular graph. To determine the heat kernel of T_k, we can use the covering theorem in the previous section. The study of eigenvalues and eigenfunctions of T_k can be found in many papers in the literature [1, 3, 9, 17, 19]. Here we will give a self-contained proof for establishing the explicit formula for the kernel of the k-tree, for $k \geq 3$. For the case of $k = 2$, T_2 is just the infinite path. This special case and its cartesian products were examined in [6].

T_k can be regarded as a covering of the following weighted path P. The vertex of P is $\{0, 1, 2, \dots\}$. For $j > 0$, the edge joining $j-1$ to j has weight $k(k-1)^{j-1}$. the covering mapping π is defined by assigning all vertices in the j-th level to vertex j in P. The Laplacian $\mathcal{L}$ for the weighted path has entries

$$\mathcal{L}(i,j) = \begin{cases} 1 & \text{if } i = j, \\ -\frac{1}{\sqrt{k}} & \text{if } (i,j) = (0,1) \text{ or } (1,0), \\ -\frac{\sqrt{k-1}}{k} & \text{if } |i-j| = 1,\ i,j \neq 0, \\ 0 & \text{otherwise.} \end{cases}$$

We observe that $\mathcal{L}$ is quite close to $I - \frac{\sqrt{k-1}}{k}M$ where M is the cyclic operator with $M(i, i+1) = M(i+1, i) = \frac{\sqrt{k-1}}{k}$ for $i \geq 0$ and 0, otherwise. Intuitively, the eigenvalues of T_k are just, for a fixed integer l,

$$1 - \frac{2\sqrt{k-1}}{k} \cos\frac{\pi j}{l} \text{ for } j = 1, \dots, l-1$$

in addition to the eigenvalues 0 and 2.

In order to examine the eigenvalues and eigenfunctions of P explicitly, we consider the following $l \times l$ matrix $\mathcal{L}^{(l)}$, for $l \geq 3$:

$$\mathcal{L}^{(l)} = \begin{pmatrix} 1 & -\frac{1}{\sqrt{k}} & 0 & \cdots & \cdots & 0 \\ -\frac{1}{\sqrt{k}} & 1 & -\frac{\sqrt{k-1}}{k} & 0 & \cdots & 0 \\ 0 & -\frac{\sqrt{k-1}}{k} & 1 & -\frac{\sqrt{k-1}}{k} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & -\frac{\sqrt{k-1}}{k} & 0 \\ 0 & \cdots & \cdots & \cdots & 1 & -\sqrt{\frac{k-1}{k}} \\ 0 & \cdots & \cdots & \cdots & -\sqrt{\frac{k-1}{k}} & 1 \end{pmatrix}$$

where

$$\mathcal{L}^{(l)}(i,j) = \begin{cases} 1 & \text{if } i = j, \\ -\frac{1}{\sqrt{k}} & \text{if } (i,j) = (0,1) \text{ or } (1,0), \\ -\frac{\sqrt{k-1}}{k} & \text{if } |i-j| = 1,\ 0 < i,j < l, \\ -\sqrt{\frac{k-1}{k}} & \text{if } (i,j) = (l-1,l) \text{ or } (l,l-1), \\ 0 & \text{otherwise.} \end{cases}$$

The eigenvalues of $\mathcal{L}^{(l)}$ are $0,\ 2$ and

$$1 - \frac{2\sqrt{k-1}}{k} \cos \frac{\pi j}{l} \text{ for } j = 1, \ldots, l-1.$$

The eigenfunction ϕ_0 associated with eigenvalue 0 is $\phi_0 = f_0/\|f_0\|$ where f_0 is defined as follows:

$$\begin{aligned} f_0(0) &= 1, \\ f_0(p) &= \sqrt{k(k-1)^{p-1}}, \qquad \text{for } 1 \leq p \leq l-1, \\ f_0(l) &= \sqrt{(k-1)^{l-1}}. \end{aligned}$$

The eigenfunction ϕ_l associated with eigenvalue 2 is $\phi_l = f_l/\|f_l\|$ where f_l is defined as follows:

$$\begin{aligned} f_l(0) &= 1, \\ f_l(p) &= (-1)^p \sqrt{k(k-1)^{p-1}}, \qquad \text{for } 1 \leq p \leq l-1, \\ f_l(l) &= (-1)^l \sqrt{(k-1)^{l-1}}. \end{aligned}$$

The eigenfunction ϕ_j, for $j = 1, \cdots, l-1$, associated with eigenvalue $1 - \frac{2\sqrt{k-1}}{k} \cos \frac{\pi j}{l}$ is $f_j/\|f_j\|$ where

$$\begin{aligned} f_j(0) &= \sqrt{\frac{k}{k-1}} \sin \frac{\pi j}{l}, \\ f_j(p) &= \sin \frac{\pi j(p+1)}{l} - \frac{1}{k-1} \sin \frac{\pi j(p-1)}{l}, \qquad \text{for } 1 \leq p \leq l-1, \\ f_j(l) &= -\frac{\sqrt{k}}{k-1} \sin \frac{\pi j}{l}. \end{aligned}$$

It is easy to compute, for $j = 1, \cdots, l-1$,

$$\|f_j\|^2 = \frac{lk^2}{2(k-1)^2}(1 - \frac{4(k-1)}{k^2}\cos^2\frac{\pi j}{l}).$$

Therefore the heat kernel $h^{(l)}$ of $P^{(l)}$ satisfies

$$h^{(l)}(0,0) = \sum_{j=1}^{l-1} \frac{e^{-t(1-\frac{2\sqrt{k-1}}{k}\cos\frac{\pi j}{l})}\sin^2\frac{\pi j}{l}}{\frac{lk}{2(k-1)}(1-\frac{4(k-1)}{k^2}\cos^2\frac{\pi j}{l})} + \frac{1}{\|f_0\|^2} + \frac{1}{\|f_l\|^2}.$$

When l approaches infinity, the heat kernel h of P satisfies:

$$h_t(0,0) = \frac{2k(k-1)}{\pi}\int_0^\pi \frac{e^{-t(1-\frac{2\sqrt{k-1}}{k}\cos x)}\sin^2 x}{k^2-4(k-1)\cos^2 x}dx.$$

In general, for $a \geq 1$, we have

$$h_t(0,a) = \frac{2\sqrt{k(k-1)}}{\pi}\int_0^\pi \frac{e^{-t(1-\frac{2\sqrt{k-1}}{k}\cos x)}\sin x[(k-1)\sin(a+1)x - \sin(a-1)x]}{k^2-4(k-1)\cos^2 x}dx.$$

For the infinite k-tree T_k, its heat kernel is denoted by H_t. For two vertices x, y in T_k, we will write $H_t(x,y) = H_t(0, d(x,y))$ where $d(x,y)$ denotes the distance of x and y in T_k. In particular, $H_t(x,x) = H_t(0,0)$ for all vertices x. Using Lemma 4 and the fact that the infinite k-tree is a covering of P, we have the following:

Theorem 2 *The heat kernel H_t of the infinite k-tree satisfies*

$$\begin{aligned} H_t(0,0) &= \frac{2k(k-1)}{\pi}\int_0^\pi \frac{e^{-t(1-\frac{2\sqrt{k-1}}{k}\cos x)}\sin^2 x}{k^2-4(k-1)\cos^2 x}dx \\ H_t(0,a) &= \frac{2}{\pi(k-1)^{a/2-1}}\int_0^\pi \frac{e^{-t(1-\frac{2\sqrt{k-1}}{k}\cos x)}\sin x[(k-1)\sin(a+1)x - \sin(a-1)x]}{k^2-4(k-1)\cos^2 x}dx. \end{aligned}$$

Corollary 4 *The heat kernel $H_t(0,0)$ of the infinite k-tree can be written as*

$$\begin{aligned} H_t(0,0) &= e^{-t}\sum_{r\geq 0}\sum_{j=0}^{r}\binom{2r}{j}\frac{2r-2j+1}{2r-j+1}(k-1)^j(\frac{t}{k})^{2r} \\ &= \frac{2(k-1)}{k}\sum_{s\geq 0}(\frac{4(k-1)}{k^2})^{2s}\frac{(2s-1)!!}{(2s+2)!!}\sum_{0\leq j\leq s}\frac{t^2 j}{(2j)!} \end{aligned}$$

where $m!!$ denotes the product of all numbers less than or equal to m and having the same parity as m.

We note that the first sum in the corollary above appeared in [15]. We remark that the heat kernel H_t of the k-tree can be viewed as a basic building block for the heat kernel of any k-regular graph, which in turn is closely related to many major invariants of the graph.

6 The heat kernel of the k-tree and the heat kernel of a k-regular graph

For a k-regular graph G, there is a natural mapping π from T_k to G so that for each vertex x in T_k, the neighbors of x are mapped to neighbors of $\pi(x)$ in G in an one-to-one fashion. Let H_t denote the heat kernel of T_k. We here abuse the notation by writing $H_t(x, y) = H_t(0, d(x, y))$ for two vertices x and y at distance $d(x, y)$ in T_k.

Lemma 5 *For a k-regular graph G, there is a covering π from T_k to G and the heat kernel h_t of G satisfies*

$$h_t(u, v) = \sum_{y \in \pi^{-1}(u)} H_t(0, d(x, y))$$

where $v = \pi(x)$, $d(x, y)$ denotes the distance between x and y in T_k and H_t denotes the heat kernel of T_k.

In a graph G, a *walk* of length s is a sequence of vertices $(v_0, v_1, \cdots, v_s)$ where $\{v_i, v_{i+1}\}$ is an edge for $i = 0, \cdots, s-1$. If $v_0 = v_s$, it is called a closed walk rooted at v_0. A walk $(v_0, v_1, \cdots, v_s)$ is said to be *irreducible* if $v_j \neq v_{j+2}$ for $j = 0, \cdots, s-2$. If $v_j = v_{j+2}$ for some j, we can reduce the walk by deleting v_j and v_{j+1}. A walk is said to be totally reducible if it can be reduced to a trivial walk of length 0. Let r_j denote the number of totally reducible walk rooted at any vertex. In McKay [15, 16], r_j's have been extensively examined. From the definition of the heat kernel, we have the following:

Lemma 6 *In a k-regular graph, the number r_s of totally reducible walks of length s rooted at any vertex satisfies*

$$H_t(0, 0) = e^{-t} \sum_{j \geq 0} r_j \frac{(t/k)^j}{j!}$$

where H_t is the heat kernel of the infinite tree T_k.

Proof: We observe that r_j is exactly the number of rooted closed walks of length j in the infinite tree T_k. From the definition of H_t we have

$$\begin{aligned} H_t &= e^{-t} \cdot e^{A/k} \\ &= e^{-t}(I + A\frac{t}{k} + A^2 \frac{(t/k)^2}{2!} + \cdots) \end{aligned}$$

where A denotes the adjacency operator. Lemma 6 then follows. □

Lemma 7 *For odd j, r_j is zero and for the even case, we have*

$$\begin{aligned} r_{2j} &= \frac{4^{j+1}k(k-1)^{j+1}}{\pi}\int_0^{\pi/2}\frac{\sin^2 x\cos^{2j}x}{k^2-4(k-1)\cos^2 x}dx \\ &\leq \frac{4^j k(k-1)^{j+1}}{2j\sqrt{\pi j}(k-2)^2}. \end{aligned}$$

Proof: The proof follows from Lemma 5 and Lemma 6 which imply:

$$\begin{aligned} r_{2j} &= \frac{\partial^{2j}}{\partial t^{2j}}(e^t H_t(0,0)) \\ &= \frac{4^{j+1}k(k-1)^{j+1}}{\pi}\int_0^{\pi/2}\frac{\sin^2 x\cos^{2j}x}{k^2-4(k-1)\cos^2 x}dx. \end{aligned}$$

Therefore we have

$$\begin{aligned} r_{2j} &\leq \frac{4^{j+1}k(k-1)^{j+1}}{\pi(k-2)^2}\int_0^{\pi/2}\sin^2 x\cos^{2j}x dx \\ &= \frac{4^{j+1}k(k-1)^{j+1}}{\pi(k-2)^2(2j+1)}\int_0^{\pi/2}\cos^{2j+2}x dx \\ &= \frac{4^{j+1}k(k-1)^{j+1}}{\pi(k-2)^2(2j+1)}\frac{2j+1}{2j+2}\frac{2j-1}{2j}\cdots\frac{1}{2}\frac{\pi}{4} \\ &\leq \frac{4^{j+1}k(k-1)^{j+1}}{\pi(k-2)^2}\frac{\sqrt{\pi}}{8(j+1)\sqrt{j}} \\ &= \frac{4^j k(k-1)^{j+1}}{2(j+1)\sqrt{\pi j}(k-2)^2}. \end{aligned}$$

□

We note that a similar upper bound was given in [16] as an asymptotic estimate for r_{2j}.

Lemma 8 *For a k-regular graph G, there is a covering π from T_k to G and the heat kernel $h_t(u,v)$ of G satisfies*

$$h_t(u,v) = \sum_{a=0}^{\infty} c_a H_t(0,a)$$

where c_a denotes the number of irreducible walks from v to u of length a.

7 Spanning trees in a k-regular graph

For a connected graph G, we consider the ζ-function

$$\zeta(s) = \sum_{i\neq 0}\frac{1}{\lambda_i^s}$$

where λ_i ranges over all nonzero eigenvalues of G.

It can be easily checked that

$$-\zeta'(0) = \sum_{i \neq 0} \log \lambda_i = \log \prod_{i \neq 0} \lambda_i$$

where log denotes the natural logarithm.

Theorem 3 *For a connected graph G, the number $\tau(G)$ of spanning trees in G is equal to*

$$\frac{\prod_x d_x}{\sum_x d_x} e^{-\zeta'(0)}$$

where d_x denotes the degree of x.

Proof: Suppose we consider the characteristic polynomial $p(x)$ of the Laplacian $\mathcal{L}$.

$$p(x) = det(\mathcal{L} - xI).$$

The coefficient of the linear term is exactly

$$-\prod_{i \neq 0} \lambda_i.$$

On the other hand,

$$p(x) = detT^{-1}det(L - xT) = (\prod_x d_x)^{-1} p_1(x).$$

By the well known matrix-tree theorem, the coefficient of the linear term of $p_1(x)$ is exactly $-\sum_x d_x$ times the number of spanning trees of G. $\square$

Thus, the number of spanning trees of a k-regular graph on n vertices satisfies

$$\tau(G) \;=\; \frac{k^{n-1}}{n} e^{-\zeta'(0)}. \tag{2}$$

In the rest of the paper, we assume that G is k-regular.

The trace function $Tr\ h_t$ of G satisfies

$$Tr\ h_t \;=\; \sum_i e^{-t\lambda_i}.$$

Therefore the zeta function satisfies

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1}(Tr\ h_t - 1)dt \tag{3}$$

by using the fact that

$$\frac{1}{\Gamma(z)} \int_0^\infty e^{-\rho t} t^{z-1} dt = \frac{1}{\rho^z}. \tag{4}$$

8 The maximum number of spanning trees in k-regular graphs

McKay [16] gave the following bounds for the maximum number of spanning trees over all k-regular graphs G_n on n vertices:

$$c_1 \frac{1}{n} C^n \leq \max \tau(G) \leq c_2 \frac{\log n}{n} C^n$$

where

$$C = \frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}}$$

and c_1 and c_2 depend only on k (in some complicated formula). He conjectured that the upper bound is the right order for $\max \tau(G_n)$. Here we will simplify the upper bound and prove that indeed it is best possible within a constant factor.

Theorem 4 *For $k \geq 3$, the number $\tau(G_n)$ of spanning trees in a k-regular graph G_n on n vertices satisfies*

$$\tau(G_n) \leq (1+o(1)) \frac{2\log n}{kn\log k} \left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}} \right)^n .$$

Theorem 5 *For $k \geq 8$, there are k-regular graphs G on n vertices having the number $\tau(G_n)$ of spanning trees satisfying*

$$\tau(G) \geq (1+o(1)) \frac{\log n}{kn\log k} \left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}} \right)^n .$$

We first need to establish the relation between the heat kernels h_t and H_t. Let r'_j denote the total number of rooted closed walks of length j which are not totally reducible. We then have

$$\begin{aligned} Tr\ h_t &= e^{-t} \sum_{j \geq 0} (nr_j + r'_j) \frac{(t/k)^j}{j!} \\ &= nH_t(0,0) + e^{-t} \sum_{j\geq 0} r'_j \frac{(t/k)^j}{j!}. \end{aligned}$$

From equation (3), we have

$$\zeta(s) =: \zeta_0(s) + \zeta_1(s)$$

where

$$\zeta_0(s) = \frac{n}{\Gamma(s)} \int_0^\infty t^{s-1} H_t(0,0) dt$$

and

$$\zeta_1(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t} \left(\sum_{j\geq 0} r'_j \frac{(t/k)^j}{j!} - e^t \right).$$

We have

$$\begin{aligned}
\zeta_0(s) &= \frac{n}{\Gamma(s)} \int_0^\infty t^{s-1} H_t(0,0) dt \\
&= \frac{2nk(k-1)}{\pi\Gamma(s)} \int_0^\infty t^{s-1} \int_0^\pi \frac{e^{-t(1-\frac{2\sqrt{k-1}}{k}\cos x)} \sin^2 x}{k^2 - 4(k-1)\cos^2 x} dx dt \\
&= \frac{2nk(k-1)}{\pi} \int_0^\pi \frac{1}{(1-\frac{2\sqrt{k-1}}{k}\cos x)^s} \cdot \frac{\sin^2 x}{k^2 - 4(k-1)\cos^2 x} dx.
\end{aligned}$$

Therefore

$$\begin{aligned}
\zeta'_0(0) &= -\frac{2nk(k-1)}{\pi} \int_0^\pi \frac{\sin^2 x}{k^2 - 4(k-1)\cos^2 x} \log(1 - \frac{2\sqrt{k-1}}{k}\cos x) dx \\
&= n \log \frac{k^{k/2}(k-2)^{k/2-1}}{(k-1)^{k-1}}. \qquad (5)
\end{aligned}$$

The above integral is evaluated by using the following formula given in [16]:

$$\frac{k}{2\pi} \int_{-\omega}^{\omega} \frac{(\omega^2 - x^2)^{1/2}}{k^2 - x^2} \log(1 - \gamma x) dx = -\log\left(\eta (\frac{k-\eta}{k-1})^{k/2-1} \right)$$

where $|\gamma| = 1/k < 1/\omega$, $\omega = 2\sqrt{k-1}$ and $\eta = \frac{1-(1-4(k-1)\gamma^2)^{1/2}}{2(k-1)\gamma^2}$.

It remains to evaluate $\zeta'_1(0)$. We note that

$$\begin{aligned}
nr_j + r'_j &= TrA^j \\
&= k^j \sum_i (1-\lambda_i)^j.
\end{aligned}$$

So, we have, for odd j,

$$\frac{r'_j}{k^j} \geq 1 + \sum_{i\neq 0} (1-\lambda_i)^j.$$

For the even case,

$$\frac{r'_{2j}}{k^{2j}} \geq 1 + \sum_{i\neq 0} (1-\lambda_i)^{2j} - \frac{n4^j k(k-1)^{j+1}}{j\sqrt{\pi j}(k-2)^2}. \qquad (6)$$

For a fixed value β (which will be chosen later), we have

$$\begin{aligned}
\zeta_1(s) &= \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}e^{-t}\left(\sum_{j\geq 0} r'_j\frac{(t/k)^j}{j!} - e^t\right)dt \\
&\geq \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}e^{-t}\left(-\sum_{j=0}^{2\beta-1}\frac{(t/k)^j}{j!}\right)dt \\
&\quad +\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}e^{-t}\left(\sum_{j>2\beta}(r'_j\frac{(t/k)^j}{j!} - \frac{(t/k)^j}{j!})\right)dt.
\end{aligned}$$

We note that for $j \geq 1$, and

$$\rho(s) = \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}e^{-t}(\frac{t^j}{j!})dt$$

we have

$$\rho'(0) = \frac{1}{j}. \tag{7}$$

Therefore

$$\begin{aligned}
\zeta'_1(0) &\geq -\sum_{j=1}^{2\beta-1}\frac{1}{j} + \zeta'_2(0) \\
&\geq -\log(2\beta) + \zeta'_2(0) \qquad (8)
\end{aligned}$$

where we define

$$\zeta_2(s) = \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}e^{-t}\left(\sum_{j\geq 2\beta}(r'_j\frac{(t/k)^j}{j!} - \frac{(t/k)^j}{j!})\right).$$

Here, we have

$$\zeta_2(s) = \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}e^{-t}\left(\sum_{j\geq 2\beta}\frac{t^j}{j!}\left(\sum_{i\neq 0}(1-\lambda_i)^j - \sum_{j\geq\beta}\frac{n4^jk(k-1)^{j+1}}{j\sqrt{\pi j}(k-2)^2k^{2j}}\right)\right).$$

By using equation (7) and inequality (8), we have

$$\begin{aligned}
\zeta'_2(0) &\geq \sum_{j\geq 2\beta}\sum_{i\neq 0}(1-\lambda_i)^j\frac{1}{j} - \sum_{j\geq\beta}\frac{n4^jk(k-1)^{j+1}}{j^2\sqrt{\pi j}(k-2)^2k^{2j}} \\
&\geq -\sum_{j\geq\beta}\frac{n4^jk(k-1)^{j+1}}{j^2\sqrt{\pi j}(k-2)^2k^{2j}} \\
&\geq -2\frac{n4^\beta k(k-1)^{\beta+1}}{\beta^2\sqrt{\pi\beta}(k-2)^2k^{2\beta}} \qquad (9)
\end{aligned}$$

by using $\lambda_i \leq 2$ and the fact that $\sum_{j\geq 2\beta}(1-\lambda_i)^j/j \geq 0$.

Now, we are ready to prove Theorem 4 and 5.

Proof of Theorem 4:

From (2) and (5), we have

$$\begin{aligned}
\tau(G) &= \frac{k^{n-1}}{n} e^{-\zeta_0'(0)-\zeta_1'(0)} \\
&= \frac{k^{n-1}}{n} \left(\frac{(k-1)^{k-1}}{k^{k/2}(k-2)^{k/2-1}} \right)^n e^{-\zeta_1'(0)} \\
&= \frac{1}{kn} \left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}} \right)^n e^{-\zeta_1'(0)}. \qquad (10)
\end{aligned}$$

By using the preceding lower bounds of ζ_1' in (8), we have

$$\tau(G) \leq \frac{2\beta}{kn} \left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}} \right)^n e^{-\zeta_2'(0)}.$$

We now choose β as:

$$\beta = \lceil \frac{\log n}{\log \frac{k^2}{4(k-1)}} \rceil.$$

From (9), we have

$$\begin{aligned}
\zeta_2'(0) &\geq -2\frac{n 4^\beta k(k-1)^{\beta+1}}{\beta^2\sqrt{\pi\beta}(k-2)^2 k^{2\beta}} \\
&\geq -2\frac{k(k-1)}{\beta^2\sqrt{\pi\beta}(k-2)^2}.
\end{aligned}$$

Therefore, we have

$$\begin{aligned}
\tau(G) &\leq \frac{2\beta}{kn} \left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}} \right)^n e^{-\zeta_2'(0)} \\
&\leq (1+o(1)) \frac{2\log n}{kn\log k} \left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}} \right)^n .
\end{aligned}$$

Theorem 4 is proved. □

Proof of Theorem 5:

For a graph with girth (the length of the smallest cycle) g, we can take $\beta = \lfloor g/2 \rfloor$ and we have

$$\begin{aligned}
\zeta_1(s) &= \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t} \left(\sum_{j \geq 0} r'_j \frac{(t/k)^j}{j!} - e^t \right) dt \\
&= \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t} \left(- \sum_{j=0}^{g} \frac{(t/k)^j}{j!} \right) dt \\
&+ \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t} \left(\sum_{j>g} (r'_j \frac{(t/k)^j}{j!} - \frac{(t/k)^j}{j!}) \right) dt.
\end{aligned}$$

$$\begin{aligned}
\zeta'_1(0) &\leq -\sum_{j=1}^{g-1} \frac{1}{j} + \zeta'_2(0) \\
&\leq -\log g + \zeta'_2(0) \qquad (11)
\end{aligned}$$

where here we will need to use some known results on random k-regular graphs. Erdős and Sachs [8] proved that with positive probability, say at least 1/2, there is a k-regular graph on n vertices having girth g satisfying

$$g = (1 + o(1)) \frac{\log n}{\log k}$$

as n approaches infinity. Friedman [10] showed that with probability approaches 1, the expected number of irreducible walks $c_j(v)$ rooted at a vertex v of length j, for $k \geq 8$, is

$$E(c_j(v)) = k(k-1)^{j-1}(\frac{1}{n} + Err_{n,j})$$

where

$$Err_{n,j} = O\left((ckj)^c (\frac{j^{2\sqrt{k}}}{n^{1+\sqrt{k-1}/2}} + \frac{1}{k^{j/2}}) \right).$$

We note that in the original paper of Friedman, only the case for even k was treated. However, the argument of counting irreducible "words" made of letters can be extended to counting walks on the k-trees for odd k in a similar way.

The expected number of closed walks of length j satisfies (see [10])

$$k^j \left(1 + (n-1)p_{j,0} + \sum_{s=1}^{j} np_{j,s} Err_{n,s} \right)$$

where $p_{j,s}$ is the probability that a random walk of length j reduces to an irreducible walk of size s. Hence, the number r'_j of not totally reducible walks of length j satisfies

$$E(\frac{r'_j}{k^j}) = 1 - p_{j,0} + \sum_{s=1}^{j} np_{j,s} Err_{n,s}.$$

Since $p_{j,s} \le 2^j k^{-j+s}$, we have

$$\begin{aligned}
\zeta_2(s) &= \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t} \left(\sum_{j \ge 2\beta} (r'_j \frac{(t/k)^j}{j!} - \frac{(t/k)^j}{j!}) \right) \\
&\le \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t} \left(\sum_{j \ge 2\beta} \frac{(t/k)^j}{j!} 2^j \sum_{s=0}^{j} k^{-j+s} (cks)^c (\frac{s^{2\sqrt{k}} 2^s}{n^{\sqrt{k-1}/2}} + \frac{1}{(k-1)^{s/2}}) \right).
\end{aligned}$$

Therefore,

$$\begin{aligned}
\zeta_2'(0) &\le \sum_{j \ge g} \frac{1}{j} \sum_{s=1}^{j} 2^j k^{-j+s} (cks)^c (\frac{s^{2\sqrt{k}} 2^s}{n^{\sqrt{k-1}/2}} + \frac{1}{(k-1)^{s/2}}) \\
&= o(1).
\end{aligned}$$

Using (10) and combining the preceding bounds , we have

$$\begin{aligned}
\tau(G) &= \frac{1}{kn} \left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}} \right)^n e^{-\zeta_1'(0)} \\
&\ge \frac{g}{kn} \left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}} \right)^n e^{-\zeta_2'(0)} \\
&\ge (1+o(1)) \frac{\log n}{kn \log k} \left(\frac{(k-1)^{k-1}}{(k^2-2k)^{k/2-1}} \right)^n.
\end{aligned}$$

This completes the proof of Theorem 5. □

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