Spectral diameter estimates for k-regular graphs

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An undirected graph is called *k-regular* if exactly k edges meet at each vertex. The eigenvalues of the adjacency matrix of a finite, k-regular graph Γ (assumed to be undirected and connected) satisfy $|\lambda_i| \leq k$, with k occurring as a simple eigenvalue. Let $\lambda(\Gamma)$ denote the maximum of $\{|\lambda_i| : |\lambda_i| \neq k\}$, and let N denote the number of vertices in Γ. The diameter of Γ can be bounded in terms of N and $\lambda(\Gamma)$. Chung ([5]) and Sarnak ([7]) have derived the estimate

$$\operatorname{diam}(\Gamma) \quad \leq \quad \frac{\operatorname{arccosh}(N-1)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)} + 1,$$

which will be our Theorem 2.

Following Brooks ([2]), we define graph-theoretic spherical functions S_λ on the universal cover of Γ, and apply the techniques of the Selberg pre-trace formula to write a spectral expression for the number of paths of length n joining two vertices x and y in Γ. Calling this number $K_n(x,y)$, we have, as Lemma 9.4,

$$K_n(x,y) \quad = \quad k(k-1)^{n-1} \sum_i S_{\lambda_i}(n) \varphi_i(x) \varphi_i(y)$$

where $\{\varphi_i\}$ is an orthonormal set of eigenfunctions for the adjacency operator, in correspondence with the eigenvalues $\{\lambda_i\}$.

We then use the spectral expression for $K_r(x,y)$, where $r \geq 1$ is the injectivity radius of Γ, along with the ideas used to prove Theorem 2, to derive a new diameter estimate in Theorem 3:

$$\operatorname{diam}(\Gamma) \;\leq\; \frac{\operatorname{arccosh}\left(\frac{N}{k(k-1)^{r-1}} - 1\right)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)} + 2r + 1.$$

Finally, in Section 12, we argue that the bound given by Theorem 3 is usually stronger than the bound in Theorem 2.

1 The adjacency matrix

Let Γ be a k-regular, connected, undirected graph with a finite number N of vertices. We assume Γ has no loops or multiple edges, so that its adjacency matrix A is a symmetric, irreducible zero-one matrix with no ones on the diagonal and exactly k ones in each row and column.

We will use the notation "$x \sim y$" to mean the vertices x and y are joined by an edge. Also "$x \in \Gamma$" will be taken to mean x is a vertex in Γ.

A *walk* in Γ is a sequence $x_0, x_1, \ldots, x_n$ of vertices such that $x_{i-1} \sim x_i$ for $i = 1, \ldots, n$. The vertices x_0 and x_n are the *endpoints* of the walk and the number n is its *length*. Let $W_n(x,y)$ denote the number of walks of length n whose endpoints are x and y. Then it is easy to see that

$$W_n(x,y) \;=\; [A^n]_{xy} \tag{1}$$

where we have used the notation $[M]_{xy}$ for the entry of the matrix M in the row associated with the vertex x and the column associated with the vertex y.

A *path* in Γ is a walk $x_0, x_1, \ldots, x_n$ such that $x_i \neq x_{i-2}$ for $i = 2, \ldots, n$. That is to say, a path does not double back by traversing the same edge twice in succession. We will let $K_n(x,y)$ denote the number of paths of length n whose endpoints are x and y. An expression for K_n in terms of A is somewhat more complicated than (1), and will be the subject of a later section.

The *distance* between two vertices x and y, denoted $\operatorname{dist}(x,y)$, is the length of the shortest walk whose endpoints are x and y. We are assuming that Γ is connected, so all distances are finite. The *diameter* of Γ is the maximum of $\mathrm{dist}(x, y)$ over all pairs (x, y).

A walk or path $x_0, x_1, \ldots, x_n$ is *closed* if $x_0 = x_n$. A graph Γ is said to be *bipartite* if it has no closed walks of odd length. In terms of our present notation, Γ is bipartite if and only if $W_n(x, x) = 0$ for all odd n and all vertices x. Because Γ is connected, the matrix A is irreducible, and the condition just stated is equivalent to the period of the matrix A being even. Since we have

$$[A^2]_{xx} \quad = \quad k \neq 0 \tag{2}$$

for all vertices x, we can say even more:

Lemma 1.1 *The period of A is 2 if Γ is bipartite, and 1 if Γ is not bipartite.*

Because A is symmetric, all its eigenvalues are real. Furthermore, the k-regularity of Γ means that all the row sums of A are equal to k. Lemma 1.1 and the Perron-Frobenius theorem then imply

Lemma 1.2 *Let A be the adjacency matrix of a finite, connected, k-regular graph Γ. Then*

(a) the number k is a simple eigenvalue of A;

(b) the number $-k$ is a simple eigenvalue of A if and only if Γ is bipartite;

(c) all other eigenvalues λ of A satisfy $|\lambda| < k$.

Let $\lambda(\Gamma)$ denote the absolute value of the next-largest eigenvalue of A, that is

$$\lambda(\Gamma) \quad = \quad \max\{|\lambda| \,:\, \lambda \in \mathrm{Spec}(A), |\lambda| \neq k\}. \tag{3}$$

2 The adjacency operator

By a *function* on Γ, we will mean a real-valued function on the vertices of Γ. If Γ has N vertices, then space of such functions is isomorphic, as a real inner-product space, with $\mathbb{R}^N$. If φ and ψ are two functions on Γ, we will write their inner product with angle brackets:

$$\langle \varphi, \psi \rangle \quad = \quad \sum_{x \in \Gamma} \varphi(x)\psi(x). \tag{4}$$

If φ is a function on Γ, then we can write φ as a column vector

$$\varphi(x) \quad = \quad (\varphi(x_1)\, \varphi(x_2)\, \cdots\, \varphi(x_N))^t \tag{5}$$

where x_i is the vertex associated with the i^{th} row of the adjacency matrix A. We then obtain a new function $A\varphi$ by matrix multiplication. In fact, the i^{th} entry of the column vector $A\varphi$ is given by

$$[A\varphi]_i \quad = \quad \sum_{x_j \sim x_i} \varphi(x_j). \tag{6}$$

In more operator-like notation, we have

$$(A\varphi)(x) \quad = \quad \sum_{y \sim x} \varphi(y). \tag{7}$$

We will take expression (7) as our definition of the adjacency operator A on the space of functions on a graph.

We have already remarked that the spectrum of A (as a matrix, but also as an operator) is a subset of the real line. In the sequel, we will write the spectrum of A as $\{\lambda_0, \lambda_1, \ldots, \lambda_{N-1}\}$ with

$$k = \lambda_0 > \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{N-1}. \tag{8}$$

Furthermore, because A is self-adjoint (it is represented by a symmetric matrix), there exists a corresponding orthonormal basis of eigenfunctions of A, which we will write

$$\{\varphi_0, \varphi_1, \ldots, \varphi_{N-1}\}. \tag{9}$$

3 Aside: the Laplacian

A more familiar operator in the field of spectral geometry is the Laplacian operator, Δ, which appears so prominently in the heat equation and the wave equation. A reasonable way to define a Laplacian operator on a graph is

$$(\Delta\varphi)(x) \quad = \quad \sum_{y\sim x} \left(\varphi(x) - \varphi(y)\right), \tag{10}$$

where φ is a function on the graph.

If Γ is k-regular, the right-hand side of (10) is easily seen to be

$$k\varphi(x) \quad - \quad \sum_{y\sim x} \varphi(y) \tag{11}$$

so that

$$\Delta \quad = \quad kI - A, \tag{12}$$

where I represents the identity operator.

It follows that the spectrum of the adjacency matrix A is the image of the spectrum of Δ under an affine transformation. Thus the number $\lambda(\Gamma)$, loosely speaking, represents the "fundamental frequency" of the graph Γ. The analogy is not perfect, because $\lambda(\Gamma)$ may correspond to either the lowest or the highest frequency among the nontrivial steady-state solutions to the wave equation on Γ. Nonetheless, we will treat $\lambda(\Gamma)$ as an "observable," and base our diameter estimates on this number.

4 The spectrum on a bipartite graph

If Γ is bipartite then, as the term suggests, we can partition the vertices of Γ into two sets with the property that no two vertices of the same set are joined by an edge. Let us arbitrarily assign a parity to each of these two sets: $\operatorname{sgn}(x)$ will be "even" if x belongs to the even set and "odd" if x belongs to the odd set.

Lemma 4.1 *Suppose Γ is bipartite. Let φ be a function on Γ such that $A\varphi = \lambda\varphi$ for some real number λ. Define a new function ψ by*

$$\psi(x) = (-1)^{\mathrm{sgn}(x)}\varphi(x). \tag{13}$$

Then $A\psi = -\lambda\psi$.

Proof.

$$\begin{aligned}
(A\psi)(x) &= \sum_{y\sim x} \psi(y) && (14)\\
&= \sum_{y\sim x} (-1)^{\mathrm{sgn}(y)}\varphi(y) && (15)\\
&= -\sum_{y\sim x} (-1)^{\mathrm{sgn}(x)}\varphi(y) && (16)\\
&= -(-1)^{\mathrm{sgn}(x)}(A\varphi)(x) && (17)\\
&= -\lambda(-1)^{\mathrm{sgn}(x)}\varphi(x) && (18)\\
&= -\lambda\psi(x) && (19)
\end{aligned}$$

□

Corollary 4.2 *Let Γ be a k-regular bipartite graph with adjacency spectrum*

$$k = \lambda_0 > \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{N-2} > \lambda_{N-1} = -k. \tag{20}$$

Let $\{\varphi_0, \varphi_1, \ldots, \varphi_{N-1}\}$ denote an orthonormal set of eigenfunctions corresponding to $\{\lambda_0, \lambda_1, \ldots, \lambda_{N-1}\}$. Then for each $i \in \{0, 1, \ldots, N-1\}$,

(a) $\lambda_{N-1-i} = -\lambda_i$;

(b) we may take $\varphi_{N-1-i}(x) = (-1)^{\mathrm{sgn}(x)}\varphi_i(x)$;

(c) in this case,

$$\varphi_{N-1-i}(x)\varphi_{N-1-i}(y) = (-1)^{\mathrm{dist}(x,y)}\varphi_i(x)\varphi_i(y). \tag{21}$$

Proof. Parts (a) and (b) follow from Lemma 4.1 and the existence of an orthonormal basis of eigenfunctions. From part (b), we have

$$\varphi_{N-1-i}(x)\varphi_{N-1-i}(y) \quad = \quad (-1)^{\mathrm{sgn}(x)+\mathrm{sgn}(y)}\varphi_i(x)\varphi_i(y). \tag{22}$$

To prove (c), we observe that $\mathrm{sgn}(x) = \mathrm{sgn}(y)$ if and only if $\mathrm{dist}(x, y)$ is even. □

5 $W_n(x, y)$

We write the walk-counting function $W_n(x, y)$ in terms of the numbers λ_i and the functions φ_i.

Lemma 5.1

$$W_n(x, y) \quad = \quad \sum_{i=0}^{N-1} \lambda_i^n \varphi_i(x)\varphi_i(y). \tag{23}$$

Proof. We have already observed that

$$W_n(x, y) \quad = \quad [A^n]_{xy}. \tag{24}$$

Let Φ be the $N \times N$ matrix whose columns are the eigenfunctions φ_i. The following are immediate

(a) Φ is unitary: $\Phi^{-1} = \Phi^t$.

(b) Φ diagonalizes A: $\Phi A \Phi^t = D$, where D is the $N \times N$ diagonal matrix with diagonal entries $\lambda_0, \lambda_1, \ldots, \lambda_{N-1}$.

Then

$$[A^n]_{xy} \quad = \quad [\Phi^t D^n \Phi]_{xy} \tag{25}$$

$$\quad = \quad \sum_{i=0}^{N-1} \lambda_i^n \varphi_i(x)\varphi_i(y). \tag{26}$$

□

6 A spectral diameter estimate

In addition to what we know about the spectrum of A on a k-regular graph, we will make use of two facts about the eigenfunctions φ_i. We state them as

Lemma 6.1 *For each vertex $x \in \Gamma$,*

(a)

$$\varphi_0(x) = \frac{1}{\sqrt{N}}; \tag{27}$$

(b)

$$\sum_{i=0}^{N-1} \varphi_i^2(x) = 1. \tag{28}$$

Proof. The constant function $\mathbf{1}$ satisfies $A\mathbf{1} = \lambda_0 \mathbf{1}$, where $\lambda_0 = k$ is a simple eigenvalue. Thus φ_0 is a multiple of the constant function, and since $\langle \varphi_0, \varphi_0 \rangle = 1$, we must have $\varphi_0 \equiv \frac{1}{\sqrt{N}}$, establishing part (a).

Part (b) follows from the orthonormality of the φ_i. If Φ is the $N \times N$ matrix whose columns are the φ_i, then Φ is unitary, so that its rows, as well as its columns, are orthonormal. A row of φ takes the form

$$(\varphi_0(x)\, \varphi_1(x)\, \cdots\, \varphi_{N-1}(x)) \tag{29}$$

and part (b) is just the assertion that this row vector has norm 1. $\square$

Our first spectral diameter estimate, which will set the pattern for those to follow, is found in [4].

Theorem 1 *Let Γ be a k-regular graph with N vertices.*

(a) If Γ is not bipartite then

$$\mathrm{diam}(\Gamma) \leq \frac{\log(N-1)}{\log k - \log \lambda(\Gamma)} + 1 \tag{30}$$

(b) If Γ is bipartite then

$$\mathrm{diam}(\Gamma) \leq \frac{\log(N-2) - \log 2}{\log k - \log \lambda(\Gamma)} + 2 \tag{31}$$

Proof. Choose x and y such that $\mathrm{dist}(x, y) = \mathrm{diam}(\Gamma)$. If n is a non-negative integer less than $\mathrm{dist}(x, y)$, then clearly $W_n(x, y) = 0$. By Lemma 5.1, then,

$$0 = \sum_{i=0}^{N-1} \lambda_i^n \varphi_i(x)\varphi_i(y). \tag{32}$$

We know that $\lambda_0 = k$ and $\varphi_0(x) = \varphi_0(y) = 1/\sqrt{N}$, so we can write

$$0 = \frac{k^n}{N} + \sum_{i=1}^{N-1} \lambda_i^n \varphi_i(x)\varphi_i(y) \tag{33}$$

which implies that

$$\frac{k^n}{N} = \left| \sum_{i=1}^{N-1} \lambda_i^n \varphi_i(x)\varphi_i(y) \right|. \tag{34}$$

Assume now that Γ is not bipartite. Then $(\lambda(\Gamma))^n$ is the greatest element of the set $\{|\lambda_i^n| : i = 1, \ldots, N-1\}$. Applying the triangle inequality, the observation just made about $\lambda(\Gamma)$, and finally the Cauchy-Schwarz inequality, we obtain, from (34),

$$\begin{aligned}
\frac{k^n}{N} &\leq \sum_{i=1}^{N-1} |\lambda_i^n||\varphi_i(x)\varphi_i(y)| && (35)\\
&\leq (\lambda(\Gamma))^n \sum_{i=1}^{N-1} |\varphi_i(x)\varphi_i(y)| && (36)\\
&\leq (\lambda(\Gamma))^n \left(\sum_{i=1}^{N-1} \varphi_i^2(x)\right)^{\frac{1}{2}} \left(\sum_{i=1}^{N-1} \varphi_i^2(y)\right)^{\frac{1}{2}}. && (37)
\end{aligned}$$

Lemma 6.1 implies that

$$\sum_{i=1}^{N-1} \varphi_i^2(y) = \sum_{i=1}^{N-1} \varphi_i^2(x) = 1 - \frac{1}{N}. \tag{38}$$

Putting this into (37), we get

$$\frac{k^n}{N} \;\leq\; (\lambda(\Gamma))^n \left(1 - \frac{1}{N}\right) \tag{39}$$

which yields the upper bound

$$n \;\leq\; \frac{\log(N-1)}{\log k - \log \lambda(\Gamma)}. \tag{40}$$

This is true for each n less than $\mathrm{dist}(x, y) = \mathrm{diam}(\Gamma)$, and we conclude that

$$\mathrm{diam}(\Gamma) \;\leq\; \frac{\log(N-1)}{\log k - \log \lambda(\Gamma)} + 1. \tag{41}$$

Now suppose Γ is bipartite. If the parity of n is different from the parity of $\mathrm{dist}(x, y)$, then parts (a) and (c) of Corollary 4.2 imply that

$$\lambda_{N-i}^n \varphi_{N-i}(x)\varphi_{N-i}(y) \;=\; -\lambda_i^n \varphi_i(x)\varphi_i(y) \tag{42}$$

for each i. In this case the right-hand side of equation (32) is trivially zero, and the equation yields no information. If, on the other hand, the parity of n agrees with the parity of $\mathrm{dist}(x, y)$, then for each i,

$$\lambda_{N-1-i}^n \varphi_{N-1-i}(x)\varphi_{N-1-i}(y) \;=\; \lambda_i^n \varphi_i(x)\varphi_i(y) \tag{43}$$

and equation (32) may be decomposed thus:

$$0 \;=\; 2\frac{k^n}{N} + \sum_{i=1}^{N-2} \lambda_i^n \varphi_i(x)\varphi_i(y). \tag{44}$$

Imitating our previous computation ((35) - (37)), we write

$$\begin{aligned} 2\frac{k^n}{N} &= \left|\sum_{i=1}^{N-2} \lambda_i^n \varphi_i(x)\varphi_i(y)\right| & (45) \\ &\leq (\lambda(\Gamma))^n \sum_{i=1}^{N-2} |\varphi_i(x)\varphi_i(y)| & (46) \\ &\leq (\lambda(\Gamma))^n \left(\sum_{i=1}^{N-2} \varphi_i^2(x)\right)^{\frac{1}{2}} \left(\sum_{i=1}^{N-2} \varphi_i^2(y)\right)^{\frac{1}{2}} & (47) \end{aligned}$$

Using the fact that $\varphi_{N-1}(x) = \pm\varphi_0(x)$ and both parts of Lemma 6.1, we find that

$$\sum_{i=1}^{N-2} \varphi_i^2(y) = \sum_{i=1}^{N-2} \varphi_i^2(x) = 1 - \frac{2}{N}. \tag{48}$$

Plugging this into (47), we continue:

$$\begin{aligned} 2\frac{k^n}{N} &\leq (\lambda(\Gamma))^n \left(1 - \frac{2}{N}\right) & (49) \\ \frac{k^n}{(\lambda(\Gamma))^n} &\leq \frac{N-2}{2} & (50) \\ n &\leq \frac{\log(N-2) - \log 2}{\log k - \log \lambda(\Gamma)}. & (51) \end{aligned}$$

We had to assume that n was less than $\mathrm{diam}(\Gamma)$ and of the same parity as $\mathrm{diam}(\Gamma)$, so we can conclude that

$$\mathrm{diam}(\Gamma) \leq \frac{\log(N-2) - \log 2}{\log k - \log \lambda(\Gamma)} + 2. \tag{52}$$

□

7 Polynomial diameter estimates

We can improve on the estimate in Theorem 1 by making better use of our observation that

$$0 = \sum_{i=0}^{N-1} \lambda_i^n \varphi_i(x)\varphi_i(y) \tag{53}$$

for any non-negative integer n less than $\mathrm{dist}(x, y)$. Let x and y be such that $\mathrm{dist}(x, y) = \mathrm{diam}(\Gamma)$, and let $\{p_n : n = 0, 1, 2, \ldots\}$ be a family of polynomials such that the degree of p_n is n. Then it follows from (53) that

$$0 = \sum_{i=0}^{N-1} p_n(\lambda_i)\varphi_i(x)\varphi_i(y) \tag{54}$$

for each n less than $\mathrm{diam}(\Gamma)$.

Proceeding as in the proof of Theorem 1, we write this as

$$0 = p_n(\lambda_0)\varphi_0(x)\varphi_0(y) + \sum_{i=1}^{N-1} p_n(\lambda_i)\varphi_i(x)\varphi_i(y). \tag{55}$$

We know that $\lambda_0 = k$ and $\varphi_0 \equiv \frac{1}{\sqrt{N}}$, and let us assume that $p_n(k)$ will be positive for each n. Then (55) implies that

$$\frac{p_n(k)}{N} = \left|\sum_{i=1}^{N-1} p_n(\lambda_i)\varphi_i(x)\varphi_i(y)\right|. \tag{56}$$

Next we apply the triangle inequality to get

$$\frac{p_n(k)}{N} \leq \sum_{i=1}^{N-1} |p_n(\lambda_i)|\,|\varphi_i(x)\varphi_i(y)|. \tag{57}$$

As in the proof of Theorem 1, our diameter estimate will turn out the be the least n for which this inequality does *not* hold. Thus it is to our advantage to make the left side of (57) as large as possible for each n, while keeping the right side small. If Γ is not bipartite (and for now we will assume that this is the case), then $|\lambda_i| \leq \lambda(\Gamma)$ for each λ_i appearing on the right side of (57). We wish to select a family $\{p_n\}$ of polynomials, then, such that

(a) $p_n(k)$ is large for each n, and

(b) $|p_n(\lambda)|$ is bounded for $|\lambda| \leq \lambda(\Gamma)$.

The Chebychev polynomials (see [1])

$$T_n(x) = \cosh(n \operatorname{arccosh}(x)) \tag{58}$$

satisfy

$$|T_n(x)| \leq 1 \quad \text{for} \quad |x| \leq 1 \tag{59}$$

and increase quite rapidly for $x > 1$. We do reasonably well by our criteria above by setting

$$\begin{aligned} p_n(\lambda) &= T_n\left(\frac{\lambda}{\lambda(\Gamma)}\right) &(60)\\ &= \cosh\left(n \operatorname{arccosh}\left(\frac{\lambda}{\lambda(\Gamma)}\right)\right). &(61)\end{aligned}$$

Then $|p_n(\lambda_i)| \leq 1$ in each term on the right side of (57), and the inequality implies that

$$\frac{p_n(k)}{N} \leq \sum_{i=1}^{N-1} |\varphi_i(x)\varphi_i(y)|. \tag{62}$$

As before, we use the Cauchy-Schwarz inequality and Lemma 6.1 to get

$$\begin{aligned} \frac{p_n(k)}{N} &\leq \left(\sum_{i=1}^{N-1} \varphi_i^2(x)\right)^{\frac{1}{2}} \left(\sum_{i=1}^{N-1} \varphi_i^2(y)\right)^{\frac{1}{2}} &(63)\\ &\leq \left(1 - \frac{1}{N}\right), &(64)\end{aligned}$$

so that

$$p_n(k) \quad \leq \quad N - 1. \tag{65}$$

Since $p_n(k) = \cosh(n \operatorname{arccosh}(\frac{k}{\lambda(\Gamma)}))$ and everything in sight is greater than 1, it follows that

$$n \operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right) \quad \leq \quad \operatorname{arccosh}(N-1), \tag{66}$$

and finally that

$$n \quad \leq \quad \frac{\operatorname{arccosh}(N-1)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)}. \tag{67}$$

This is true, in particular, for $n = \operatorname{diam}(\Gamma) - 1$, and we have proved part (a) of the following theorem. Part (b) depends on a minor modification of the same argument.

Theorem 2 *Let Γ be a k-regular, connected graph with N vertices.*

(a) If Γ is not bipartite then

$$\operatorname{diam}(\Gamma) \quad \leq \quad \frac{\operatorname{arccosh}(N-1)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)} + 1. \tag{68}$$

(b) If Γ is bipartite then

$$\operatorname{diam}(\Gamma) \quad \leq \quad \frac{\operatorname{arccosh}\left(\frac{N}{2}-1\right)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)} + 2. \tag{69}$$

Sarnak uses the same technique, but expresses the result slightly differently in [7]. Chung presents a more general form of this theorem, not requiring k-regularity, in [5].

8 Polynomial estimates are better

Note that the approach we have used to prove Theorem 2 yields exactly the result in Theorem 1 if, instead of using the Chebychev polynomials, we define the family $\{p_n\}$ by

$$p_n(\lambda) \;=\; \left(\frac{\lambda}{\lambda(\Gamma)}\right)^n. \tag{70}$$

In fact, since this family of polynomials also satisfies

$$|p_n(\lambda)| \leq 1 \quad \text{for} \quad |\lambda| \leq \lambda(\Gamma), \tag{71}$$

we could write a proof of Theorem 1 identical to our proof of Theorem 2 except in the last step, where we would use logarithms, rather than the inverse hyperbolic cosine, to dig out the number n.

In Theorem 1, the diameter bound is one more than the greatest n such that

$$\left(\frac{k}{\lambda(\Gamma)}\right)^n \;\leq\; N-1 \tag{72}$$

and in Theorem 2 the bound is one more than the greatest n such that

$$\cosh\left(n \,\mathrm{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)\right) \;\leq\; N-1. \tag{73}$$

To verify that the estimate in Theorem 2 is actually stronger than the estimate in Theorem 1, then, we need only verify that

$$\cosh\left(n \,\mathrm{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)\right) \;\geq\; \left(\frac{k}{\lambda(\Gamma)}\right)^n \tag{74}$$

for each n. Since $k > \lambda(\Gamma)$, this requirement may be phrased more succinctly as

$$\cosh(n \,\mathrm{arccosh}(x)) \geq x^n \quad \text{for} \quad x > 1,\ n \geq 0. \tag{75}$$

This is true, and may be verified as follows.

Lemma 8.1 *Let* $T_n(x) = \cosh(n \operatorname{arccosh}(x))$*. Let* $x > 1$*. Then*

(a) $T_0(x) = x^0$*;* $T_1(x) = x^1$*.*

(b) If $n > 1$ *then* $T_n(x) > x^n$*.*

Proof. Both statements in part (a) are immediate from the definitions. For part (b), we wish to show that, under the stated conditions,

$$\cosh(n \operatorname{arccosh}(x)) \quad > \quad x^n. \tag{76}$$

Since both sides of this inequality are greater than 1 (by hypothesis), we can take the inverse hyperbolic cosine and find that the required inequality is equivalent to

$$n \operatorname{arccosh}(x) \quad > \quad \operatorname{arccosh}(x^n). \tag{77}$$

We will show that the expression

$$n \operatorname{arccosh}(x) \quad - \quad \operatorname{arccosh}(x^n) \tag{78}$$

is positive for $x > 1$ and $n > 1$. Recalling (or looking up) the derivative of arccosh, we write (78) as

$$n \int_1^x \frac{1}{\sqrt{t^2 - 1}}\, dt \quad - \quad n \int_1^x \frac{t^{n-1}}{\sqrt{t^{2n} - 1}}\, dt. \tag{79}$$

We combine the two integrals to get

$$n \int_1^x \frac{\sqrt{t^{2n} - 1} \;-\; t^{n-1}\sqrt{t^2 - 1}}{\sqrt{(t^2 - 1)(t^{2n} - 1)}}\, dt. \tag{80}$$

The denominator in the integrand is positive throughout the interval $(1, x)$, so we need only verify that the numerator is positive. (Since we already know the antiderivative, we may safely assume that the integral converges.) The numerator is positive if

$$\sqrt{t^{2n} - 1} \quad > \quad \sqrt{t^{2n} - t^{2n-2}}. \tag{81}$$

Since $n > 1$ and $t > 1$, the subtrahend t^{2n-2} is greater than 1, so the inequality holds.

$\square$

9 $K_n(x, y)$

Next we turn to the function $K_n(x, y)$, which counts the number of paths of length n whose endpoints are x and y.

Let Γ be a k-regular graph with N vertices, and let Γ_k be the k-tree, which is the universal cover of Γ. The adjacency operator on the space of functions on Γ_k will be denoted by A, and is defined analogously to the adjacency operator on Γ, by expression (7).

Lemma 9.1 *Let $x \in \Gamma_k$, $\lambda \in \mathbb{R}$. Then there is a unique function $S_{\lambda,x}$ on Γ_k such that*

(a) $S_{\lambda,x}(x) = 1$

(b) $AS_{\lambda,x} = \lambda S_{\lambda,x}$

(c) $S_{\lambda,x}(y) = S_{\lambda,x}(z)$ *if* $\mathrm{dist}(x, y) = \mathrm{dist}(x, z)$.

Proof. Let $C(x, r)$ denote the set of vertices $\{y \in \Gamma_k : \mathrm{dist}(x, y) = r\}$. If $r = 0$, then the set $C(x, r)$ contains just the vertex x. If $r \geq 1$ then $C(x, r)$ contains exactly $k(k-1)^{r-1}$ vertices.

By condition (c), the function $S_{\lambda,x}$ is constant on each set $C(x, r)$. We will use the notation $S_\lambda(r)$ to denote the common value of $S_{\lambda,x}$ on $C(x, r)$.

Condition (a) fixes $S_\lambda(0)$. The value of $S_\lambda(1)$ is determined by

$$\begin{aligned} \lambda &= \lambda S_\lambda(0) && (82) \\ &= (AS_{\lambda,x})(x) && (83) \\ &= \sum_{y \sim x} S_{\lambda,x}(y) && (84) \\ &= kS_\lambda(1) && (85) \end{aligned}$$

implying that $S_\lambda(1) = \lambda/k$.

If $r \geq 1$ and $y \in C(x, r)$ then we have

$$AS_{\lambda,x}(y) = S_{\lambda,x}(z_1) + (k-1)S_{\lambda,x}(z_2) \quad (86)$$

where z_1 is some vertex in $C(x, r-1)$ and z_2 is some vertex in $C(x, r+1)$. Thus

$$\lambda S_\lambda(r) \;=\; S_\lambda(r-1) + (k-1)S_\lambda(r+1). \tag{87}$$

This determines $S_\lambda(r+1)$ in terms of $S_\lambda(r)$ and $S_\lambda(r-1)$, and we conclude that S_λ is uniquely determined for all integers $r \geq 0$, and thus that $S_{\lambda,x}$ is determined on all of Γ_k. $\square$

We extract from this proof the following corollary:

Corollary 9.2 *$S_\lambda(r)$ is an r^{th}-degree polynomial in λ. Moreover, for $r \geq 1$, $k(k-1)^{r-1}S_\lambda(r)$ is a monic r^{th}-degree polynomial in λ. If r is even, then $S_\lambda(r)$ is even, and if r is odd, then $S_\lambda(r)$ is odd.*

Proof. In the preceding proof, we remarked that

$$S_\lambda(0) \;=\; 1 \tag{88}$$

$$S_\lambda(1) \;=\; \frac{1}{k}\lambda \tag{89}$$

establishing our present claim for $r = 0$ and $r = 1$. For $r \geq 2$, we refer to (87), and adjust the index to rewrite the equation this way:

$$(k-1)S_\lambda(r) \;=\; \lambda S_\lambda(r-1) - S_\lambda(r-2). \tag{90}$$

Multiplying through by $k(k-1)^{r-2}$, we obtain

$$\begin{aligned} &k(k-1)^{r-1}S_\lambda(r) = \\ &\quad \lambda k(k-1)^{r-2}S_\lambda(r-1) - k(k-1)^{r-2}S_\lambda(r-2). \end{aligned} \tag{91}$$

By induction, $k(k-1)^{r-2}S_\lambda(r-1)$ is a monic, $(r-1)^{\text{th}}$-degree polynomial in λ with parity equal to that of $r-1$. Therefore the first term on the right in (91) is a monic, r^{th}-degree polynomial in λ with the same parity as r. The second term on the right is a polynomial of degree $r-2$. Its parity (given by $r-2$) is also the same as the parity of r. The sum of the two terms is thus monic of degree r, with parity equal to the parity of r, as claimed. $\square$

We note that Brooks, in [2], solves the difference equation (87), and the resulting closed-form expression yields much information about the behavior of the function S_λ. We will not need such detailed information here, however, and will make do with the basic properties of S_λ given in the preceding lemma and corollary.

Let φ be a function on Γ such that $A\varphi = \lambda\varphi$. Let $\tilde{\varphi}$ denote the lift of φ to the universal cover, Γ_k. Let $x \in \Gamma$ and pick some lift $\tilde{x}$ of x. Let $\tilde{\varphi}^\sharp$ denote the spherical average of $\tilde{\varphi}$ about $\tilde{x}$, that is

$$\begin{aligned} \tilde{\varphi}^\sharp(\tilde{x}) &= \tilde{\varphi}(\tilde{x}) && (92) \\ \tilde{\varphi}^\sharp(\tilde{y}) &= \frac{1}{k(k-1)^{r-1}} \sum_{\tilde{y} \in C(\tilde{x},r)} \tilde{\varphi}(\tilde{y}) \quad \text{for } \mathrm{dist}(\tilde{x},\tilde{y}) = r \geq 1. && (93) \end{aligned}$$

Then we have

Lemma 9.3

$$\tilde{\varphi}^\sharp = \varphi(x) S_{\lambda,\tilde{x}}. \qquad (94)$$

Proof. Clearly the value of $\tilde{\varphi}^\sharp(\tilde{y})$ depends only on the distance from $\tilde{x}$ to $\tilde{y}$, that is, $\tilde{\varphi}^\sharp$ is constant on each set $C(\tilde{x}, r)$.

We claim that

$$A\tilde{\varphi}^\sharp = \lambda\tilde{\varphi}^\sharp \qquad (95)$$

where A is the adjacency operator on Γ_k, as given by (7). To see this, consider $(A\tilde{\varphi}^\sharp)(\tilde{y})$, where $\mathrm{dist}(\tilde{x},\tilde{y}) = r \geq 1$. Because Γ_k is simply connected, we have

$$(A\tilde{\varphi}^\sharp)(\tilde{y}) = \tilde{\varphi}^\sharp(\tilde{z}_1) + (k-1)\tilde{\varphi}^\sharp(\tilde{z}_2) \qquad (96)$$

where $\tilde{z}_1$ is any element of $C(\tilde{x}, r-1)$ and $\tilde{z}_2$ is any element of $C(\tilde{x}, r+1)$. We sum this equation, letting $\tilde{y}$ run through $C(\tilde{x}, r)$, which contains $k(k-1)^{r-1}$ vertices.

$$\begin{aligned} \sum_{\tilde{y} \in C(\tilde{x},r)} (A\tilde{\varphi}^\sharp)(\tilde{y}) &= && (97) \\ k(k-1)^{r-1}(A\tilde{\varphi}^\sharp)(\tilde{y}) &= k(k-1)^{r-1}\tilde{\varphi}^\sharp(\tilde{z}_1) + k(k-1)^r\tilde{\varphi}^\sharp(\tilde{z}_2) && (98) \end{aligned}$$

$$= (k-1)\sum_{\tilde{z}\in C(\tilde{x},r-1)}\tilde{\varphi}(\tilde{z}) + \sum_{\tilde{z}\in C(\tilde{x},r+1)}\tilde{\varphi}(\tilde{z}) \quad (99)$$

$$= \sum_{\tilde{y}\in C(\tilde{x},r)}(A\tilde{\varphi})(\tilde{y}) \quad (100)$$

$$= \lambda\sum_{\tilde{y}\in C(\tilde{x},r)}\tilde{\varphi}(\tilde{y}) \quad (101)$$

$$= \lambda k(k-1)^{r-1}\tilde{\varphi}^{\sharp}(\tilde{y}). \quad (102)$$

From (102) and the left side of (98), we conclude that

$$(A\tilde{\varphi}^{\sharp})(\tilde{y}) = \lambda\tilde{\varphi}^{\sharp}(\tilde{y}) \quad (103)$$

for $\mathrm{dist}(\tilde{x},\tilde{y}) \geq 1$.

If $\mathrm{dist}(\tilde{x},\tilde{y}) = 0$, then $\tilde{y} = \tilde{x}$, and we get

$$(A\tilde{\varphi}^{\sharp})(\tilde{x}) = \sum_{\tilde{y}\in C(\tilde{x},1)}\tilde{\varphi}^{\sharp}(\tilde{y}) \quad (104)$$

$$= \sum_{\tilde{y}\in C(\tilde{x},1)}\tilde{\varphi}(\tilde{y}) \quad (105)$$

$$= (A\tilde{\varphi})(\tilde{x}) \quad (106)$$

$$= \lambda\tilde{\varphi}(\tilde{x}) \quad (107)$$

$$= \lambda\tilde{\varphi}^{\sharp}(\tilde{x}) \quad (108)$$

and we have established our claim (95).

If $\tilde{\varphi}(\tilde{x})$ is not zero, then the function

$$f(\tilde{y}) = \frac{1}{\tilde{\varphi}(\tilde{x})}\tilde{\varphi}^{\sharp}(\tilde{y}) \quad (109)$$

depends only on $\mathrm{dist}(\tilde{x},\tilde{y})$, and satisfies $Af = \lambda f$ and $f(\tilde{x}) = 1$. Therefore, by Lemma 9.1, we have

$$f = S_{\lambda,\tilde{x}} \quad (110)$$

so

$$
\begin{aligned}
\tilde{\varphi}^{\sharp} &= \tilde{\varphi}(\tilde{x}) S_{\lambda,\tilde{x}} &(111)\\
&= \varphi(x) S_{\lambda,\tilde{x}}. &(112)
\end{aligned}
$$

If $\tilde{\varphi}(\tilde{x}) = 0$, then $\tilde{\varphi}^{\sharp}(\tilde{x}) = 0$. Using this fact and an induction argument based on (103), it is easy to show that $\tilde{\varphi}^{\sharp}$ is identically zero, and so the lemma holds in this case, as well. □

Consider the function k_n on $\Gamma_k \times \Gamma_k$ given by

$$
k_n(\tilde{x}, \tilde{y}) = \begin{cases} 1 & \text{if } \operatorname{dist}(\tilde{x}, \tilde{y}) = n \\ 0 & \text{otherwise} \end{cases} \tag{113}
$$

Let K_n be the sum of the covering-map images of k_n, that is to say, let $K_n : \Gamma \times \Gamma \to \mathbb{R}$ by

$$
K_n(x, y) = \sum_{g \in G} k_n(\tilde{x}, g\tilde{y}) \tag{114}
$$

where $\tilde{x}$ is some lift of x, $\tilde{y}$ is some lift of y, and G is the group of covering transformations of Γ_k over Γ.

The sum on the right in (114) contains a 1 for each lift $\tilde{y}$ of y in $C(\tilde{x}, n)$. The unique path in Γ_k from $\tilde{x}$ to each $\tilde{y}$ projects down to a path of length n from x to y in Γ. Conversely, the lift of any path of length n from x to y in Γ, when the lift is started at $\tilde{x}$, will terminate at some lift of y in $C(\tilde{x}, n)$.

This establishes that the function $K_n(x, y)$ is equal to the number of paths of length n from x to y. We now have ready the machinery which will allow us to write a spectral expression, in the spirit of the Selberg pre-trace formula, for K_n.

We want to express K_n in this form:

$$
K_n(x, y) = \sum_{i,j} a_{ij} \varphi_i(x) \varphi_j(y) \tag{115}
$$

for some coefficients a_{ij}. Integrating both sides of (115) against the function $\varphi_k(y)$, we get

$$\begin{aligned}
\sum_{y\in\Gamma} K_n(x,y)\varphi_k(y) &= \sum_{i,j} a_{ij}\varphi_i(x)\sum_{y\in\Gamma}\varphi_j(y)\varphi_k(y) && (116)\\
&= \sum_{i,j} a_{ij}\varphi_i(x)\delta_{j,k} && (117)\\
&= \sum_{i} a_{ik}\varphi_i(x). && (118)
\end{aligned}$$

Turning our attention to the expression on the left side of (116), we let $\tilde{\varphi}_k$ be the lift of φ_k to Γ_k and use the definition of K_n, (114), to write the expression as a summation over vertices in Γ_k:

$$\sum_{y\in\Gamma} K_n(x,y)\varphi_k(y) = \sum_{y\in\Gamma}\sum_{g\in G} k_n(\tilde{x}, g\tilde{y})\tilde{\varphi}_k(\tilde{y}) \tag{119}$$

where $\tilde{x}$ is some lift of x and $\tilde{y}$ denotes some lift of each $y \in \Gamma$. Because $\tilde{\varphi}_k$ is G-invariant, we can express the right side of (119) as

$$\sum_{y\in\Gamma}\sum_{g\in G} k_n(\tilde{x}, g\tilde{y})\tilde{\varphi}_k(g\tilde{y}). \tag{120}$$

As g runs through G and y through Γ, the image $g\tilde{y}$ hits every vertex in Γ_k exactly once, so we get

$$\sum_{y\in\Gamma} K_n(x,y)\varphi_k(y) = \sum_{\tilde{y}\in\Gamma_k} k_n(\tilde{x}, \tilde{y})\tilde{\varphi}_k(\tilde{y}). \tag{121}$$

By the definition of k_n, (113), this is equal to

$$\sum_{\tilde{y}\in C(\tilde{x},n)} \tilde{\varphi}_k(\tilde{y}). \tag{122}$$

We now assume $n \geq 1$ and apply definition (93) to see that this is equal to

$$k(k-1)^{n-1}\tilde{\varphi}_k^{\sharp}(\tilde{y}) \tag{123}$$

where $\tilde{y}$ is any vertex in $C(\tilde{x}, n)$. By Lemma 9.3,

$$\tilde{\varphi}_k^\sharp = \varphi_k(x) S_{\lambda_k, \tilde{x}}, \tag{124}$$

so that (122) is equal to

$$k(k-1)^{n-1} \varphi_k(x) S_{\lambda_k}(n). \tag{125}$$

Substituting this back into (116), we get

$$k(k-1)^{n-1} \varphi_k(x) S_{\lambda_k}(n) \quad = \quad \sum_i a_{ik} \varphi_i(x) \tag{126}$$

which implies that $a_{ik} = 0$ if $i \neq k$ and

$$a_{ii} \quad = \quad k(k-1)^{n-1} S_{\lambda_i}(n). \tag{127}$$

We have shown:

Lemma 9.4 *For $n \geq 1$,*

$$K_n(x, y) \quad = \quad k(k-1)^{n-1} \sum_i S_{\lambda_i}(n) \varphi_i(x) \varphi_i(y). \tag{128}$$

10 Broken paths

Let x and y be two vertices in Γ, and consider the expression

$$\sum_{z \in \Gamma} K_n(x, z) K_m(z, y). \tag{129}$$

The term corresponding to a single z in the sum is equal to the number of paths of length n from x to z times the number of paths of length m from z to y. In other words, it is the number of walks from x to y which are made up of a path of length n ending at z followed by a path of length m from z to y. The entire expression, then, is equal to the number of walks from x to y

of length $m+n$ which do not double back, except possibly at the n^{th} vertex, counting from x.

We can use this idea to derive a spectral diameter estimate for k-regular graphs which depends explicitly on the injectivity radius.

We define the *girth* of a graph to be the length of its shortest closed path (excluding closed paths of length zero). Let g be the girth of Γ and let $r = \lfloor \frac{g-1}{2} \rfloor$. Then the ball of radius r about any vertex in Γ is simply connected, and therefore isomorphic to a ball of radius r in the k-tree. We will call r the *injectivity radius* of Γ.

Lemma 10.1 *Let Γ be a k-regular graph with N vertices, injectivity radius r, and adjacency spectrum $\{\lambda_0, \lambda_1, \ldots, \lambda_{N-1}\}$. Let $\{\varphi_0, \varphi_1, \ldots, \varphi_{N-1}\}$ be corresponding orthonormal eigenfunctions. Then for each vertex $x \in \Gamma$,*

$$\sum_{i=0}^{N-1} S^2_{\lambda_i}(r)\varphi_i^2(x) \quad = \quad \frac{1}{k(k-1)^{r-1}}. \tag{130}$$

Proof. Consider the expression

$$\sum_{y\in\Gamma} K_r(x,y)K_r(y,x) \tag{131}$$

This is equal to the number of walks, beginning and ending at x, comprising a path of length r followed by a second path of length r. Because the ball of radius r about x is simply connected, the second path must coincide (except for orientation) with the first. The vertex where the two paths join together is at a distance r from x, and each vertex at this distance from x determines exactly one walk of length $2r$, beginning and ending at x. Thus expression (131) is equal to the number of vertices at distance r from x.

The ball of radius r about x is isometric with a ball of radius r in the k-tree, so the number of such vertices is $k(k-1)^{r-1}$.

We apply Lemma 9.4:

$$\begin{aligned} &k(k-1)^{r-1} \\ &\quad = \sum_{y\in\Gamma} K_r(x,y)K_r(y,x) \\ &\quad = k^2(k-1)^{2(r-1)} \sum_{y\in\Gamma}\sum_{i=0}^{N-1} S_{\lambda_i}(r)\varphi_i(x)\varphi_i(y) \sum_{j=0}^{N-1} S_{\lambda_j}(r)\varphi_j(y)\varphi_j(x) \end{aligned} \tag{132}$$

so that

$$k(k-1)^{r-1} \\ = k^2(k-1)^{2(r-1)} \sum_{i,j=0}^{N-1} S_{\lambda_i}(r) S_{\lambda_j}(r) \varphi_i(x)\varphi_j(x) \sum_{y\in\Gamma} \varphi_i(y)\varphi_j(y). \tag{133}$$

The functions φ_i are orthonormal, so

$$\sum_{y\in\Gamma} \varphi_i(y)\varphi_j(y) = \delta_{i,j}, \tag{134}$$

and the right side of (133) becomes a summation over a single index:

$$k(k-1)^{r-1} = k^2(k-1)^{2(r-1)} \sum_{i=0}^{N-1} S^2_{\lambda_i}(r)\varphi_i^2(x). \tag{135}$$

We divide each side by $k^2(k-1)^{2(r-1)}$ to complete the proof. □

11 Injectivity radius and diameter

We are now ready to state and prove our third diameter estimate, which depends explicitly on the injectivity radius of the graph.

Theorem 3 *Let Γ be a k-regular, connected graph with N vertices and injectivity radius $r \geq 1$.*

(a) If Γ is not bipartite, then

$$\mathrm{diam}(\Gamma) \leq \frac{\operatorname{arccosh}\left(\frac{N}{k(k-1)^{r-1}} - 1\right)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)} + 2r + 1. \tag{136}$$

(b) If Γ is bipartite, then

$$\mathrm{diam}(\Gamma) \leq \frac{\operatorname{arccosh}\left(\frac{N}{2k(k-1)^{r-1}} - 1\right)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)} + 2r + 2. \tag{137}$$

Proof. Let x_0 and y_0 be vertices in Γ such that $\mathrm{dist}(x_0, y_0) = \mathrm{diam}(\Gamma)$. Let n be a positive integer such that $n + 2r < \mathrm{dist}(x_0, y_0)$. Consider the expression

$$\sum_{x,y\in\Gamma} K_r(x_0, x)W_n(x, y)K_r(y, y_0). \tag{138}$$

This is equal to the number of walks from x_0 to y_0 comprising a path of length r followed by a walk of length n and then a second path of length r. The total length of such a walk is $n + 2r$. But the distance from x_0 to y_0 is greater than $n + 2r$, so there are no such walks, and the expression must be equal to zero.

Using the spectral expansions of K_r and W_n in Lemmas 9.4 and 5.1 respectively, we conclude that

$$0 = \sum_{x,y\in\Gamma} \sum_{i=0}^{N-1} S_{\lambda_i}(r)\varphi_i(x_0)\varphi_i(x) \sum_{j=0}^{N-1} \lambda_j^n \varphi_j(x)\varphi_j(y) \sum_{l=0}^{N-1} S_{\lambda_l}(r)\varphi_l(y)\varphi_l(y_0) \tag{139}$$

where we have divided out the constant factors $k(k-1)^{r-1}$. Sorting out this multiple summation, we get

$$0 = \sum_{i,j,l=0}^{N-1} S_{\lambda_i}(r)\varphi_i(x_0)\lambda_j^n S_{\lambda_l}(r)\varphi_l(y_0) \sum_{x\in\Gamma} \varphi_i(x)\varphi_j(x) \sum_{y\in\Gamma} \varphi_j(y)\varphi_l(y). \tag{140}$$

The functions φ_i are orthonormal, so

$$\sum_{x\in\Gamma} \varphi_i(x)\varphi_j(x) = \delta_{i,j} \quad \text{and} \quad \sum_{y\in\Gamma} \varphi_j(y)\varphi_l(y) = \delta_{j,l} \tag{141}$$

and the entire summation collapses to a single index:

$$0 \;=\; \sum_{i=0}^{N-1} S_{\lambda_i}^2(r)\lambda_i^n \varphi_i(x_0)\varphi_i(y_0). \tag{142}$$

This holds for each exponent n less than $\mathrm{dist}(x_0, y_0) - 2r$, so, summing over n, we obtain

$$0 = \sum_{i=0}^{N-1} S_{\lambda_i}^2(r) p_n(\lambda_i) \varphi_i(x_0) \varphi_i(y_0) \tag{143}$$

where p_n is any polynomial of degree $n < \mathrm{dist}(x_0, y_0) - 2r$. We set

$$p_n(\lambda) = \cosh\left(n \operatorname{arccosh}\left(\frac{\lambda}{\lambda(\Gamma)}\right)\right). \tag{144}$$

Assume that Γ is not bipartite. We write (143) as

$$\begin{aligned} 0 = \; & p_n(\lambda_0) S_{\lambda_0}^2(r) \varphi_0(x_0) \varphi_0(y_0) \\ & + \sum_{i=1}^{N-1} p_n(\lambda_i) S_{\lambda_i}^2(r) \varphi_i(x_0) \varphi_i(y_0). \end{aligned} \tag{145}$$

All the factors in the first term on the right are known: $\lambda_0 = k$, S_{λ_0} is constantly equal to 1, and $\varphi_0 \equiv \frac{1}{\sqrt{N}}$. Plugging these values in, we determine that

$$\frac{p_n(k)}{N} = \left| \sum_{i=1}^{N-1} p_n(\lambda_i) S_{\lambda_i}^2(r) \varphi_i(x_0) \varphi_i(y_0) \right|. \tag{146}$$

Because Γ is not bipartite, we have $|\lambda_i| \leq \lambda(\Gamma)$ for $i = 1, 2, \ldots, N-1$, so that

$$|p_n(\lambda_i)| \leq 1 \quad \text{for} \quad i = 1, 2, \ldots, N-1. \tag{147}$$

By the triangle inequality, then, we get

$$\frac{p_n(k)}{N} \leq \sum_{i=1}^{N-1} |S_{\lambda_i}(r) \varphi_i(x_0) S_{\lambda_i}(r) \varphi_i(y_0)|. \tag{148}$$

We apply the Cauchy-Schwarz inequality:

$$\frac{p_n(k)}{N} \leq \left(\sum_{i=1}^{N-1} S^2_{\lambda_i}(r)\varphi_i^2(x_0)\right)^{\frac{1}{2}} \left(\sum_{i=1}^{N-1} S^2_{\lambda_i}(r)\varphi_i^2(y_0)\right)^{\frac{1}{2}}. \tag{149}$$

Using Lemma 10.1 and the known (constant) values for S_{λ_0} and φ_0, we find that each factor on the right is equal to

$$\left(\frac{1}{k(k-1)^{r-1}} - \frac{1}{N}\right)^{\frac{1}{2}}, \tag{150}$$

thus

$$p_n(k) \leq \frac{N}{k(k-1)^{r-1}} - 1 \tag{151}$$

$$\cosh\left(n \operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)\right) \leq \frac{N}{k(k-1)^{r-1}} - 1 \tag{152}$$

$$n \leq \frac{\operatorname{arccosh}\left(\frac{N}{k(k-1)^{r-1}} - 1\right)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)}. \tag{153}$$

This holds for $n = \operatorname{dist}(x_0, y_0) - 2r - 1$, and result (a) follows.

Assume now that Γ is bipartite. Then for each i, $\lambda_{N-1-i} = -\lambda_i$. The polynomial $p_n(\lambda)$ is even if n is even and odd if n is odd, so

$$p_n(\lambda_{N-1-i}) = (-1)^n p_n(\lambda_i) \tag{154}$$

for each i. The functions $S_\lambda(r)$, considered as r^{th}-degree polynomials in λ, have the same parity property (Corollary 9.2), so that

$$S^2_{\lambda_{N-1-i}}(r) = S^2_{\lambda_i}(r) \tag{155}$$

for each i.

Using these observations and part (c) of Lemma 6.1, we conclude that, if the parity of n is different from the parity of $\operatorname{dist}(x_0, y_0)$,

$$\begin{aligned}&p_n(\lambda_{N-1-i})S^2_{\lambda_{N-1-i}}(r)\varphi_{N-1-i}(x_0)\varphi_{N-1-i}(y_0)\\&\quad=-p_n(\lambda_i)S^2_{\lambda_i}(r)\varphi_i(x_0)\varphi_i(y_0)\end{aligned}\tag{156}$$

so that the right side of (143) is trivially zero, and the equation yields no information.

If, however, the parity of n agrees with the parity of $\operatorname{dist}(x_0, y_0)$, then we have

$$\begin{aligned}&p_n(\lambda_{N-1})S^2_{\lambda_{N-1}}(r)\varphi_{N-1}(x_0)\varphi_{N-1}(y_0)\\&\quad=p_n(\lambda_0)S^2_{\lambda_0}(r)\varphi_0(x_0)\varphi_0(y_0)\\&\quad=\frac{p_n(k)}{N}\end{aligned}\tag{157}$$

and equation (143) implies that

$$2\frac{p_n(k)}{N} \quad = \quad \left|\sum_{i=1}^{N-2} p_n(\lambda_i)S^2_{\lambda_i}(r)\varphi_i(x_0)\varphi_i(y_0)\right|. \tag{158}$$

Becuase $|\lambda_i| \leq \lambda(\Gamma)$ for $i = 1, 2, \ldots, N-2$, we have

$$|p_n(\lambda_i)| \leq 1 \quad \text{for} \quad i = 1, 2, \ldots, N-2. \tag{159}$$

Applying this and the triangle inequality to (158), we get

$$2\frac{p_n(k)}{N} \quad \leq \quad \sum_{i=1}^{N-2} |S_{\lambda_i}(r)\varphi_i(x_0)S_{\lambda_i}(r)\varphi_i(y_0)|. \tag{160}$$

As before, we apply the Cauchy-Schwarz inequality:

$$2\frac{p_n(k)}{N} \quad \leq \quad \left(\sum_{i=1}^{N-2} S^2_{\lambda_i}(r)\varphi_i^2(x_0)\right)^{\frac{1}{2}} \left(\sum_{i=1}^{N-2} S^2_{\lambda_i}(r)\varphi_i^2(y_0)\right)^{\frac{1}{2}}. \tag{161}$$

We use Lemma 10.1 to evaluate each summation on the right. The $i = 0$ and $i = N - 1$ terms are missing, so each factor is equal to

$$\left(\frac{1}{k(k-1)^{r-1}} - \frac{2}{N}\right)^{\frac{1}{2}}, \tag{162}$$

and we have

$$\begin{aligned} 2p_n(k) &\leq \frac{N}{k(k-1)^{r-1}} - 2 & (163)\\ \cosh\left(n \operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)\right) &\leq \frac{N}{2k(k-1)^{r-1}} - 1 & (164)\\ n &\leq \frac{\operatorname{arccosh}\left(\frac{N}{2k(k-1)^{r-1}} - 1\right)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)}. & (165) \end{aligned}$$

This is true for each n less than $\operatorname{dist}(x_0, y_0) - 2r$, provided the parity of n is the same as that of $\operatorname{dist}(x_0, y_0)$. We set $n = \operatorname{dist}(x_0, y_0) - 2r - 2$, and the proof is complete. $\square$

12 Using the injectivity radius is worth it

We verify that Theorem 3 actually improves upon Theorem 2, at least in a very large number of cases. Specifically, we will show, in these cases, that

$$\frac{\operatorname{arccosh}\left(\frac{N}{k(k-1)^{r-1}} - 1\right)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)} + 2r \quad < \quad \frac{\operatorname{arccosh}(N-1)}{\operatorname{arccosh}\left(\frac{k}{\lambda(\Gamma)}\right)}. \tag{166}$$

Clearly, this inequality will be "more unequal," and therefore easier to establish, when $\lambda(\Gamma)$ is close to k, so that the denominators of the fractions are small. We will show that (166) holds provided $\lambda(\Gamma) \geq 2\sqrt{k-1}$.

To show that this situation is quite general, we appeal to a result in the spectral geometry of manifolds. Cheng's theorem ([3]) gives an upper bound on the first eigenvalue of the Laplacian on a compact, hyperbolic surface S. It says that if S is large, then the first eigenvalue of the Laplacian can't be much greater than 1/4. There is an analogous theorem for k-regular graphs (see [7], Proposition 3.2.7 and [2] Theorem 4.4) giving a lower bound on $\lambda(\Gamma)$. This theorem states that

$$\lambda(\Gamma) \quad \geq \quad 2\sqrt{k-1} - \epsilon(\Gamma) \tag{167}$$

where ϵ is some positive function which goes to zero as Γ gets large.

Our proof of inequality (166) will begin with the hypothesis $\lambda(\Gamma) \geq 2\sqrt{k-1}$, but there will be a little slack in the computation — that is, the result will really be proved for $\lambda(\Gamma)$ slightly less than $2\sqrt{k-1}$ as well as $\lambda(\Gamma) \geq 2\sqrt{k-1}$. For simplicity, we will not try to determine exactly how much less, but, because of Cheng's theorem, any amount of slack allows us to infer the result for all sufficiently large graphs, in addition to all smaller graphs with $\lambda(\Gamma) \geq 2\sqrt{k-1}$.

We will make use of the following lemma.

Lemma 12.1 *Let $1 \leq r < s$. Then*

$$\operatorname{arccosh}(s) - \operatorname{arccosh}(r) \quad > \quad \log(s) - \log(r). \tag{168}$$

Proof.

$$\operatorname{arccosh}(s) - \operatorname{arccosh}(r) = \int_r^s \frac{dt}{\sqrt{t^2-1}} > \int_r^s \frac{dt}{t} = \log(s) - \log(r). \tag{169}$$

□

We now state (166) as

Lemma 12.2 *For $r \geq 1$, $k \geq 3$, $N > k(k-1)^{r-1}$, and $\lambda \geq 2\sqrt{k-1}$,*

$$\frac{\operatorname{arccosh}\left(\frac{N}{k(k-1)^{r-1}} - 1\right)}{\operatorname{arccosh}\left(\frac{k}{\lambda}\right)} + 2r \quad < \quad \frac{\operatorname{arccosh}(N-1)}{\operatorname{arccosh}\left(\frac{k}{\lambda}\right)}. \tag{170}$$

Proof. From $\lambda \geq 2\sqrt{k-1}$, we get

$$\frac{k}{\lambda} \quad \leq \quad \frac{k}{2\sqrt{k-1}}. \tag{171}$$

We observe that $\cosh(\log\sqrt{k-1}) = \dfrac{k}{2\sqrt{k-1}}$ and take the arccosh of both sides of (171):

$$\operatorname{arccosh}\left(\frac{k}{\lambda}\right) \le \log\sqrt{k-1}. \tag{172}$$

It follows that

$$2r\operatorname{arccosh}\left(\frac{k}{\lambda}\right) \le r\,\log(k-1). \tag{173}$$

From the hypotheses, $\dfrac{k}{k-1}$ and $\dfrac{N-1}{N-k(k-1)^{r-1}}$ are both greater than 1, so we can add their logarithms to the right side (this is where the slack first comes in):

$$\begin{aligned}
&2r\operatorname{arccosh}\left(\frac{k}{\lambda}\right)\\
&\quad< r\,\log(k-1)+\log\left(\frac{k}{k-1}\right)+\log\left(\frac{N-1}{N-k(k-1)^{r-1}}\right)\\
&\quad=\log(N-1)-\log\left(\frac{N}{k(k-1)^{r-1}}-1\right).
\end{aligned} \tag{174}$$

Now we apply Lemma 12.1 (another source of slack), to get

$$\begin{aligned}
&2r\operatorname{arccosh}\left(\frac{k}{\lambda}\right)\\
&\quad<\operatorname{arccosh}(N-1)-\operatorname{arccosh}\left(\frac{N}{k(k-1)^{r-1}}-1\right).
\end{aligned} \tag{175}$$

Dividing through by $\operatorname{arccosh}(\frac{k}{\lambda})$ and rearranging the terms in the obvious way gives the result. □

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