Eigenvalue comparisons in graph theory

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1 Introduction

A standard technique for estimating the eigenvalues of the Laplacian on a compact Riemannian manifold M with bounded curvature is to pack the manifold with disjoint geodesic balls. The smallest Dirichlet eigenvalues of the Laplacian on the balls (which may be easier to estimate) can then be used as lower bounds for certain eigenvalues of the Laplacian on M.

In this paper, we explore what happens when the same techniques are applied to the problem of estimating eigenvalues of the adjacency operator on finite graphs of bounded degree. In Theorem 7, we show how eigenvalues of the adjacency operator on a finite graph Γ may be bounded in terms of the biggest eigenvalues of the adjacency operator on "geodesic balls" in Γ. We find explicit bounds for the eigenvalues on the balls (Theorem 6), and in Theorem 8, we turn these into explicit estimates on certain eigenvalues of the adjacency operator on Γ.

2 The setting: Linear algebra on Graphs

We begin by introducing the principal notions in the spectral theory of graphs and recalling a few results we will need from linear algebra.

Let Γ be a connected, undirected graph with a finite number n of vertices. We will denote the vertices $x_1, x_2, \ldots, x_n$. A *function* on Γ is a map from

the vertex set of Γ to the real numbers. The set of functions on Γ forms an n-dimensional vector space over $\mathbb{R}$. A canonical basis for this space is made up of the functions $\delta_1, \delta_2, \ldots \delta_n$, where

$$\delta_i(x_j) = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

There is also a canonical inner product on this function space. If f and g are functions on Γ, define

$$\langle f, g \rangle = \sum_{i=1}^{n} f(x_i) g(x_i),$$

and note that the canonical basis is orthonormal with respect to this inner product. We will denote the space of functions on Γ (now a Hilbert space) as $L^2(\Gamma)$.

There is a natural self-adjoint linear operator on $L^2(\Gamma)$, called the *adjacency operator*, and denoted A. It is defined by

$$(Af)(x) = \sum_{y \sim x} f(y),$$

where $y \sim x$ means the vertex y is joined to the vertex x by an edge. The easy way to see that A is indeed self-adjoint is to observe that its matrix with respect to the canonical basis is simply the adjacency matrix of Γ which, since Γ is undirected, must be symmetric.

The sequence of eigenvalues of A forms the *spectrum of* Γ. The study of spectral graph theory involves looking for relations between the spectrum of a graph and its geometric properties. This is analogous to the field of spectral geometry on manifolds, where the spectrum of another self-adjoint operator, the Laplacian, is related to geometric features of a manifold. The analogy is very close, because any reasonable definition of a "Laplacian" on a graph (some operator that looks like heat diffusion) involves the adjacency operator in an important way. Consider, for example, a graph Γ which is k-regular, meaning that every vertex in Γ has degree k. A Laplacian operator Δ on such a graph, trying to look like minus the divergence of the gradient, might be defined as

$$\Delta f(x) = \sum_{y \sim x} (f(x) - f(y)) \tag{1}$$

$$= ((kI - A)f)(x), \tag{2}$$

where I denotes the identity operator on $L^2(\Gamma)$.

A basic result in spectral geometry is a theorem of Cheng [4], giving upper bounds on the eigenvalues of the Laplacian on a compact Riemannian manifold M in terms of the diameter of M and curvature bounds on M. Intuitively, this result says that big manifolds have low fundamental frequencies. Our purpose here is to formulate the graph-theory analogue to Cheng's theorem, and derive lower bounds on the eigenvalues of the adjacency operator on a finite graph Γ in terms of the diameter of Γ and bounds on the degrees of its vertices. Our sample Laplacian in line (2) shows that the adjacency operator has the opposite sign from the usual Laplacian, so that lower bounds on eigenvalues of A are the correct analogue to upper bounds on eigenvalues of Δ.

If a graph Γ is finite and k-regular, then the number k is in the spectrum of Γ; the constant function is an eigenfunction for the value k. Furthermore, if Γ is bipartite (meaning it contains no cycles of odd length) then the number $-k$ is also in the spectrum of Γ, corresponding to an eigenfunction with value 1 on half the vertices and -1 on the other half. A finite, k-regular graph is called *Ramanujan* if every eigenvalue λ in its spectrum satisfies either $|\lambda| = k$ or $|\lambda| \leq 2\sqrt{k-1}$.

Among other things, our results will explain the significance of the number $2\sqrt{k-1}$ in this context, and clarify the assertion ([5]) that the second-greatest eigenvalue of a finite, k-regular graph Γ approaches $2\sqrt{k-1}$ as Γ gets large.

We conclude this section by recalling two results from linear algebra: the variational characterization of eigenvalues and the Perron-Frobenius theorem.

Let A be a self-adjoint linear operator on an n-dimensional Hilbert space V, so that A has n real eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ with corresponding eigenvectors $v_1, v_2, \ldots, v_n$. Let v be a non-zero vector in V. The *Rayleigh quotient* for v is the quotient $\langle Av, v\rangle / \langle v, v\rangle$. Clearly, if v happens to be an eigenvector v_i of A, then the Rayleigh quotient for v is equal to λ_i. In fact, each eigenvalue of A is an extreme value of the Rayleigh quotient over an appropriate subspace of V. We will use this version of the variational characterization of eigenvalues:

Theorem (Rayleigh's Principle) *With notation as above, for each index* $1 \leq i \leq n$,

$$\lambda_i = \max_{v \perp T_{i-1}} \frac{\langle Av, v \rangle}{\langle v, v \rangle},$$

where T_{i-1} *is the subspace of* V *spanned by the eigenvectors* $v_1, v_2, \ldots, v_{i-1}$.

For a proof, see [9] or [6].

The Perron-Frobenius theorem is stated in terms of matrices rather than operators.

A real matrix $M = (m_{ij})$ is called *non-negative* if each of its entries is non-negative. A non-negative, square matrix M is called *irreducible* if for each pair (i, j), there is a non-negative integer p such that the $(i, j)^{\text{th}}$ entry of M^p is strictly positive. Since the $(i, j)^{\text{th}}$ entry of the pth power of the adjacency matrix of a graph Γ is equal to the number of edge sequences of length p connecting vertex i to vertex j, it is clear that the adjacency matrix of a connected graph is irreducible.

For each i, the *row sum* r_i of a matrix $M = (m_{ij})$ is given by

$$r_i = \sum_j m_{ij}. \tag{3}$$

Theorem (Perron-Frobenius) *Let* M *be a non-negative, square matrix, and suppose* M *is irreducible. Let* $r_{\min}$ *and* $r_{\max}$ *be the minimum and maximum row sums of* M*, respectively. There is a unique eigenvector* v *of* M *all of whose entries are positive. The eigenvalue* λ *corresponding to* v *is the largest eigenvalue of* M *and satisfies* $r_{\min} \leq \lambda \leq r_{\max}$.

For a proof, see [8].

3 Trees and spherical functions

For each integer $k \geq 3$, let Γ_k denote the k-tree, that is, the simply-connected infinite graph each of whose vertices has degree k. The k-tree is the graph-theoretic analogue of a symmetric space. The number k plays the role of

negative curvature, in that the number of vertices in a ball of fixed radius in a k-tree (formal definitions to follow) increases with k, just as the volume of a unit ball in a symmetric space of negative curvature increases as the curvature gets "more negative."

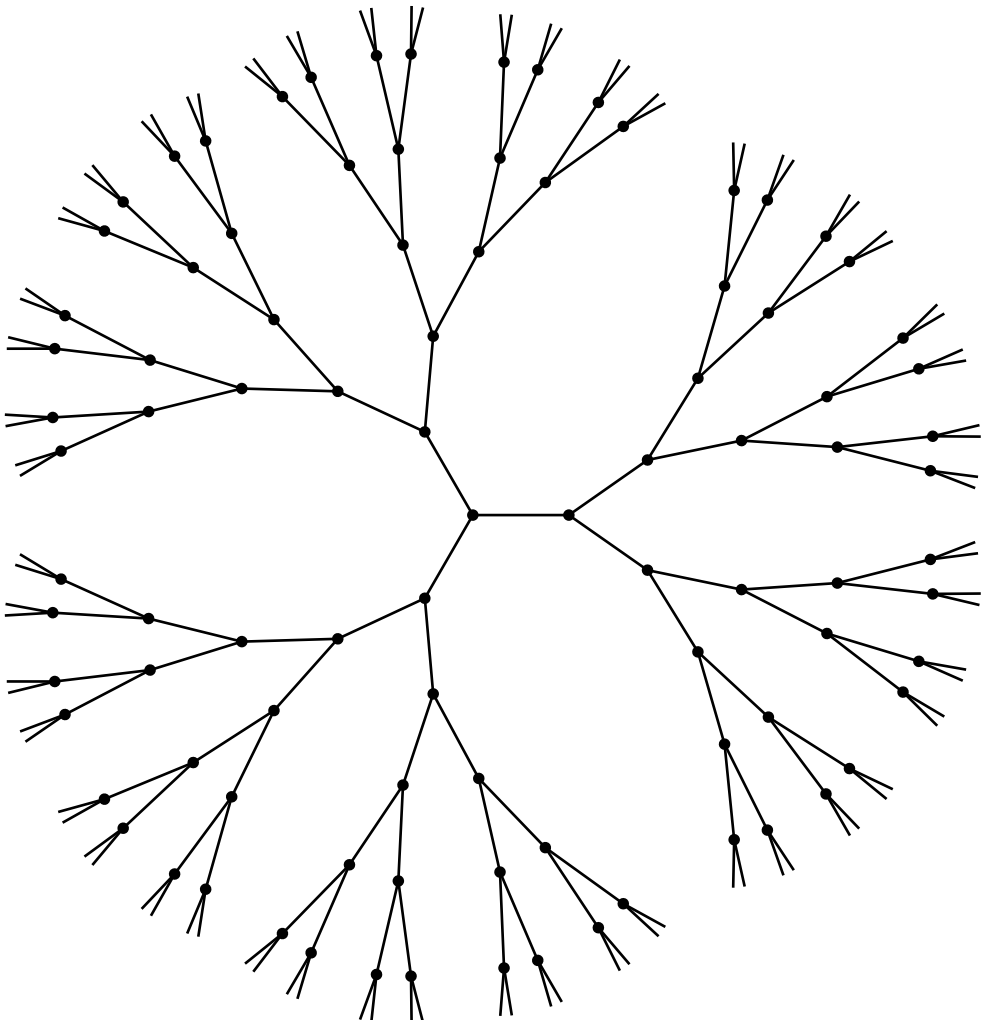

Figure 1: Part of the 3-tree

Our reference point in spectral graph theory is the family of spherical eigenfunctions of the adjacency operator on Γ_k. These are analogous to the spherical eigenfunctions of the Laplacian on a symmetric space which one con-

structs using Bessel or Legendre functions (see [3]).

Given $\lambda \in (0, 2\sqrt{k-1})$ and $x_0 \in \Gamma_k$, the *spherical eigenfunction* S_λ on Γ centered at x_0 is the function satisfying

1. $AS_\lambda = \lambda S_\lambda$
2. $S_\lambda(x_0) = 1$
3. $S_\lambda(x)$ depends only on the distance from x to x_0.

We claim that there is a unique such function for each choice of λ, x_0, and $k \geq 3$, and will demonstrate this by constructing the function.

Since the value of $S_\lambda(x)$ depends only on the distance from x to x_0, we can consider S_λ as a function on the non-negative integers, and construct it as follows. Conditions (1) and (2) above imply that S_λ satisfies the difference equation

$$S_\lambda(r-1) + (k-1)S_\lambda(r+1) = \lambda S_\lambda(r) \tag{4}$$

for $r \geq 1$, with initial conditions given by

$$S_\lambda(0) = 1 \tag{5}$$
$$kS_\lambda(1) = \lambda. \tag{6}$$

If we write

$$S_\lambda(r) = c_1 x_1^r + c_2 x_2^r, \tag{7}$$

where c_1 and c_2 are coefficients to be determined later, then the difference equation (4) implies that x_1 and x_2 must satisfy the quadratic equation $1 + (k-1)x^2 = \lambda x$. Thus we have

$$x_{1,2} = \frac{\lambda \pm \sqrt{\lambda^2 - 4(k-1)}}{2(k-1)}. \tag{8}$$

Since we have assumed $0 < \lambda < 2\sqrt{k-1}$, equation (8) implies that x_1 and x_2 are complex numbers with modulus $1/\sqrt{k-1}$. This suggests writing

$$x_{1,2} = \frac{1}{\sqrt{k-1}} \left(\frac{\lambda \pm \sqrt{\lambda^2 - 4(k-1)}}{2\sqrt{k-1}} \right). \tag{9}$$

Let

$$\theta = \arg \left(\frac{\lambda + \sqrt{\lambda^2 - 4(k-1)}}{2\sqrt{k-1}} \right) \tag{10}$$

so that $0 < \theta < \frac{\pi}{2}$. Then

$$\begin{aligned} S_\lambda(r) &= c_1 x_1^r + c_2 x_2^r && (11) \\ &= \frac{1}{\sqrt{k-1}^r} \left(c_1 e^{ir\theta} + c_2 e^{-ir\theta} \right) && (12) \\ &= \frac{1}{\sqrt{k-1}^r} \left(c_3 \cos r\theta + c_4 \sin r\theta \right). && (13) \end{aligned}$$

Using the initial conditions $S_\lambda(0) = 1$ and $S_\lambda(1) = \lambda/k$, we can determine that $c_3 = 1$ and $c_4 = \frac{k-2}{k} \cot\theta$. Thus our spherical eigenfunction on the k-tree is represented by the function

$$S_\lambda(r) = \frac{1}{\sqrt{k-1}^r} \left(\cos r\theta + \frac{k-2}{k} \cot\theta \sin r\theta \right). \tag{14}$$

Reading S_λ as a function of a continuous variable r, we observe that it has the form of a sine wave with period $2\pi/\theta$ and exponentially decaying amplitude. If we rewrite S_λ as

$$S_\lambda(r) = \frac{c_5}{\sqrt{k-1}^r} \sin(r\theta + \alpha), \tag{15}$$

equate this with our other expression for S_λ, and use the addition formula for sine, we can determine that the phase shift α is given by

$$\tan\alpha = \frac{k}{k-2}\tan\theta \tag{16}$$

with $0 < \alpha < \frac{\pi}{2}$, and that $c_5 = \csc\alpha$.

Figure 2 shows some curves $y = S_\lambda(x)$ for $k = 3$. The values of λ, given in the order in which the curves cross the x-axis, are 0.5, 1, 1.5, 2, and 2.5.

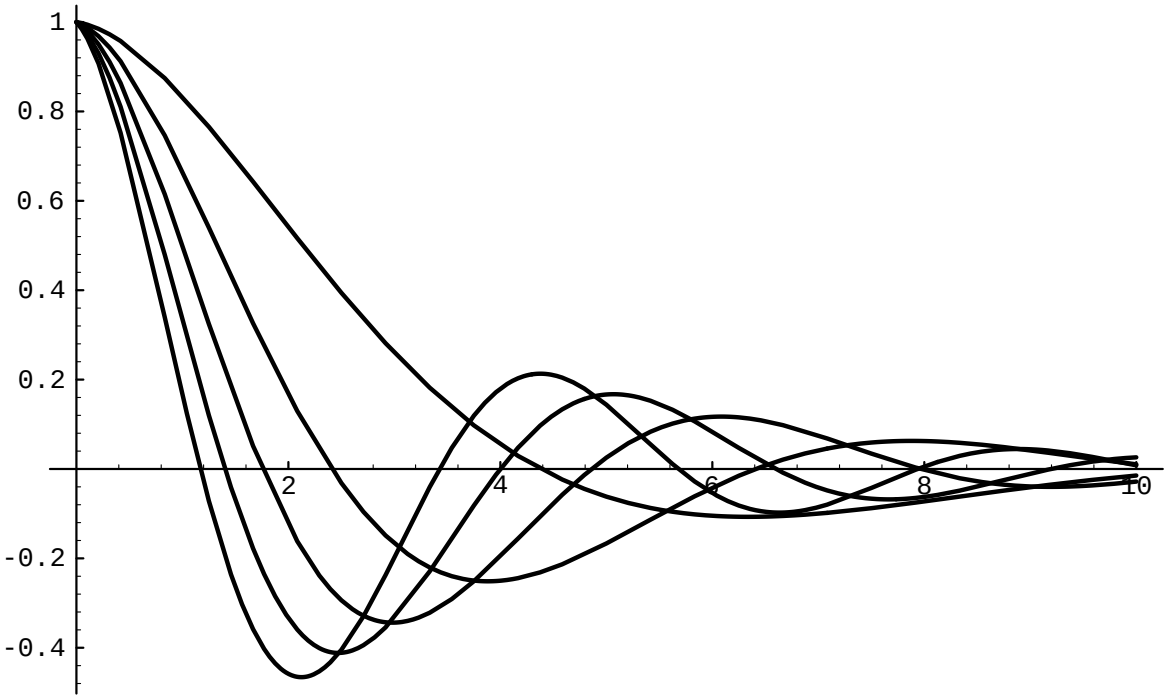

Figure 2: Graphs of some S_λ functions

We summarize our investigation of spherical eigenfunctions in the following theorem.

Theorem 1 *Let $k \geq 3$ be an integer and let $\lambda \in (0, 2\sqrt{k-1})$. Let*

$$\theta \;=\; \arg\left(\frac{\lambda + \sqrt{\lambda^2 - 4(k-1)}}{2\sqrt{k-1}}\right).$$

Then the function

$$S_\lambda(r) \quad = \quad \frac{\csc\alpha}{\sqrt{k-1}^{\,r}}\sin(r\theta+\alpha), \tag{17}$$

where $\alpha = \arctan\left(\dfrac{k}{k-2}\tan\theta\right)$*, is a spherical* λ*-eigenfunction of* A *on* Γ_k*, in the sense that a function* φ *on* Γ_k *given by* $\varphi(x) = S_\lambda(\mathrm{dist}(x, x_0))$*, for some fixed* x_0*, satisfies* $A\varphi = \lambda\varphi$ *and* $S_\lambda(x_0) = 1$*.*

We remark that the restriction $\lambda \in (0, 2\sqrt{k-1})$ is artificial. An eigenfunction S_λ can be constructed for any $\lambda \in \mathbb{R}$ by making only minor changes to the development outlined above. See [2] or [7] for the details. In this paper, we will need only the functions S_λ with $\lambda \in (0, 2\sqrt{k-1})$ and unless otherwise specified, any λ we discuss will lie in this interval.

4 Zeroes of spherical functions

Regarding S_λ once again as a function of a continuous variable r, we now investigate where the first zero of S_λ occurs. That is, we wish to identify the least positive r such that $S_\lambda(r) = 0$. Figure 2 suggests that the first positive root of S_λ increases with λ. We establish this in the following theorem.

Lemma 2 *Let* S_λ *denote the spherical eigenfunction with eigenvalue* λ *on the* k*-tree. For each* $r_0 > 1$*, there is a real number* $\lambda \in (0, 2\sqrt{k-1})$ *such that* $S_\lambda(r) > 0$ *for* $0 \le r < r_0$ *and* $S_\lambda(r_0) = 0$*.*

Proof We use the form of S_λ given in Theorem 1, that is, S_λ is equal to some positive exponential times the function $\sin(r\theta+\alpha)$. By the construction, we know $S_\lambda(0) = 1$, so $\sin(0+\alpha)$ is strictly positive. Since θ and α are both positive, the first zero of $\sin(r\theta+\alpha)$ occurs when $r\theta+\alpha = \pi$. Solving for r, we find that the first zero of S_λ occurs when

$$r = \frac{\pi - \alpha}{\theta}. \tag{18}$$

From the definition of θ (equation (10)), we get

$$\cos\theta = \frac{\lambda}{2\sqrt{k-1}}, \tag{19}$$

which shows that θ is a continuous, monotone decreasing function of λ for $0 < \lambda < 2\sqrt{k-1}$. As we noted earlier, the range of θ is the interval $(0, \frac{\pi}{2})$. The relation

$$\tan\alpha = \frac{k}{k-2}\tan\theta \tag{20}$$

(equation (16)) shows that α is a continuous, monotone increasing function of θ for $0 < \theta < \frac{\pi}{2}$, and thus that α is a continuous, monotone decreasing function of λ.

Now the "first-zero" function $r = (\pi - \alpha)/\theta$ is a continuous, monotone increasing function of λ on $0 < \lambda < 2\sqrt{k-1}$. Furthermore, as λ increases toward $2\sqrt{k-1}$, both θ and α decrease to 0, and the value of r at the first zero increases without bound. As λ decreases toward 0, both θ and α increase to $\frac{\pi}{2}$, and the value of r at the first zero decreases toward 1. Since the range of the "first-zero" function is $(1, \infty)$ and the function is monotone, there is an inverse function giving, for each $r \in (1, \infty)$ the unique value of λ between 0 and $2\sqrt{k-1}$ such that r is the first zero of S_λ. ∎

We will use the notation $\Lambda(r)$ for the function constructed in Lemma 2. That is, for each $r > 1$, the number r will be the first zero of $S_{\Lambda(r)}$. In the next lemma, we derive an estimate on $\Lambda(r)$.

Lemma 3 *For $r > 1$,*

$$\Lambda(r) > 2\sqrt{k-1}\cos\left(\frac{\pi}{r+1}\right).$$

Proof Let $\lambda = \Lambda(r)$, so that the first zero of S_λ occurs at $r = (\pi - \alpha)/\theta$, where θ and α are the angles corresponding to the eigenvalue λ. Since θ and α both lie in $(0, \frac{\pi}{2})$ and $\tan\alpha = \frac{k}{k-2}\tan\theta$, we know $\tan\alpha > \tan\theta$, and thus that $\alpha > \theta$. This yields

$$r = \frac{\pi - \alpha}{\theta} < \frac{\pi - \theta}{\theta}. \tag{21}$$

Solving for θ gives

$$\theta \quad < \quad \frac{\pi}{r+1}. \tag{22}$$

Taking the cosine of both sides changes the direction of the inequality, giving

$$\cos\theta \quad > \quad \cos\left(\frac{\pi}{r+1}\right). \tag{23}$$

Now $\cos\theta = \dfrac{\lambda}{2\sqrt{k-1}}$, so we have

$$\frac{\lambda}{2\sqrt{k-1}} \quad > \quad \cos\left(\frac{\pi}{r+1}\right), \tag{24}$$

from which the result follows. ■

We will need one more result concerning the functions S_λ, which we state in the following lemma.

Lemma 4 *Let $r_0 \geq 1$ be an integer and let $\lambda = \Lambda(r_0)$. Then the function S_λ is monotone decreasing on the integers $0, 1, \ldots, r_0$.*

Proof We know that S_λ is positive on the integers $0, 1, \ldots, r_0 - 1$, that $S_\lambda(0) = 1$, and that S_λ satisfies the difference equation (4).

We proceed by induction, first noting that the difference equation for S_λ implies that $S_\lambda(1) = \lambda/k$. Since $\lambda < 2\sqrt{k-1}$, we get

$$S_\lambda(1) \quad < \quad \frac{2\sqrt{k-1}}{k}. \tag{25}$$

For $k \geq 3$, the expression on the right is always less than 1. Thus we have established the base case, that $S_\lambda(1) < S_\lambda(0)$.

Now assume that $1 \leq r \leq r_0 - 1$ and $S_\lambda(r) < S_\lambda(r-1)$. The difference equation for S_λ implies that

$$(k-1)S_\lambda(r+1) = \lambda S_\lambda(r) - S_\lambda(r-1). \tag{26}$$

Since $S_\lambda(r-1) > S_\lambda(r)$ and $\lambda < 2\sqrt{k-1}$, equation (26) gives the inequality

$$\begin{aligned} (k-1)S_\lambda(r+1) &< (\lambda - 1)S_\lambda(r) \\ &< (2\sqrt{k-1} - 1)S_\lambda(r) \\ S_\lambda(r+1) &< \frac{2\sqrt{k-1}-1}{k-1} S_\lambda(r). \end{aligned}$$

For $k \geq 3$, the coefficient $\dfrac{2\sqrt{k-1}-1}{k-1}$ is always less than 1, and since $S_\lambda(r)$ is positive (because $r \leq r_0 - 1$), we have established that $S_\lambda(r+1) < S_\lambda(r)$.

■

5 Graph-theoretic balls

Next we examine the graph-theoretic analogues of geodesic balls in symmetric spaces and on manifolds.

We define the *distance* between two vertices x and y on a graph Γ to be the number of edges traversed in the shortest path connecting x to y. We denote the distance from x to y as $\mathrm{dist}(x, y)$. In a connected graph, $\mathrm{dist}(x, y)$ is always defined, and it is easy to check that it is a valid distance function.

Let x_0 be a vertex in a graph Γ, and let n be a non-negative integer. The *ball of radius n about x_0*, denoted $B(x_0, n)$, is the subgraph of Γ induced by the set of vertices x in Γ with $\mathrm{dist}(x_0, x) \leq n$. (The subgraph *induced* by a set S of the vertices of Γ is a graph whose vertices are the elements of S and whose edges are all the edges of Γ which have both endpoints in S.)

Our reference graphs will be balls in the k-tree. Let x_0 be a vertex in Γ_k, and let n be a non-negative integer. Because of the symmetry of Γ_k, the ball

of radius n around x_0 is isomorphic to the ball of radius n around any other vertex in Γ_k. The shape of the ball does of course depend on k, and so we will use the notation V_n^k to denote the ball of radius n in Γ_k.

The quantity of interest to us is the largest eigenvalue of the adjacency operator on V_n^k, which we will denote $\lambda_1(V_n^k)$.

Theorem 5 *For $n \geq 1$ and $k \geq 3$,*

$$\lambda_1(V_n^k) \quad > \quad 2\sqrt{k-1}\cos\left(\frac{\pi}{n+2}\right).$$

Proof Let x_0 be the center of V_n^k, and define a test function φ on V_n^k by

$$\varphi(x) \quad = \quad S_\lambda(\mathrm{dist}(x, x_0)), \tag{27}$$

where $\lambda = \Lambda(n+1)$. We claim that φ is an eigenfunction of the adjacency operator A on V_n^k with eigenvalue λ. To verify this, we examine $A\varphi(x)$ in three cases.

1. $x = x_0$. Then $A\varphi(x)$ is a sum of $\varphi(y)$ over the k vertices y which are joined to x_0. The value of φ at each such vertex is $S_\lambda(1)$, and we get $A\varphi(x) = kS_\lambda(1) = \lambda S_\lambda(0) = \lambda\varphi(x)$.

2. $1 \leq r = \mathrm{dist}(x, x_0) \leq n-1$. The neighbors of x include one vertex y at distance $r-1$ from x_0 and $k-1$ vertices z at distance $r+1$ from x_0. Thus

$$\begin{aligned} A\varphi(x) &= \varphi(y) + (k-1)\varphi(z) \\ &= S_\lambda(r-1) + (k-1)S_\lambda(r+1) \\ &= \lambda S_\lambda(r) \\ &= \lambda\varphi(x). \end{aligned}$$

3. $\mathrm{dist}(x, x_0) = n$. The vertex x is joined to only one vertex y in V_n^k, and $\mathrm{dist}(x_0, y) = n-1$. We also know that $S_\lambda(n+1) = 0$, so we can write

$$\begin{aligned} A\varphi(x) &= \varphi(y) \\ &= S_\lambda(n-1) \\ &= S_\lambda(n-1) + (k-1)S_\lambda(n+1) \\ &= \lambda S_\lambda(n) \\ &= \lambda\varphi(x). \end{aligned}$$

Since λ is an eigenvalue of the adjacency operator on V_n^k, we must have

$$\lambda_1(V_n^k) \geq \lambda = \Lambda(n+1) > 2\sqrt{k-1}\cos\left(\frac{\pi}{n+2}\right). \tag{28}$$

■

The idea of using S_λ to define a test function on a graph is called *transplantation*. This technique is very flexible, and can be applied to graphs other than Γ_k. In the next theorem, for example, we allow the graph Γ to be multiply connected, and we even relax the k-regularity requirement.

A graph Γ will be said to have *minimal degree* k if every vertex of Γ has degree greater than or equal to k.

Theorem 6 *Let Γ be a graph with minimal degree $k \geq 3$. Let x_0 be a vertex in Γ, let n be a positive integer, and let $B = B(x_0, n)$ denote the ball around x_0 of radius n. Then the greatest eigenvalue of the adjacency operator on B, denoted $\lambda_1(B)$, satisfies*

$$\lambda_1(B) \quad > \quad 2\sqrt{k-1}\cos\left(\frac{\pi}{n+2}\right). \tag{29}$$

Proof As in the proof of Theorem 5, we begin by defining a function φ on B by

$$\varphi(x) \quad = \quad S_\lambda(\mathrm{dist}(x, x_0)), \tag{30}$$

where $\lambda = \Lambda(n+1)$. Since distances on Γ are well-defined, our function φ is well-defined, and since all points in B are within n units of x_0, φ is strictly positive on B.

We claim that the Rayleigh quotient for φ, $\langle A\varphi, \varphi\rangle \,/\, \langle \varphi, \varphi\rangle$, is greater than or equal to λ. Because the Rayleigh quotient for φ is a lower bound for $\lambda_1(B)$, and λ (by Theorem 3) is greater than $2\sqrt{k-1}\cos(\frac{\pi}{n+2})$, we will be finished once we have established this claim.

The Rayleigh quotient for φ is greater than or equal to λ because $A\varphi$ is, pointwise, greater than or equal to $\lambda\varphi$. To see this, we examine $A\varphi(x)$ in three cases.

1. $x = x_0$. Then $A\varphi(x)$ is the sum of $\varphi(y)$ over all the vertices y which are joined to x_0 by an edge. Since the degree of x_0 is at least k, this is a sum over at least k vertices y, and the value of φ at each such vertex is $S_\lambda(1)$. Since $S_\lambda(1)$ is positive, the sum is at least as large as $kS_\lambda(1)$, which is equal to $\lambda S_\lambda(0)$, which, in turn, is equal to $\lambda\varphi(x_0)$.

2. $1 \leq r = \mathrm{dist}(x, x_0) \leq n-1$. Among the neighbors of x, there must be one vertex y whose distance to x_0 is $r-1$. All the other neighbors z of x must lie within $r+1$ units of x_0, and there must be at least $k-1$ of them. Since S_λ is decreasing, φ must decrease with distance from x_0, and therefore the value of φ at each z is greater than or equal to $S_\lambda(r+1)$. This, along with the fact that S_λ is positive in the relevant domain, gives us the following chain of inequalities.

$$\begin{aligned} A\varphi(x) &= \varphi(y) + \sum_z \varphi(z) \\ &\geq S_\lambda(r-1) + \sum_z S_\lambda(r+1) \\ &\geq S_\lambda(r-1) + (k-1)S_\lambda(r+1) \\ &= \lambda S_\lambda(r) \\ &= \lambda\varphi(x). \end{aligned}$$

3. $\mathrm{dist}(x, x_0) = n$. In this case, x must have at least one neighbor y whose distance to x_0 is $n-1$. Any other neighbors z of x satisfy $\varphi(z) > 0$. Also, $S_\lambda(n+1) = 0$, by our choice of λ. These observations justify the following chain of inequalities.

$$\begin{aligned} A\varphi(x) &= \varphi(y) + \sum_z \varphi(z) \\ &\geq \varphi(y) \\ &= S_\lambda(n-1) + (k-1)\cdot 0 \\ &= S_\lambda(n-1) + (k-1)S_\lambda(n+1) \\ &= \lambda S_\lambda(n) \\ &= \lambda\varphi(x). \end{aligned}$$

We have established that $A\varphi(x) \geq \lambda\varphi(x)$ for each $x \in B$, and we know that $\varphi(x) > 0$ for each $x \in B$, so

$$\begin{aligned} \langle A\varphi, \varphi \rangle &= \sum_{x \in B} A\varphi(x)\varphi(x) \\ &\geq \sum_{x \in B} \lambda\varphi(x)\varphi(x) \\ &= \lambda \langle \varphi, \varphi \rangle , \end{aligned}$$

showing that the Rayleigh quotient for φ is indeed greater than λ. ■

We remark here that if B itself has minimal degree k_1, then the Perron-Frobenius theorem guarantees that $\lambda_1(B) \geq k_1$. However a ball B in a graph Γ with minimum degree k can easily have vertices on its frontier with degree less than k. The balls V_n^k, for example, always contain vertices of degree 1.

6 Eigenvalue estimates

We will say that two balls B_1 and B_2 in a graph Γ are *edge-disjoint* if the vertex set of B_1 is disjoint from that of B_2 and there is no edge in Γ joining any vertex of B_1 to any vertex of B_2.

Theorem 7 *Let Γ be a finite graph. Let $B_1, B_2, \ldots, B_m$ be balls in Γ which are pairwise edge-disjoint. Then the mth largest eigenvalue of the adjacency operator on Γ, denoted $\lambda_m(\Gamma)$, satisfies*

$$\lambda_m(\Gamma) \geq \min_i \lambda_1(B_i),$$

where $\lambda_1(B_i)$ denotes the largest eigenvalue of the adjacency operator on the subgraph B_i.

Proof Let $\varphi_1, \ldots, \varphi_{m-1}$ be a set of eigenfunctions corresponding to the eigenvalues $\lambda_1, \ldots, \lambda_{m-1}$ of the adjacency operator A on Γ. Because A is self-adjoint, we know that the φ_i can be chosen so that they are orthogonal,

and thus they span an $m-1$-dimensional subspace T_{m-1} of $L^2(\Gamma)$. The eigenvalue λ_m is characterized by

$$\lambda_m = \max_{\psi \perp T_{m-1}} \frac{\langle A\psi, \psi \rangle}{\langle \psi, \psi \rangle}. \tag{31}$$

We will construct a test function from the eigenfunctions of the adjacency operators on all the balls B_i. For now, let A_i denote the adjacency operator on the ball B_i. Let ψ_i denote an eigenfunction corresponding to the first eigenvalue $\lambda_1(B_i)$ of the operator A_i on each B_i. Extend each function ψ_i to a function $\tilde{\psi}_i$ on all of Γ by setting $\tilde{\psi}_i(x) = 0$ for $x \notin B_i$. Because the balls B_i are disjoint, the support of $\tilde{\psi}_i$ is disjoint from the support of $\tilde{\psi}_j$ if $i \neq j$, so the functions $\tilde{\psi}_i$ are all orthogonal to one another. The subspace of $L^2(\Gamma)$ spanned by the $\tilde{\psi}_i$ is therefore m-dimensional, and so it must contain a function which is orthogonal to T_{m-1}. That is, there are coefficients γ_i such that the function

$$\tilde{\psi} = \sum_{i=1}^{m} \gamma_i \tilde{\psi}_i \tag{32}$$

is orthogonal to every function in T_{m-1}. The Rayleigh quotient of $\tilde{\psi}_i$ will therefore be a lower bound for $\lambda_m(\Gamma)$.

To estimate this Rayleigh quotient, we observe first that for each i, the equality $\left\langle A\tilde{\psi}_i, \tilde{\psi}_i \right\rangle = \langle A_i\psi_i, \psi_i \rangle$ holds, where A is the adjacency operator on all of Γ, and A_i is the adjacency operator on just B_i. This fact, from which it follows that $\left\langle A\tilde{\psi}_i, \tilde{\psi}_i \right\rangle$ is actually equal to $\lambda_1(B_i)$, can be verified as follows.

$$\begin{aligned}
\left\langle A\tilde{\psi}_i, \tilde{\psi}_i \right\rangle &= \sum_{x \in \Gamma} \sum_{\substack{y \sim x \\ y \in \Gamma}} \tilde{\psi}_i(y)\tilde{\psi}_i(x) \\
&= \sum_{x \in B_i} \sum_{\substack{y \sim x \\ y \in B_i}} \tilde{\psi}_i(y)\tilde{\psi}_i(x) \quad (\mathrm{supp}(\tilde{\psi}_i) = B_i) \\
&= \sum_{x \in B_i} \sum_{\substack{y \sim x \\ y \in B_i}} \psi_i(y)\psi_i(x) \\
&= \langle A\psi_i, \psi_i \rangle .
\end{aligned}$$

We next make use of the fact that the B_i are edge-disjoint to show that $\left\langle A\tilde{\psi}_i, \tilde{\psi}_j \right\rangle = 0$ for $i \neq j$. We have

$$\begin{aligned} \left\langle A\tilde{\psi}_i, \tilde{\psi}_j \right\rangle &= \sum_{x\in\Gamma} \sum_{y\sim x} \tilde{\psi}_i(y)\tilde{\psi}_j(x) \\ &= \sum_{x\in B_j} \sum_{y\sim x} \tilde{\psi}_i(y)\tilde{\psi}_j(x). \end{aligned}$$

But B_i and B_j are edge-disjoint, so $y \sim x$ and $x \in B_j$ imply that $y \notin B_i$, and thus that $\tilde{\psi}_i(y) = 0$. Thus $\left\langle A\tilde{\psi}_i, \tilde{\psi}_j \right\rangle = 0$.

And now we will compute the Rayleigh quotient for $\tilde{\psi}$ in two parts. First the numerator:

$$\begin{aligned} \left\langle A\tilde{\psi}, \tilde{\psi} \right\rangle &= \left\langle A \sum_i \gamma_i \tilde{\psi}_i, \sum_j \gamma_j \tilde{\psi}_j \right\rangle \\ &= \sum_{i,j} \gamma_i \gamma_j \left\langle A\tilde{\psi}_i, \tilde{\psi}_j \right\rangle \\ &= \sum_i \gamma_i^2 \left\langle A\tilde{\psi}_i, \tilde{\psi}_i \right\rangle \\ &= \sum_i \lambda_1(B_i)\gamma_i^2 \left\langle \tilde{\psi}_i, \tilde{\psi}_i \right\rangle. \end{aligned}$$

In computing the denominator, we will use the fact that the functions $\tilde{\psi}_i$ are mutually orthogonal.

$$\begin{aligned} \left\langle \tilde{\psi}, \tilde{\psi} \right\rangle &= \left\langle \sum_i \gamma_i \tilde{\psi}_i, \sum_j \gamma_j \tilde{\psi}_j \right\rangle \\ &= \sum_{i,j} \gamma_i \gamma_j \left\langle \tilde{\psi}_i, \tilde{\psi}_j \right\rangle \\ &= \sum_i \gamma_i^2 \left\langle \tilde{\psi}_i, \tilde{\psi}_i \right\rangle. \end{aligned}$$

For each i, let $\zeta_i = \gamma_i^2 \left\langle \tilde{\psi}_i, \tilde{\psi}_i \right\rangle$, and let $Z = \sum \zeta_i$. Then the Rayleigh quotient for $\tilde{\psi}$ is equal to

$$\sum_i \frac{\zeta_i}{Z} \lambda_1(B_i). \tag{33}$$

Since the coefficients ζ_i/Z are all positive and add up to 1, this Rayleigh quotient must be greater than $\min_i \lambda_1(B_i)$, and the proof is complete. ∎

In the next theorem, we will bring into play our explicit estimates of the eigenvalues $\lambda_1(B_i)$, assuming bounded degree, to derive explicit lower bounds on $\lambda_m(\Gamma)$ for $m \geq 2$. For the moment, however, let us examine what Theorem 7 says about $\lambda_1(\Gamma)$. Since all the balls in the set $\{B_1\}$ are pairwise edge-disjoint (there are no pairs of them), B_1 may be taken to be any ball in Γ, and the theorem tells us that $\lambda_1(\Gamma) \geq \lambda_1(B_1)$, where B_1 is any ball in Γ. If the degree of Γ is bounded below by k and the radius of B_1 is n, Theorem 6 implies that $\lambda_1(B_1) > 2\sqrt{k-1}\cos(\pi/(n+2))$. We may take n as large as we like (since B_1 will never intersect another ball, no matter what), so we can conclude that $\lambda_1(\Gamma) \geq 2\sqrt{k-1}$. Unfortunately, this estimate is easily beaten by the Perron-Frobenius theorem, which says that if the degree of Γ is bounded below by k, then $\lambda_1(\Gamma)$ is at least k. If, however, we can find a B_1 which is slightly smaller than Γ and which has a minimal degree k_1 greater than k, then Theorem 7 applied with B_1 may yield a better estimate on λ_1 than Perron-Frobenius theorem does when applied to Γ directly.

The *diameter* of a finite graph Γ is the maximum of $\mathrm{dist}(x, y)$ over all pairs of vertices x and y in Γ. In the next theorem, we estimate the eigenvalues of the adjacency operator on Γ in terms of the diameter of Γ.

Theorem 8 *Let Γ be a finite graph with diameter d and minimal degree $k \geq 3$. Then for $2 \leq m \leq 1 + d/4$, the mth eigenvalue of the adjacency operator on Γ satisfies*

$$\lambda_m(\Gamma) \quad > \quad 2\sqrt{k-1}\cos\left(\frac{\pi}{r+1}\right),$$

where r is the greatest integer less than or equal to $\dfrac{d}{2(m-1)}$.

Proof We claim there are m vertices in Γ, separated pairwise by distances of at least $2r$. If not, then the distance between any two vertices in Γ less than $(m-1)(2r) \leq d$, contradicting the fact that the diameter of Γ is d. Choose m such vertices $x_1, x_2, \ldots, x_m$, and for each one, let $B_i = B(x_i, r-1)$. The balls B_i are edge-disjoint, because if $x \in B(x_i, r-1)$ and $y \in B(x_j, r-1)$ (with $i \neq j$) and x and y are joined by an edge, then the distance between x_i and x_j is less than or equal to $2(r-1)+1 = 2r-1$, contrary to our choice of x_i and x_j. Applying Theorem 7, we conclude that $\lambda_m(\Gamma) \geq \min_i \lambda_1(B_i)$. Theorem 6 then tells us that each $\lambda_1(B_i)$ is greater than $2\sqrt{k-1}\cos\left(\frac{\pi}{r+1}\right)$, and the result follows. ■

One consequence of Theorem 8 for large (but finite) k-regular graphs may be seen as follows. The largest eigenvalue of A on such a graph is k, and Theorem 8 gives the lower bound for $\lambda_2(\Gamma)$ as

$$\lambda_2(\Gamma) \quad > \quad 2\sqrt{k-1}\cos\left(\frac{\pi}{r+1}\right) \tag{34}$$

where r is essentially $d/2$. As d gets large, the right side of (34) increases toward $2\sqrt{k-1}$, so if $\Gamma_1, \Gamma_2, \ldots$ is a sequence of k-regular graphs such that

$$\lim_{n\to\infty} \operatorname{diam}(\Gamma_n) \quad = \quad \infty, \tag{35}$$

we can conclude that

$$\liminf_{n\to\infty} \lambda_2(\Gamma_n) \geq 2\sqrt{k-1}. \tag{36}$$

Even for moderately large k-regular graphs, Theorem 8 does not allow λ_2 to be very far inside the interval $[-2\sqrt{k-1}, 2\sqrt{k-1}]$. The k-regular graphs which, in spite of this crowding effect, have λ_2 and all other eigenvalues except $\pm k$ in the given interval are honored with the name Ramanujan.

7 Boundary case: radius zero

We can get an interesting application of Theorem 7 using balls of radius 0. Mostly for notational convenience, all our previous theorems excluded this boundary case, but it is easy to state what happens when balls of radius zero

are considered. Briefly, we will need to define $\Lambda(1)$ (it turns out to be 0), and so we will need to look at the function S_λ when $\lambda = 0$. Here are the boundary cases of our previous theorems, given in the order in which the theorems originally appeared.

Theorem 9 (Compare with Theorem 1) *Let $k \geq 3$ be an integer. Then the function*

$$S_0(r) \quad = \quad \frac{1}{\sqrt{k-1}^{\,r}} \sin\left(\frac{r\pi}{2} + \frac{\pi}{2}\right)$$

is a spherical 0*-eigenfunction of A on Γ_k.*

Proof This is just a matter of plugging $\lambda = 0$ into the development of S_λ in section 3. The value of θ turns out to be $\frac{\pi}{2}$, as does the value of α. ■

Lemma 10 (Compare with Lemma 2) *$S_0(r)$ is the unique spherical eigenfunction on the k-tree which takes on the value* 0 *at $r = 1$.*

Proof The difference equation defining S_λ requires $\lambda S_\lambda(0) = kS_\lambda(1)$. Since $S_\lambda(1) = 0$ and $S_\lambda(0) = 1$, we conclude that $\lambda = 0$. ■

Lemma 11 (Compare with Lemma 3) $\Lambda(1) = 0$.

Proof Immediate. ■

A ball of radius 0 is a single vertex x. Since no other vertices are connected to x, the adjacency operator on a ball of radius 0 is the zero operator, and its only (and therefore largest) eigenvalue is 0. Thus the boundary case of Theorem 5 is

Theorem 12 $\lambda_1(V_0^k) = 0$.

Packing balls of radius 0 into a finite graph yields the following boundary case of Theorem 8.

Theorem 13 *Let Γ be a finite graph with minimum degree $k \geq 3$ and diameter d. Let n be the greatest integer less than or equal to $1 + d/2$. Then at least n eigenvalues of the adjacency operator on Γ are non-negative. Let p be the greatest integer less than or equal to $1 + d/4$. Then at least p eigenvalues of the adjacency operator on Γ are positive.*

Proof Γ must contain n vertices separated from one another by distance at least 2. If not, then the diameter of Γ is less than $2(n-1)$, and therefore less than d, contrary to hypothesis. We consider these n vertices as n balls of radius 0, and apply Theorems 7 and 12 to conclude that $\lambda_n(\Gamma) \geq 0$. The second assertion is immediate from Theorem 8. ∎

References

[1] Pierre Bérard. *Spectral geometry: direct and inverse problems.* Number 1207 in Lecture notes in mathematics. Springer Verlag, Berlin, 1986.

[2] Robert Brooks. The spectral geometry of k-regular graphs. *Journal d'Analyse*, 57:120–151, 1991.

[3] Isaac Chavel. *Eigenvalues in Riemannian Geometry.* Academic Press, Inc., Orlando, FL, 1984.

[4] Shiu-Yuen Cheng. Eigenvalue comparison theorems and its geometric applications. *Math. Z.*, 143:289–297, 1975.

[5] A. Lubotzky, R. Phillips, and P. Sarnak. Ramanujan graphs. *Combinatorica*, 8(3):261–277, 1988.

[6] Ben Noble and James W. Daniel. *Applied Linear Algebra.* Prentice-Hall, Englewood Cliffs, NJ, 1977.

[7] Gregory Quenell. Spectral diameter estimates for k-regular graphs. *Advances in mathematics*, 106(1):122–148, 1994.

[8] E. Seneta. *Non-negative matrices and Markov chains.* Springer-Verlag, New York, 1981.

[9] Hans F. Weinberger. *Variational Methods for Eigenvalue Approximation.* Number 15 in Regional Conference Series in Applied Mathematics. Society for Industrial and Applied Mathematics, Philadelphia, 1974.

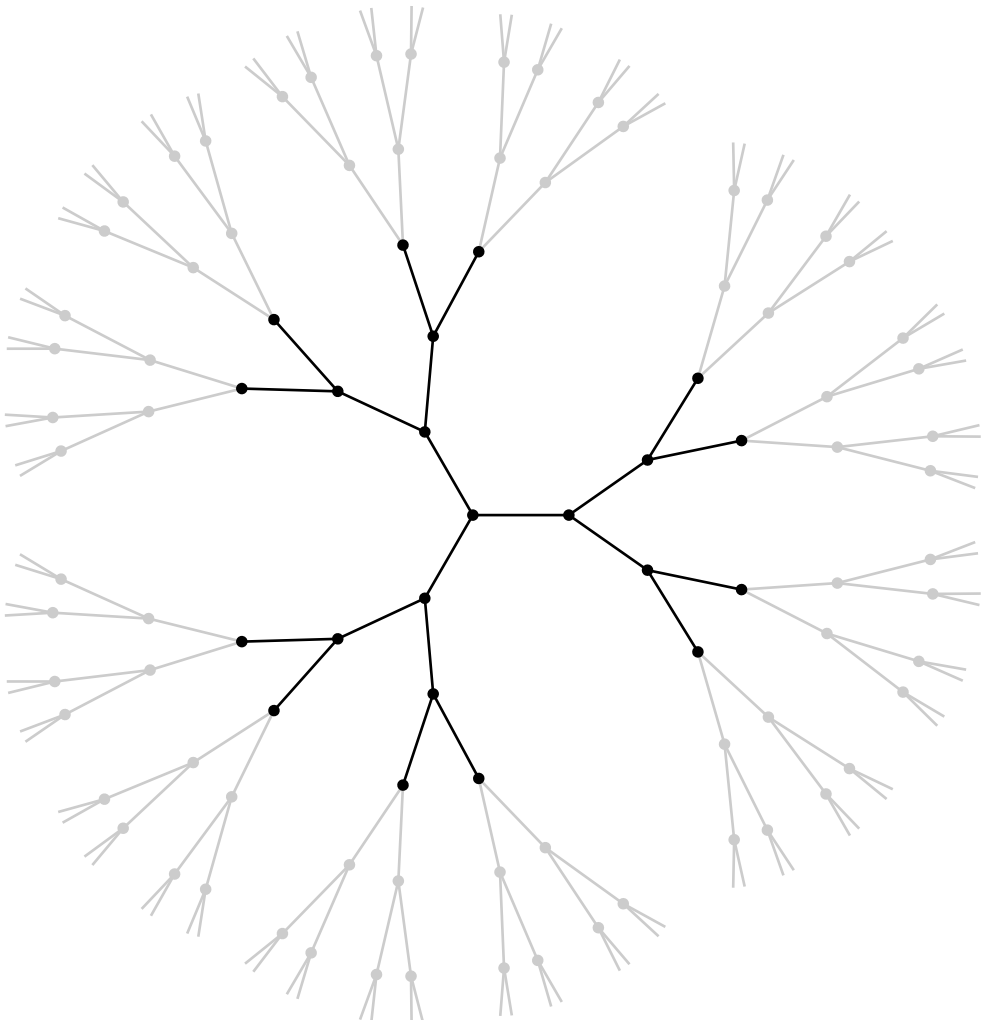

Figure 3: V_3^3 in the 3-tree