Trees with Cantor Eigenvalue Distribution

Li He * Xiangwei Liu † Gilbert Strang ‡

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Abstract

We study a family of trees with degree k at all interior nodes and degree 1 at boundary nodes. The eigenvalues of the adjacency matrix have high multiplicities. As the trees grow, the graphs of those eigenvalues approach a piecewise-constant "Cantor function". For each value of $\frac{m}{n}$, we will find the fraction of the eigenvalues that are given by $\lambda = 2\sqrt{k-1}\cos(\frac{\pi m}{n})$.

1 Introduction

A tree is an attractive and deceptively simple graph. It has no loops, so the path connecting node i to node j is unique. A systematic construction can ensure that all interior nodes have the same degree k and all boundary nodes have degree 1. This finite tree is a subgraph of an infinite homogeneous tree. As the tree grows, it is natural to expect important properties (like the eigenvalues of the adjacency matrix A or the Laplacian) to approach the corresponding properties of the infinite tree. In our case this doesn't happen.

This small note computes the eigenvalues of A for a growing family of trees, and finds an entirely different limit. Repeated eigenvalues occur with astonishing multiplicities. The spectral distribution function looks like a singular Cantor function, constant almost everywhere but nevertheless increasing continuously from $\lambda_{min} = -2\sqrt{k-1}$ to $\lambda_{max} = 2\sqrt{k-1}$. We will see that everything depends on the boundary condition.

2 Construction

Choose any degree $k > 2$. The tree T_1 has a central node x_0 with k edges going out to nodes $x_1, x_2, \ldots, x_k$. The tree T_2 has $k-1$ new edges going out from each of those

*Department of Mathematics, MIT, Cambridge, MA 02139, lihe@math.mit.edu
†Department of Mathematics, MIT, Cambridge, MA 02139, xwliu@math.mit.edu
‡Department of Mathematics, MIT, Cambridge, MA 02139, gs@math.mit.edu

k nodes (previously boundary nodes, now interior nodes). There are $k(k-1)$ new boundary nodes. Figure 1 shows the first two trees for $k = 3$.

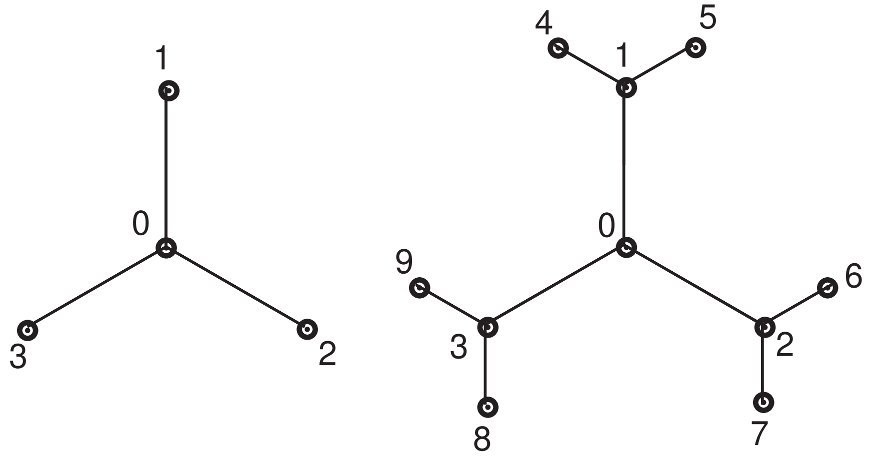

Figure 1: The trees T_1 and T_2 with $B_1 = 3$ and $B_2 = 6$ boundary nodes

After r steps, the tree T_r of radius r will have $B_r = k(k-1)^{r-1}$ boundary nodes. The number of interior nodes is:

$$1 + k + k(k-1) + \cdots + k(k-1)^{r-2} = \frac{k(k-1)^{r-1} - 2}{k-2}$$

The total number of nodes (boundary plus interior, so one more term in the sum) is given by the same expression with r in place of $r-1$:

$$N_r = N(k,r) = \frac{k(k-1)^r - 2}{k-2}$$

The number of interior nodes at stage r is the number N_{r-1} of all nodes at stage $r-1$. Boundary nodes outnumber interior nodes for large r by roughly $k:1$.

The excluded case $k = 2$ is degenerate but very familiar (and important). The tree T_r becomes simply a chain of $2r+1$ nodes, two on the boundary and $2r-1$ inside. The eigenvalues of the adjacency matrix are *cosines.* We will see those same cosines in the degree k construction, but now the eigenvalues will be repeated with high multiplicity.

The N_r by N_r adjacency matrix has $a_{ij} = 1$ if an edge connects node i to node j. In the absence of such an edge $a_{ij} = 0$ (in particular $a_{ii} = 0$). With $k = 3$ the matrices for the trees T_1 and T_2 have orders $N_1 = 4$ and $N_2 = 10$:

$$A_1 = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \quad \text{and} \quad A_2 = \begin{bmatrix} A_1 & C_2 \\ C_2^T & 0 \end{bmatrix}$$

The key to our analysis will be this recursive form of the adjacency matrix, so we go carefully. The zero block on the diagonal of A_r represents no edges between boundary nodes of the tree. The rectangular block C_r represents edges connecting interior nodes to boundary nodes. Thus C_r is an N_{r-1} by B_r matrix, but its only nonzeros will be in a submatrix D_r. This submatrix indicates the new edges connecting B_{r-1} previous boundary nodes to B_r new boundary nodes. In our example with $k = 3$, the matrix D_2 has $B_1 = 3$ rows (nodes 1,2,3) and $B_2 = 6$ columns (nodes 4,5,6,7,8,9):

$$C_2 = \begin{bmatrix} 0 \\ D_2 \end{bmatrix} \quad \text{and} \quad D_2 = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

The $k-1$ ones in each row of D_r represent the $k-1$ new edges going out from each of the earlier boundary points. The symmetry of the adjacency matrix ensures that its remaining block must be C_2^T.

For any k and r, the adjacency matrices of the trees have this same recursive form. We need to indicate the shapes of all submatrices, so our counts of eigenvalues and eigenvectors are consistent. Recall that $B_r = k(k-1)^{r-1}$:

Adjacency matrix: $$A_r = \begin{bmatrix} A_{r-1} & C_r \\ C_r^T & 0 \end{bmatrix}_{(N_r \times N_r)} \qquad N_{r-1} + B_r = N_r$$

Interior to boundary: $$C_r = \begin{bmatrix} 0 \\ D_r \end{bmatrix}_{(N_{r-1} \times B_r)} \qquad N_{r-2} + B_{r-1} = N_{r-1}$$

Old boundary to new boundary:

$$D_r = \begin{bmatrix} 1 & \dots & 1 & & & & & & \\ & & & 1 & \dots & 1 & & & \\ & & & & & & \dots & & \\ & & & & & & 1 & \dots & 1 \end{bmatrix}_{(B_{r-1} \times B_r)} \qquad k-1 \text{ ones in each row.}$$

3 The eigenvalues of the adjacency matrix

Our paper began with a MATLAB computation of the eigenvalues of A_r. The result of a typical experiment $plot(sort(eig(A)))$ is shown in Figure 2. The eigenvalues are

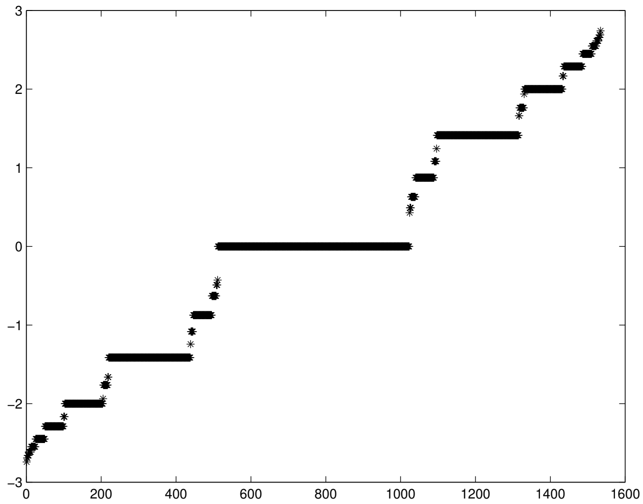

Figure 2: The eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{N_r}$ of the adjacency matrix for $k = 3$, $r = 9$, $N_r = 1534$. There are 512 zero eigenvalues.

plotted in increasing order, from λ_1 to λ_{1534}. The features of this graph caught our attention immediately. Actually Henrik Eriksson did the first experiment in joint work [2] on models for "small-world" graphs. Those graphs are partly structured and partly random, following the experiments of Watts and Strogatz [7], [8]. Those are not trees! And the eigenvalues do not look at all like those in Figure 2.

For the tree we have a piecewise-constant eigenvalue distribution that reminds us of a Cantor singular function. We will prove that this is indeed the limit as $r \to \infty$. The zero eigenvalue in Figure 2 is repeated 512 times out of $N_r = 1534$ eigenvalues, and this fraction approaches $\frac{1}{3}$ as $r \to \infty$. For degree k this limiting fraction is $\frac{(k-2)^2}{k^2-2k}$. Almost all the eigenvalues have the form $\lambda = 2\sqrt{k-1}\cos(\frac{\pi m}{n})$, and for each $\frac{m}{n}$ we will find the asymptotic fraction with this constant value. Those fractions add to 1. (In Cantor's famous "middle thirds" construction, the function is constant on one interval of length $\frac{1}{3}$, two intervals of length $\frac{1}{9}$, four of length $\frac{1}{27}$, ... , and $\sum_{n=1}^{\infty} \frac{2^{n-1}}{3^n} = 1$. Our limiting functions are different.)

One notices that the eigenvalues occur in plus-minus pairs. This is true whenever the graph is a tree. A diagonal similarity verifies that A_r is similar to $-A_r$, as Ahmed Sourour pointed out to us. (The diagonal matrix D has entries $d_{ii} = +1$ or -1 according to whether node i is an even or odd distance from node 0. Then $D^{-1}A_rD =$

$-A_r$ and $-\lambda$ is an eigenvalue when λ is an eigenvalue.) The book by Godsil [4] goes much more deeply into the algebra that connects matrices (and polynomials) that come from graphs.

Another family of trees, closely related to our T_r, starts from two nodes (thus a single edge instead of a single node). The graph with $r = 1$ connects $k-1$ new nodes to each node (thus $n = 2k$). At every stage we add $k-1$ edges to every boundary node, as before. The analysis of this family of trees, and the asymptotic fraction of eigenvalues given by $\lambda = 2\sqrt{k-1}\cos(\frac{\pi m}{n})$, will be the same.

We must emphasize that this piecewise-constant Cantor distribution is *not* the spectral distribution for the infinite homogeneous tree. The infinite case is linked to beautiful mathematics [3] of group representations, and there are no boundary nodes of degree one to produce a singular limit. The valuable book [1] by Fan Chung connects these eigenvalues to other properties of the graph.

For our trees, the diameter (maximum distance between nodes) is explicit:

$$\text{Diameter} \quad D = 2r, \qquad \text{so} \quad D \approx 2\log_2 \frac{N_r}{3}$$

The *average* distance between nodes can also be computed (averaged over all pairs):

$$\begin{aligned} \text{average distance} &= \frac{2(N_r+2)^2}{N_r(N_r-1)}\log_2\frac{N_r+2}{3} - \frac{10N_r+14}{3N_r} \\ &\approx 2\log_2\frac{N_r}{3} - \frac{10}{3} \approx D - \frac{10}{3} \end{aligned}$$

This logarithmic growth is also seen for random graphs and small-world graphs, but with entirely different eigenvalues.

To find the eigenvalues of the adjacency matrix A_r, we first study its characteristic polynomial $P_r(\lambda)$:

$$\begin{aligned} P_r(\lambda) &= \det(A_r - \lambda I) \\ &= \det\begin{bmatrix} A_{r-1} - \lambda I & C_r \\ C_r^T & -\lambda I \end{bmatrix} \\ &= \det\begin{bmatrix} A_{r-1} - \lambda I + \lambda^{-1}C_rC_r^T & 0 \\ C_r^T & -\lambda I \end{bmatrix} \\ &= (-\lambda)^{B_r}\det(A_{r-1} - \lambda I + \lambda^{-1}C_rC_r^T) \end{aligned} \tag{3.1}$$

The size of I is N_r or N_{r-1} or B_r, indicated by its position. From the structure of C_r, we have:

$$C_rC_r^T = \begin{bmatrix} 0 \\ D_r \end{bmatrix}\begin{bmatrix} 0 & D_r^T \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & D_rD_r^T \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & (k-1)I \end{bmatrix}$$

The $k-1$ ones in each row of D_r immediately give $D_r D_r^T = (k-1)I$ (of order B_{r-1}). So we have a recursive structure

$$\begin{aligned} P_r(\lambda) &= (-\lambda)^{B_r} \det(A_{r-1} - \lambda I + \lambda^{-1} C_r C_r^T) \\ &= (-\lambda)^{B_r} \det \begin{bmatrix} A_{r-2} - \lambda I & C_{r-1} \\ C_{r-1}^T & -(\lambda - (k-1)\lambda^{-1})I \end{bmatrix} \end{aligned} \tag{3.2}$$

This recursion is the key, if we can solve a more general problem: Find an expression for

$$f(r, \lambda, \omega) = \det \begin{bmatrix} A_{r-1} - \lambda I & C_r \\ C_r^T & -\omega I \end{bmatrix} \tag{3.3}$$

$P_r(\lambda)$ is the special case where $\omega = \lambda$. So an explicit expression for $f(r, \lambda, \lambda)$ yields the characteristic polynomial of A_r.

To compute (3.3), we follow the same steps that led from (3.1) to (3.2). The backward recursive expression from r to $r-1$ becomes:

$$f(r, \lambda, \omega) = (-\omega)^{B_r} f(r-1, \lambda, \lambda - (k-1)\omega^{-1}) \tag{3.4}$$

Three things are worth noticing in the recursion (3.4):

1. $B_r = k(k-1)^{r-1}$ is an even number for $r \geq 2$. Thus $(-\lambda)^{B_r} = \lambda^{B_r}$.

2. The third argument of $f(n, \lambda, q_{r+1-n})$ follows a recursive relation $q_n = \lambda - (k-1)q_{n-1}^{-1}$, with $q_1 = \lambda$.

3. The backward recursion for f stops at radius $r = 1$, where

$$f(1, \lambda, \omega) = \det \begin{bmatrix} -\lambda & 1 & 1 & \dots & 1 \\ 1 & -\omega & 0 & \dots & 0 \\ & \dots & & \dots & \\ 1 & 0 & 0 & \dots & -\omega \end{bmatrix} = (-1)^{k-1}\omega^{k-1}(\lambda\omega - k)$$

Now our characteristic polynomial $P_r(\lambda)$ is

$$\begin{aligned} f(r, \lambda, \lambda) &= \lambda^{B_r} f(r-1, \lambda, q_2(\lambda)) \\ &= q_1^{B_r} q_2^{B_{r-1}} f(r-2, \lambda, q_3(\lambda)) \end{aligned}$$

Continuing the recursion we obtain

$$\begin{aligned} f(r, \lambda, \lambda) &= q_1^{B_r} q_2^{B_{r-1}} \dots q_{r-1}^{B_2} f(1, \lambda, q_r) \\ &= (-1)^{k-1} q_1^{B_r} q_2^{B_{r-1}} \dots q_{r-1}^{B_2} q_r^{k-1} (\lambda q_r - k) \end{aligned} \tag{3.5}$$

So if we could find an expression for q_n, then we have the characteristic polynomial.

To do this, let $p_1 = \lambda$ and $p_2 = q_2 p_1 = \lambda^2 - (k-1)$. The relation satisfied by $p_n = q_n p_{n-1}$ is:

$$\begin{aligned} p_n &= (\lambda - (k-1)q_{n-1}^{-1})p_{n-1} \\ &= (\lambda - (k-1)\frac{p_{n-2}}{p_{n-1}})p_{n-1} \\ &= \lambda p_{n-1} - (k-1)p_{n-2} \end{aligned}$$

These polynomials $p_n(\lambda)$ of degree n are the coefficients in the generating function

$$g(t,\lambda) = \sum_{n=0}^{\infty} p_n(\lambda)t^n$$

From the recursive relation, we have

$$\begin{aligned} & p_{n+1}t^n = \lambda p_n t^n - (k-1)p_{n-1}t^n \\ \Rightarrow \quad & \frac{1}{t}\sum_{n=0}^{\infty} p_{n+1}t^{n+1} = \lambda \sum_{n=0}^{\infty} p_n t^n - t(k-1)\sum_{n=0}^{\infty} p_{n-1}t^{n-1} \\ \Rightarrow \quad & \frac{1}{t}(g(t,\lambda) - 1) = \lambda g(t,\lambda) - (k-1)tg(t,\lambda) \\ \Rightarrow \quad & g(t,\lambda) = \frac{1}{1 - \lambda t + (k-1)t^2} \end{aligned}$$

Fix λ, and solve $1 - \lambda t + (k-1)t^2 = 0$ for the two roots

$$\alpha = \frac{\lambda + \sqrt{\lambda^2 - 4(k-1)}}{2(k-1)} \quad \text{and} \quad \beta = \frac{\lambda - \sqrt{\lambda^2 - 4(k-1)}}{2(k-1)}$$

So we have

$$g(t,\lambda) = \frac{1}{(k-1)(\alpha-\beta)}(\frac{1}{t-\alpha} - \frac{1}{t-\beta}) = \frac{1}{(k-1)(\alpha-\beta)}(\frac{1}{\beta}\sum_{n=0}^{\infty}\frac{t^n}{\beta^n} - \frac{1}{\alpha}\sum_{n=0}^{\infty}\frac{t^n}{\alpha^n})$$

The coefficient of t^n is

$$p_n = \frac{1}{(k-1)(\alpha-\beta)}(\frac{1}{\beta^{n+1}} - \frac{1}{\alpha^{n+1}})$$

Returning to the characteristic polynomial,

$$\begin{aligned} P_r(\lambda) = f(r,\lambda,\lambda) &= p_1^{B_r}(\frac{p_2}{p_1})^{B_{r-1}}(\frac{p_3}{p_2})^{B_{r-2}} \ldots (\frac{p_r}{p_{r-1}})^k(\lambda - \frac{kp_{r-1}}{p_r}) \\ &= p_1^{B_r - B_{r-1}} p_2^{B_{r-1}-B_{r-2}} \ldots p_{r-1}^{k(k-2)} p_r^{k-1}(\lambda p_r - kp_{r-1}) \end{aligned} \tag{3.6}$$

So all the eigenvalues are roots of p_n $(1 \le n \le r)$ or roots of $\lambda p_r - kp_{r-1}$. The n roots of $p_n(\lambda)$ come from $\alpha^{n+1} = \beta^{n+1}$:

$$\begin{aligned} & (\lambda + \sqrt{\lambda^2 - 4(k-1)})^{n+1} = (\lambda - \sqrt{\lambda^2 - 4(k-1)})^{n+1} \\ \Rightarrow \quad & \frac{\lambda + \sqrt{\lambda^2 - 4(k-1)}}{\lambda - \sqrt{\lambda^2 - 4(k-1)}} = e^{i\frac{2\pi m}{n+1}} \qquad 1 \le m \le n \end{aligned}$$

($m = 0$ is excluded because that will make $\sqrt{\lambda^2 - 4(k-1)}$ zero, but this term appears in the denominator of p_n). Solving for λ, the roots of $p_n(\lambda)$ are now

$$\lambda = 2\sqrt{k-1}\cos(\frac{\pi m}{n+1}) \qquad 1 \le m \le n \tag{3.7}$$

So the eigenvalues of A_r are cosines with $1 \le m \le n \le r$, multiplied by $2\sqrt{k-1}$ (which is a crucial number for k-regular graphs), plus the roots of $\lambda p_r - kp_{r-1}$. Those $r+1$ roots only account for a negligible portion of the N_r eigenvalues for large r.

We take a closer look at the eigenvalues of the adjacency matrix. The roots of p_r are $\lambda = 2\sqrt{k-1}\cos(\frac{\pi m}{r+1})$, $1 \le m \le r$. The following table illustrates the pattern of the appearance of new eigenvalues:

radius	roots of p_r	new terms	number of new terms
$r=1$	$2\sqrt{k-1}\cos(\frac{\pi m}{2})$	$m=1$	$\varphi(2)$
$r=2$	$2\sqrt{k-1}\cos(\frac{\pi m}{3})$	$m=1,2$	$\varphi(3)$
$r=3$	$2\sqrt{k-1}\cos(\frac{\pi m}{4})$	$m=1,3$	$\varphi(4)$
$r=4$	$2\sqrt{k-1}\cos(\frac{\pi m}{5})$	$m=1,2,3,4$	$\varphi(5)$
$r=5$	$2\sqrt{k-1}\cos(\frac{\pi m}{6})$	$m=1,5$	$\varphi(6)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

φ is the Euler Totient Function, so that $\varphi(r+1)$ counts the positive integers $m \le r+1$ that are relatively prime to $r+1$. These correspond to the new angles $\frac{\pi m}{r+1}$ and new cosines.

Thus each new p_r brings us $\varphi(r+1)$ new eigenvalues. (The other roots of p_r are repeats of old eigenvalues – the numbers m and $r+1$ have a common factor and the angle $\frac{\pi m}{r+1}$ was seen earlier.) The total number of eigenvalues is $N_r = B_r + I_r = 1 + \frac{k}{k-2}((k-1)^r - 1)$. Now we can study their multiplicity:

1. $\cos(\frac{\pi}{2})$ appears in the roots of $p_1, p_3, \ldots, p_{2n+1}, \ldots$, so its multiplicity is

$$\begin{aligned} h_1(r) = \quad & (B_r - B_{r-1}) + (B_{r-2} - B_{r-3}) + \cdots + (B_{r-2n} - B_{r-2n-1}) + \ldots \\ = \quad & k(k-2)[(k-1)^{r-2} + (k-1)^{r-4} + (k-1)^{r-6} + \ldots] \end{aligned} \tag{3.8}$$

Asymptotically this is

$$h_1(r) \quad \approx \quad k(k-2)\frac{(k-1)^r}{(k-1)^2-1} \qquad \text{as} \quad r \to \infty$$

This zero eigenvalue accounts for a fraction $\frac{h_1(r)}{N_r} = \frac{(k-2)^2}{(k-1)^2-1}$ of all eigenvalues. For $k = 3$, this fraction is $\frac{1}{3}$.

2. $\cos(\frac{\pi}{3})$ and $\cos(\frac{2\pi}{3})$ appear in the roots of p_2, p_5, p_8, $\ldots$, so their multiplicity is

$$\begin{aligned} h_2(r) &= (B_{r-1} - B_{r-2}) + (B_{r-4} - B_{r-5}) + (B_{r-7} - B_{r-8}) + \ldots \\ &= k(k-2)[(k-1)^{r-3} + (k-1)^{r-6} + (k-1)^{r-9} + \ldots] \\ &\approx k(k-2)\frac{(k-1)^r}{(k-1)^3-1} \qquad \text{as} \quad r \to \infty \end{aligned}$$

This accounts for a fraction $\frac{h_2(r)}{N_r} = \frac{(k-2)^2}{(k-1)^3-1}$ of all eigenvalues. For $k = 3$, this fraction is $\frac{1}{7}$.

3. Each of the $\varphi(n+1)$ new zeros brought in by p_n appears in the roots of p_n, p_{2n+1}, p_{3n+2}, $\ldots$. Following the same steps, its multiplicity is asymptotically

$$h_n(r) \approx k(k-2)\frac{(k-1)^r}{(k-1)^{n+1}-1} \qquad \text{as} \quad r \to \infty$$

This is a fraction $\frac{(k-2)^2}{(k-1)^{n+1}-1}$ of all eigenvalues of A_r. For $k = 3$, this fraction is $\frac{1}{2^{n+1}-1}$.

The fractions we get here agree with the distribution of eigenvalues from direct calculation, as shown in the graph. To verify the asymptotic result, we now sum all the fractions multiplied by φ (and hope that their sum is 1).

An important property of Euler's Totient Function is that

$$\sum_{n=1}^{\infty} \frac{\varphi(n)x^n}{1-x^n} = \frac{x}{(1-x)^2} \qquad \text{for} \quad |x| < 1$$

Substitute $x = \frac{1}{k-1}$ and recall that $\varphi(1) = 1$:

$$\sum_{n=1}^{\infty} \frac{\varphi(n)}{(k-1)^n - 1} = \frac{k-1}{(k-2)^2}$$

Then the sum of fractions multiplied by $\varphi(n)$ is

$$\sum_{n=2}^{\infty} \frac{\varphi(n)(k-2)^2}{(k-1)^n-1} = (k-1) - \frac{\varphi(1)(k-2)^2}{(k-1)^1-1} = 1$$

So all eigenvalues of A_r are asymptotically accounted for as $r \to \infty$.

The zero eigenvalue of T_r has largest multiplicity. According to (3.8), this multiplicity satisfies

$$h_1(r) = h_1(r-2) + k(k-2)(k-1)^{r-2}$$

Johnson and Leal Duarte [5] have connected this maximum multiplicity to the minimum number $P(T_r)$ of disjoint paths that cover all vertices of T_r. To apply their theory to our graphs, we want to show that this path count $P(T_r)$ satisfies the same recursion as $h_1(r)$.

Start from the tree T_{r-2}. Then T_{r-1} has $B_{r-1} = k(k-1)^{r-2}$ new nodes. Each of those nodes grows $k-1$ new edges in T_r, so we have B_{r-1} small stars. Each star (one node in T_{r-1} and $k-1$ new nodes in T_r) is easily covered by $k-2$ disjoint paths. (One path has three nodes and the others have only one; these optimal covering paths are pathetically short.) Therefore this path count $P(T_r)$ increases from $P(T_{r-2})$ in the same way that $h_1(r-2)$ increases to $h_1(r)$. It is easy to check equality for $r = 0, 1, 2$.

We still have to confirm that our count is the *minimum* number of disjoint paths that cover T_r. The main theorem in [5] establishes in several steps that

$$\text{maximum multiplicity} = \text{minimum path count.}$$

There the multiplicities refer to *all* symmetric matrices that have $a_{ij} = 0$ when no edge connects nodes i and j $(i \neq j)$. Our path count agrees with the maximum multiplicity for one particular matrix in this family (the adjacency matrix A_r). But if another matrix in the family had an eigenvalue of higher multiplicity, or if our path count were not minimal, the equation above will be violated.

We turn now to the eigenvectors.

4 The null space of the adjacency matrix

The nullspace of A_r contains the eigenvectors with eigenvalue $\lambda = 0$. Denote this space by $E_r(0)$. We solve $A_r x = 0$ to find the interior components x_i and boundary components x_b of these eigenvectors:

$$A_r x = \begin{bmatrix} A_{r-1} & C_r \\ C_r^T & 0 \end{bmatrix} \begin{bmatrix} x_i \\ x_b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

There will be two orthogonal subspaces of eigenvectors, those concentrated entirely at the boundary (with $x_i = 0$) and those not concentrated at the boundary (with $x_i \neq 0$).

1. Eigenvectors at the boundary: If $x_i = 0$, then we need $C_r x_b = 0$. The vector x_b has B_r components and the matrix C_r has rank B_{r-1}:

$$C_r = \begin{bmatrix} 0 \\ D_r \end{bmatrix}$$

So $B_r - B_{r-1}$ eigenvectors come from the equation $C_r x_b = 0$ which reduces to $D_r x_b = 0$:

$$D_r x_b = \begin{bmatrix} 1 & \dots & 1 & & & & & \\ & & & \cdots & & & & \\ & & & & \cdots & & & \\ & & & & & 1 & \dots & 1 \end{bmatrix} \begin{bmatrix} x_{b,1} \\ \vdots \\ x_{b,k-1} \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \vdots \end{bmatrix}$$

Each row of D_r corresponds to the $k-1$ boundary nodes that come from an interior node. The one equation coming from a typical row has $k-1$ terms:

$$x_{b,1} + x_{b,2} + \cdots + x_{b,k-1} = 0$$

This has $k-2$ independent solutions as illustrated in Figure 3.

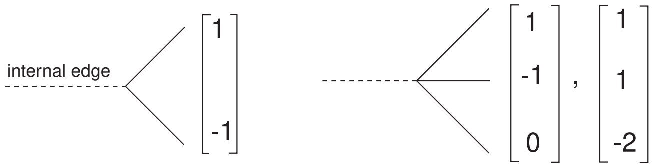

Figure 3: Boundary eigenvectors for $\lambda = 0$ in the case $k = 3$ and $k = 4$

The boundary edges are "fluttering" and there is no movement in the interior. Again, the number of these eigenvectors is

$$B_r - B_{r-1} = k(k-1)^{r-1} - k(k-1)^{r-2} = k(k-2)(k-1)^{r-2}$$

2. Eigenvectors not concentrated at the boundary. If $x_i \neq 0$, then the interior components x_i solve

$$A_{r-1}x_i + C_r x_b = \begin{bmatrix} A_{r-2} & C_{r-1} \\ C_{r-1}^T & 0 \end{bmatrix} \begin{bmatrix} x_{ii} \\ x_{ib} \end{bmatrix} + \begin{bmatrix} 0 \\ D_r x_b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{4.1}$$

$$C_r^T x_i = \begin{bmatrix} 0 & D_r^T \end{bmatrix} \begin{bmatrix} x_{ii} \\ x_{ib} \end{bmatrix} = D_r^T x_{ib} = 0 \tag{4.2}$$

From the second equation, we have

$$D_r^T x_{ib} = \begin{bmatrix} 1 & & \\ \vdots & & \\ 1 & & \\ & \vdots & \\ & & 1 \\ & & \vdots \\ & & 1 \end{bmatrix} \begin{bmatrix} x_{ib,1} \\ \vdots \\ \vdots \\ x_{ib,B_{r-1}} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix} \Rightarrow x_{ib} = 0$$

The first equation now reduces to $A_{r-2}x_{ii} = 0$ and $C_{r-1}^T x_{ii} + D_r x_b = 0$, which means that x_{ii} is in the null space of A_{r-2} and for each such x_{ii}, we can uniquely solve for a x_b that is orthogonal to the boundary eigenvectors. This gives us yet another recursion! We get $B_{r-2} - B_{r-3}$ direct eigenvectors here, plus the null space of A_{r-4}. So the dimension of the nullspace $E_r(0)$, which counts the eigenvectors of A_r for $\lambda = 0$, is:

$$(B_r - B_{r-1}) + (B_{r-2} - B_{r-3}) + (B_{r-4} - B_{r-5}) + \dots$$

This agrees with the number $h_1(r)$ of zero eigenvalues $\lambda = \cos\frac{\pi}{2}$ in Section 3.

5 The eigenspaces of the adjacency matrix

For the eigenspace $E_r(\lambda)$, with eigenvalue $\lambda \neq 0$, we solve $(A_r - \lambda I)x = 0$ to find the eigenvectors:

$$(A_r - \lambda I)x = \begin{bmatrix} A_{r-1} - \lambda I & C_r \\ C_r^T & -\lambda I \end{bmatrix} \begin{bmatrix} x_i \\ x_b \end{bmatrix} = 0 \tag{5.1}$$

This gives us two equations:

$$(A_{r-1} - \lambda I)x_i + C_r x_b = 0 \tag{5.2}$$

$$C_r^T x_i - \lambda x_b = 0 \tag{5.3}$$

Multiply (5.3) by C_r to find

$$\begin{aligned} & C_r C_r^T x_i - \lambda C_r x_b = 0 \\ \Rightarrow \quad & C_r x_b = \lambda^{-1} \begin{bmatrix} 0 & 0 \\ 0 & (k-1)I \end{bmatrix} x_i \end{aligned} \tag{5.4}$$

Substitute (5.4) into (5.2):

$$(A_{r-1} - \lambda I + \begin{bmatrix} 0 & 0 \\ 0 & (k-1)\lambda^{-1} I \end{bmatrix}) x_i = \begin{bmatrix} A_{r-2} - \lambda I & C_{r-1} \\ C_{r-1}^T & -(\lambda - (k-1)\lambda^{-1}) I \end{bmatrix} x_i = 0 \tag{5.5}$$

So x_i is the solution of (5.5) while x_b is uniquely decided by x_i through (5.4).

Not surprisingly, we see that the matrix in (5.5) is actually the same as the matrix we get when calculating eigenvalues. This backward recursion can be carried on as long as the term in the lower right corner of the matrix is nonzero.

If the eigenvalue λ results from $p_n(\lambda) = 0$, we will hit a zero at the $(n-1)$th step of the backward recursion. At that point, the equation is

$$\begin{bmatrix} A_{r-n} - \lambda I & C_{r-n+1} \\ C_{r-n+1}^T & 0 \end{bmatrix} \begin{bmatrix} y_i \\ y_b \end{bmatrix} = 0$$

1. If $y_i = 0$, we have $C_{r-n+1} y_b = 0$. This produces $B_{r-n+1} - B_{r-n}$ boundary eigenvectors.

2. If $y_i \neq 0$, let $y_i = [y_{ii} \quad y_{ib}]^T$, following the similar procedures in the null space calculation, we have $y_{ib} = 0$, $(A_{r-n-1} - \lambda I) y_{ii} = 0$ and $C_{r-n} y_{ii} + C_{r-n+1} y_b = 0$. Thus, y_{ii} is the eigenvector of A_{r-n-1} with eigenvalue λ and for each such y_{ii}, we can uniquely solve for a y_b that is orthogonal to the boundary eigenvectors. This gives us another recursion.

From the recursion, the number of eigenvectors is:

$$\begin{aligned} & (B_{r-n+1} - B_{r-n}) + (B_{r-2n} - B_{r-2n-1}) + (B_{r-3n-1} - B_{r-3n-2}) + \ldots \\ = \quad & k(k-2)[(k-1)^{r-n-1} + (k-1)^{r-2n-2} + (k-1)^{r-3n-3} + \ldots] \\ \approx \quad & k(k-2) \frac{(k-1)^r}{(k-1)^{n+1} - 1} \qquad \text{as} \quad r \to \infty \end{aligned}$$

This agrees with the multiplicity of the eigenvalue λ computed in Section 3.

6 Change of boundary condition

We could increase the degree of the boundary nodes by connecting them to other boundary nodes. At present the degree is 1, and two possibilities have natural interest:

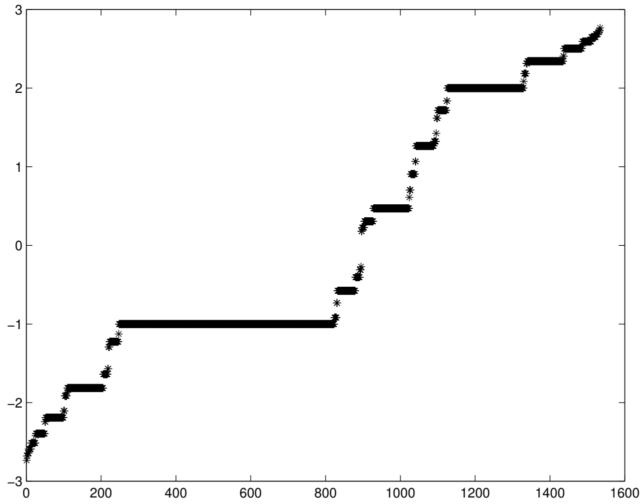

Figure 4: The eigenvalues of the adjacency matrix for $k = 3$, $r = 9$, $N_r = 1534$ with boundary degree 2 (case A).

A. Connect each boundary node to the other $k - 2$ boundary nodes that go out from the same interior node. Then each boundary node has degree $k - 1$. The degree in the interior is still k.

B. Stack up k copies of the original graph, and identify the boundary nodes. This reduces each stack of k boundary nodes, all of degree 1, to a single node of degree k. The graph becomes k-regular.

These graphs are not trees. In both cases, we can again find a recursion for the eigenvalues. The piecewise-constant "Cantor distributions" are shown in Figures 4 and 5. The eigenvalue $\lambda = -1$ is now repeated most frequently in Figure 4, because the zero block in A_r (no connections between boundary nodes) is replaced by a nearly full block. This block is the all-ones matrix, minus the identity. So $\lambda = -1$ is a multiple eigenvalue.

Another way to convert the trees in Figure 1 into 3-regular graphs is to connect the boundary nodes by an outer loop. New edges will connect nodes 1 2 3 1 in T_1 and 4 5 6 7 8 9 4 in T_2. The recursion is gone because the new edges are shortcuts between different branches of the tree.

Figure 6 shows the eigenvalues for this "tree plus outer loop". The limiting distribution as $r \to \infty$ was found by McKay [6], and it is repeated for the partly random graphs discussed in [2]. Our great multiplicities have sadly disappeared. The limiting distribution is no longer singular.

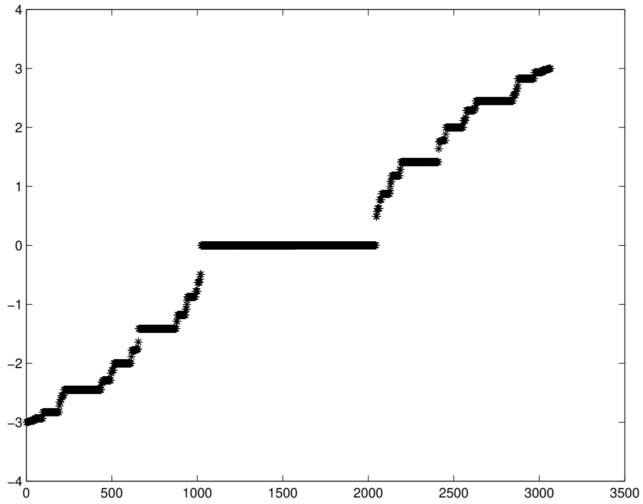

Figure 5: The eigenvalues of the adjacency matrix for $k = 3$, $r = 9$, $N_r = 3066$ with boundary degree 3 (case B).

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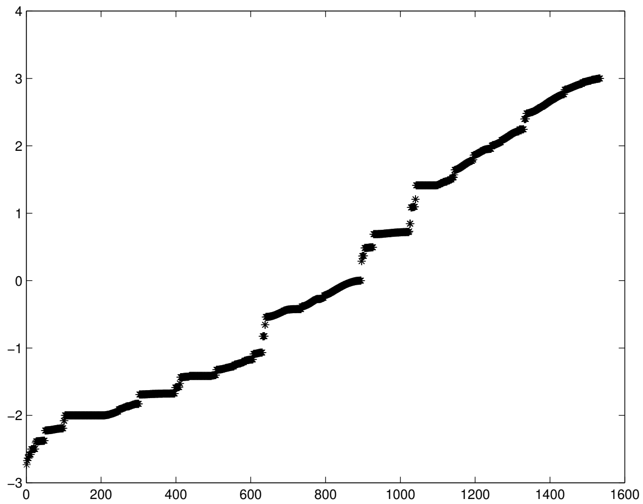

Figure 6: The eigenvalues of the adjacency matrix for $k = 3$, $r = 9$, $N_r = 1534$ with an outer loop.