

Spectrum of some regular graphs with widely spaced modifications

by

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B.S., University of Science and Technology of China, June 1996

Submitted to the Department of Mathematics

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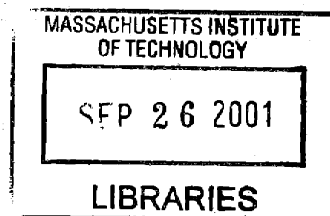
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ABSTRACT

This thesis has two parts. The first part studies the spectrum of a family of growing trees, we show that the eigenvalues of the adjacency matrix and Laplacian matrix have high multiplicities. As the trees grow, the graphs of those eigenvalues approach a piecewise-constant “Cantor function”, which is different from the corresponding properties of the infinite tree. The second part studies the effect of “widely spaced” modifications on the spectrum of some type of structured matrices. We show that by applying those modifications, new eigenvectors that are localized near the components that correspond to the modified rows appear. By knowing the approximate form of those eigenvectors, we also determine a very close (and simple) approximation to the eigenvalues, and then we show that this approximation is indeed the limit as the matrix grows.

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1 Introduction

1.1 Spectrum of a type of growing trees

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 L) to approach the corresponding properties of the infinite tree. In our case this doesn't happen.

In this thesis, we compute the eigenvalues of A for a growing family of trees, and find 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.

We also compute the eigenvalues of L and show that the most frequently repeated eigenvalue $\lambda = 1$ approaches a constant fraction of the number of nodes.

We are grateful to the referee of our paper on this subject for pointing out Gutman's important paper [6] on the characteristic polynomials of a wide class of growing trees (including ours). Where our construction grows the new tree T_r from the boundary of T_{r-1} , Gutman connects d_r copies of T_r to a new root vertex. Heilmann and Lieb [7] studied these trees with d_r independent of r (and with valuable applications to physical chemistry). Our trees appear in this alternative construction by choosing $d_1 = k$ and $d_r = k-1$ for $r > 1$, which constitutes a new special case of independent interest. We also construct the eigenvectors of A .

1.2 Localized eigenvectors from widely spaced matrix modifications

This part is about the eigenvalues and eigenvectors of familiar structured matrices, after changes in a small number of entries. The actual changes need not be small, so we refer to them as modifications rather than perturbations. The *number* of changes is small relative to the size of the matrix, because the modifications are required to be “widely spaced”. They occur in entries that are far apart. They produce new eigenvectors that are localized near the components that correspond to the modified rows. By knowing the approximate form of those eigenvectors, we also determine a very close (and simple) approximation to the eigenvalues.

Imagine a large number of nodes around a circle. Edges go only to the two neighbors of every node. Each row of the adjacency matrix A of this cyclic graph has two 1’s. The matrix is a circulant with 1’s on the first subdiagonal and superdiagonal, coming from the neighbors to the left and right. Now add a few edges going “across” the circle, so that the nodes involved are widely spaced. The modified graph has an adjacency matrix (symmetric if the added edges are undirected, but this is not required) with 1 in the i,j entry when an edge connects node i to node j . A typical example of our work is to find the “new” eigenvalues and eigenvectors of this modified matrix.

Professor Gilbert Strang mentioned in *SIAM News* (April 2000) the simplest case of this example. Only one undirected edge crosses the circle, from node i to a distant node j . This added edge modifies A by setting $a_{ij} = a_{ji} = 1$, in other words by a widely spaced submatrix with entries from

$$B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

The two new 1’s in the modified matrix are far from the main diagonal. *The*

two new eigenvalues are almost exactly $\sqrt{5}$ and $-\sqrt{5}$. The corresponding eigenvectors show a sum or difference of two spikes, as in Figure 1.1, centered at the

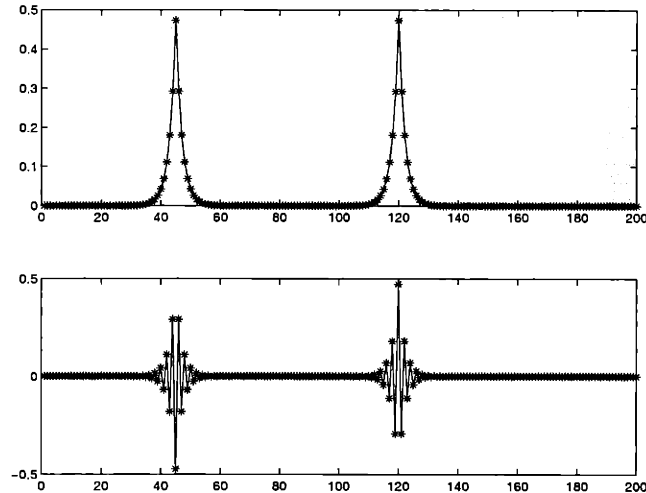


Figure 1.1: The eigenvectors for the maximal and minimal eigenvalues of the adjacency matrix of a 200-node cycle with an edge added between nodes $i = 45$ and $j = 120$

positions i and j connected by the “shortcut edge”. The remaining eigenvalues stay in the interval $[-2, 2]$ that contains all eigenvalues of the original A . Their eigenvectors still oscillate like the original eigenvectors, but orthogonality to the new ones produces the pinching that is illustrated by Figure 1.2.

This brief report in *SIAM News* brought suggested proofs from three friends, Beresford Parlett and Bill Trench and Jackie Shen. All three approaches are different! Shen connected the problem to the theory of perturbed Schrödinger operators, and we believe that our work can be seen as a small contribution (possibly not new) to that established theory. In the first section of this thesis, we study the case when the original matrix is the tridiagonal adjacency matrix of a linear chain, and we find the following formula linking the (nearly exact)

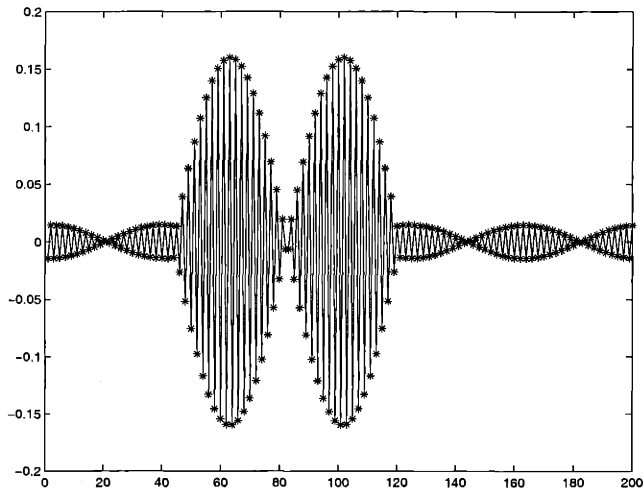


Figure 1.2: A typical eigenvector corresponding to an eigenvalue in the range of $[-2, 2]$ for the perturbed adjacency matrix.

new eigenvalues λ to the eigenvalues μ of B :

$$\lambda = \text{sign}(\mu) \sqrt{4 + \mu^2}$$

The rank two perturbation from one undirected edge and

$$B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

has $\mu = 1$ and -1 , confirming that $\lambda = \sqrt{5}$ and $-\sqrt{5}$. In the two localized eigenvectors, the heights of the “spikes” are given by the eigenvectors of B . We also determine the ratio t between neighboring entries near the spikes (a smaller t means a sharper spike and a more localized eigenvector). This pattern extends to any widely spaced modification by a nonsingular B .

Later sections of the thesis extend the theory beyond a string of nodes and its particular adjacency matrix A . We mention that a circle of nodes would give the same results. We also show that when the underlying matrix is a

general symmetric toeplitz matrix or the adjacency matrix of a 2-dimensional grid, a widely spaced modification will also produce localized eigenvector and we will deduce the equation that can be used to determine the special eigenvalue corresponding to localized eigenvectors.

The work in the first part of the thesis appeared in [9] and [10], and we are preparing another paper [13] that will include most of the work in the second part of the thesis. The author of this thesis took the lead in numerical experiments and their mathematical analysis, and Professor Strang took the lead in writing the papers which are reproduced in this thesis with added materials.

2 Spectrum of a type of growing trees

The tree we study here has degree k at all interior nodes and degree 1 at boundary nodes. First, let's explain in detail how the trees can be constructed.

2.1 Tree 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, \dots, x_k . The tree T_2 has $k - 1$ new edges going out from each of those k nodes (previously boundary nodes, now interior nodes). There are $k(k - 1)$ new boundary nodes. Figure 2.1 shows the first two trees for $k = 3$.

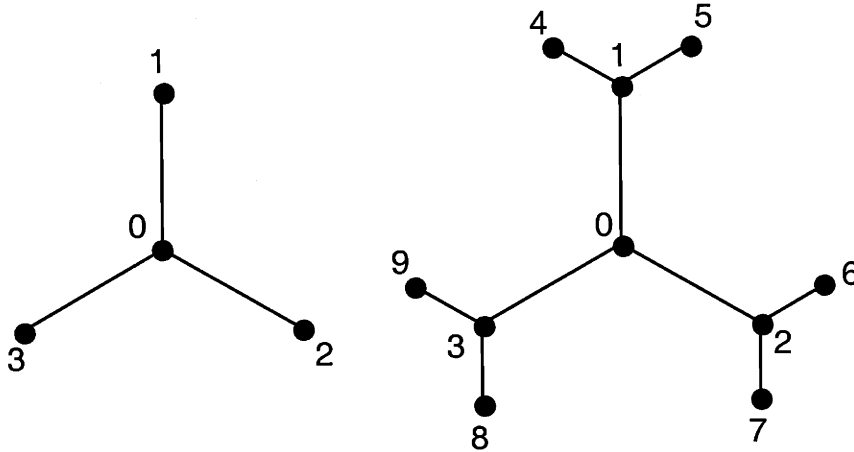


Figure 2.1: The trees T_1 and T_2 with $B_1 = 3$ and $B_2 = 6$ boundary nodes

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:

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

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 linear chain of $2r + 1$ nodes, two on the boundary and $2r - 1$ inside. It is well known that the characteristic polynomial of such a linear chain is $U_{2r+1}(\frac{1}{2}x)$ where $U_n(x) = \sin((n + 1)\theta)/\sin(\theta)$, $\theta = \cos^{-1}(x)$ is the Chebyshev polynomial of the second kind of degree n (See for example [7]). Thus, the eigenvalues of T_r are $2 \cos(\frac{k\pi}{2r+2})$, $k = 1, 2, \dots, 2r + 1$. We will see those same cosines in the degree k construction, but now the eigenvalues will be repeated with high multiplicity.

First, let's look at the adjacency matrix of T_r .

2.2 The adjacency matrix of T_r

The N_r by N_r adjacency matrix of T_r 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 $B_r = k(k - 1)^{r-1}$:

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

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

Old boundary to new boundary:

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

2.2.1 The eigenvalues of the adjacency matrix

We began our study with a MATLAB computation of the eigenvalues of A_r . The result of a typical experiment $\text{plot}(\text{sort}(\text{eig}(A)))$ is shown in Figure 2.2.

The eigenvalues are plotted in increasing order, from λ_1 to λ_{1534} . The features

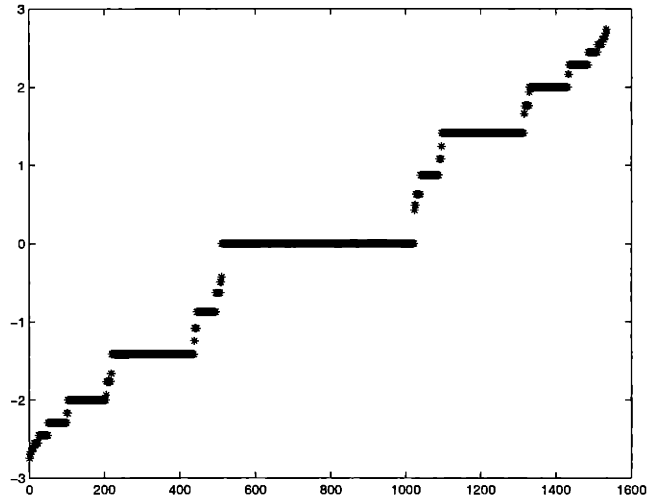


Figure 2.2: The eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{N_r}$ of the adjacency matrix for $k = 3$, $r = 9$, $N_r = 1534$. There are 512 zero eigenvalues.

of this graph caught our attention immediately. Actually Henrik Eriksson did the first experiment in joint work [3] on models for “small-world” graphs. Those graphs are partly structured and partly random, following the experiments of Watts and Strogatz [14], [15], [16]. Those are not trees! And the eigenvalues do not look at all like those in Figure 2.2.

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 $r \rightarrow \infty$. The zero eigenvalue in Figure 2.2 is repeated 512 times out of $N_r = 1534$ eigenvalues, and this fraction approaches $\frac{1}{3}$ as $r \rightarrow \infty$. 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 $\frac{1}{27}$, \dots , 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 [5] 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 [4] 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:

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

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 $P_r(\lambda)$:

$$\begin{aligned}
P_r(\lambda) &= \det(A_r - \lambda I) \\
&= \det \begin{bmatrix} A_{r-1} - \lambda I & C_r \\ C_r^T & -\lambda I \end{bmatrix} \\
&= \det \begin{bmatrix} A_{r-1} - \lambda I + \lambda^{-1} C_r C_r^T & 0 \\ C_r^T & -\lambda I \end{bmatrix} \\
&= (-\lambda)^{B_r} \det(A_{r-1} - \lambda I + \lambda^{-1} C_r C_r^T)
\end{aligned} \tag{2.2.1}$$

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:

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

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

$$\begin{aligned}
P_r(\lambda) &= (-\lambda)^{B_r} \det(A_{r-1} - \lambda I + \lambda^{-1} C_r C_r^T) \\
&= (-\lambda)^{B_r} \det \begin{bmatrix} A_{r-2} - \lambda I & C_{r-1} \\ C_{r-1}^T & -(\lambda - (k-1)\lambda^{-1})I \end{bmatrix}
\end{aligned} \tag{2.2.2}$$

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

$$f(r, \lambda, \omega) = \det \begin{bmatrix} A_{r-1} - \lambda I & C_r \\ C_r^T & -\omega I \end{bmatrix} \tag{2.2.3}$$

$P_r(\lambda)$ 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 (2.2.3), we follow the same steps that led from (2.2.1) to (2.2.2). The backward recursive expression from r to $r - 1$ becomes:

$$f(r, \lambda, \omega) = (-\omega)^{B_r} f(r - 1, \lambda, \lambda - (k - 1)\omega^{-1}) \quad (2.2.4)$$

Three things are worth noticing in the recursion (2.2.4):

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

$$\begin{aligned} f(r, \lambda, \lambda) &= q_1^{B_r} q_2^{B_{r-1}} \dots q_{r-1}^{B_2} f(1, \lambda, q_r) \\ &= (-1)^{k-1} q_1^{B_r} q_2^{B_{r-1}} \dots q_{r-1}^{B_2} q_r^{k-1} (\lambda q_r - k) \end{aligned} \quad (2.2.5)$$

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

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

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

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

The coefficient of t^n is

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

Returning to the characteristic polynomial,

$$\begin{aligned} P_r(\lambda) = f(r, \lambda, \lambda) &= p_1^{B_r} \left(\frac{p_2}{p_1} \right)^{B_{r-1}} \left(\frac{p_3}{p_2} \right)^{B_{r-2}} \dots \left(\frac{p_r}{p_{r-1}} \right)^k \left(\lambda - \frac{kp_{r-1}}{p_r} \right) \\ &= p_1^{B_r - B_{r-1}} p_2^{B_{r-1} - B_{r-2}} \dots p_{r-1}^{k(k-2)} p_r^{k-1} (\lambda p_r - kp_{r-1}) \end{aligned} \quad (2.2.6)$$

So all the eigenvalues are roots of p_n ($1 \leq n \leq r$) or roots of $\lambda p_r - kp_{r-1}$.

The n roots of $p_n(\lambda)$ come from $\alpha^{n+1} = \beta^{n+1}$:

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

($m = 0$ 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

$$\lambda = 2\sqrt{k-1} \cos\left(\frac{\pi m}{n+1}\right) \quad 1 \leq m \leq n \quad (2.2.7)$$

So the eigenvalues of A_r are cosines with $1 \leq m \leq n \leq r$, multiplied by $2\sqrt{k-1}$ (which is a crucial number for k -regular graphs), plus the roots of $\lambda p_r - k p_{r-1}$. 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 $\lambda = 2\sqrt{k-1} \cos\left(\frac{\pi m}{r+1}\right)$, $1 \leq m \leq r$. The following table illustrates the pattern of the appearance of new eigenvalues:

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

φ is the Euler Totient Function, so that $\varphi(r+1)$ counts the positive integers $m \leq r+1$ 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 $p_1, p_3, \dots, p_{2n+1}, \dots$, so its multiplicity is

$$\begin{aligned} h_1(r) &= (B_r - B_{r-1}) + (B_{r-2} - B_{r-3}) + \dots + (B_{r-2n} - B_{r-2n-1}) + \dots \\ &= k(k-2)[(k-1)^{r-2} + (k-1)^{r-4} + (k-1)^{r-6} + \dots] \end{aligned} \tag{2.2.8}$$

Asymptotically this is

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

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, \dots , so their multiplicity is

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

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 $p_n, p_{2n+1}, p_{3n+2}, \dots$. Following the same steps, its multiplicity is asymptotically

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

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

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

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 $r \rightarrow \infty$.

The zero eigenvalue of T_r has largest multiplicity. According to (2.2.8), this multiplicity satisfies

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

Johnson and Leal Duarte [8] 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 [8] establishes in several steps that

maximum multiplicity = 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.

2.2.2 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 $D_r x_b = 0$:

$$A_{r-1}x_i + C_r x_b = \begin{bmatrix} A_{r-2} & C_{r-1} \\ C_{r-1}^T & 0 \end{bmatrix} \begin{bmatrix} x_{ii} \\ x_{ib} \end{bmatrix} + \begin{bmatrix} 0 \\ D_r x_b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (2.2.9)$$

$$C_r^T x_i = \begin{bmatrix} 0 & D_r^T \end{bmatrix} \begin{bmatrix} x_{ii} \\ x_{ib} \end{bmatrix} = D_r^T x_{ib} = 0 \quad (2.2.10)$$

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 2.2.1.

2.2.3 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:

$$(A_r - \lambda I)x = \begin{bmatrix} A_{r-1} - \lambda I & C_r \\ C_r^T & -\lambda I \end{bmatrix} \begin{bmatrix} x_i \\ x_b \end{bmatrix} = 0 \quad (2.2.11)$$

This gives us two equations:

$$(A_{r-1} - \lambda I)x_i + C_r x_b = 0 \quad (2.2.12)$$

$$C_r^T x_i - \lambda x_b = 0 \quad (2.2.13)$$

Multiply (2.2.13) by C_r to find

$$\begin{aligned} C_r C_r^T x_i - \lambda C_r x_b &= 0 \\ \Rightarrow C_r x_b &= \lambda^{-1} \begin{bmatrix} 0 & 0 \\ 0 & (k-1)I \end{bmatrix} x_i \end{aligned} \quad (2.2.14)$$

Substitute (2.2.14) into (2.2.12):

$$(A_{r-1} - \lambda I + \begin{bmatrix} 0 & 0 \\ 0 & (k-1)\lambda^{-1}I \end{bmatrix})x_i = \begin{bmatrix} A_{r-2} - \lambda I & C_{r-1} \\ C_{r-1}^T & -(\lambda - (k-1)\lambda^{-1})I \end{bmatrix} x_i = 0 \quad (2.2.15)$$

So x_i is the solution of (2.2.15) while x_b is uniquely decided by x_i through (2.2.14).

Not surprisingly, we see that the matrix in (2.2.15) 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 $y_i = [y_{ii} \ y_{ib}]^T$, 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:

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

This agrees with the multiplicity of the eigenvalue λ computed in Section 2.2.1.

2.3 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:

- 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

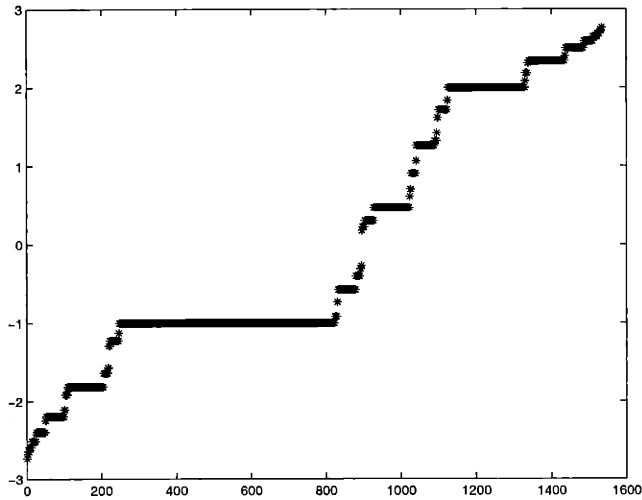


Figure 2.4: The eigenvalues of the adjacency matrix for $k = 3$, $r = 9$, $N_r = 1534$ with boundary degree 2 (case A).

in Figures 2.4 and 2.5. The eigenvalue $\lambda = -1$ is now repeated most frequently in Figure 2.4, 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 2.1 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 2.6 shows the eigenvalues for this “tree plus outer loop”. The limiting distribution as $r \rightarrow \infty$ was found by McKay [11], and it is repeated for the partly random graphs discussed in [3]. Our great multiplicities have sadly disappeared. The limiting distribution is no longer singular.

Now we return to our trees with the original boundary conditions, and we look at the Laplacian matrix of T_r .

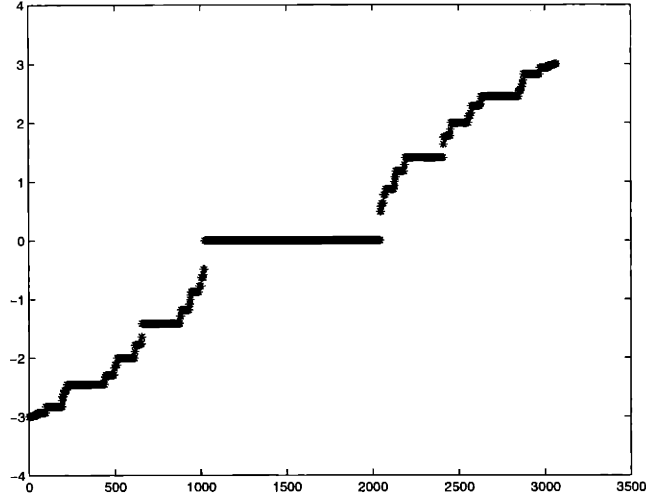


Figure 2.5: The eigenvalues of the adjacency matrix for $k = 3$, $r = 9$, $N_r = 3066$ with boundary degree 3 (case B).

2.4 The Laplacian matrix of T_r

The N_r by N_r Laplacian matrix L_r satisfies the relationship $L_r = H_r - A_r$ where H_r is a diagonal matrix that has h_{ii} equal to the degree of node i . Then the sum along each row of L is zero. With $k = 3$ the Laplacian matrices for the trees T_1 and T_2 have orders $N_1 = 4$ and $N_2 = 10$:

$$L_1 = \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad L_2 = \begin{bmatrix} 3I - A_1 & -C_2 \\ -C_2^T & I \end{bmatrix}$$

This recursive relationship between L_r and A_r , the Laplacian matrix and the adjacency matrix, is key to our analysis of the Laplacian matrix. Similar to what we have shown in Section 2.2, the identity block on the diagonal of L_r represents no edges between boundary nodes of the tree. The rectangular block

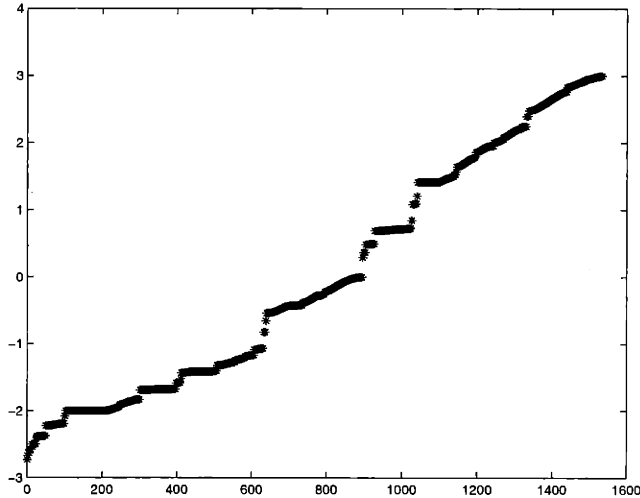


Figure 2.6: The eigenvalues of the adjacency matrix for $k = 3$, $r = 9$, $N_r = 1534$ with an outer loop.

C_r represents edges connecting interior nodes to boundary nodes.

For any k and r , the Laplacian matrices of the trees have this same recursive form. We will use this to compute the characteristic polynomial of L_r .

2.4.1 The eigenvalues of the Laplacian matrix

The result of a typical experiment $plot(sort(eig(L)))$ is shown in Figure 2.7. The eigenvalues are plotted in increasing order, from λ_1 to λ_{1534} . Not surprisingly, here we have again a piecewise-constant eigenvalue distribution that resembles a Cantor singular function. The eigenvalue 1 in Figure 2.7 is repeated 410 times out of $N_r = 1534$ eigenvalues, and we will show that this fraction approaches $\frac{4}{15}$ as $r \rightarrow \infty$.

To find the eigenvalues of the Laplacian matrix L_r , we first study its char-

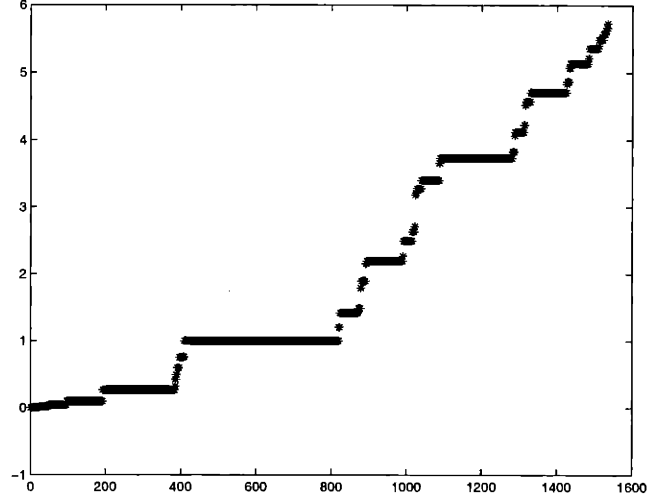


Figure 2.7: The eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{N_r}$ of the Laplacian matrix for $k = 3$, $r = 9$, $N_r = 1534$. There are 410 ones.

acteristic polynomial $\tilde{P}_r(\lambda)$:

$$\begin{aligned}
 \tilde{P}_r(\lambda) &= \det(\lambda I - L_r) \\
 &= \det \begin{bmatrix} A_{r-1} + (\lambda - k)I & C_r \\ C_r^T & (\lambda - 1)I \end{bmatrix} \\
 &= \det \begin{bmatrix} A_{r-1} + (\lambda - k)I - (\lambda - 1)^{-1}C_r C_r^T & 0 \\ C_r^T & (\lambda - 1)I \end{bmatrix} \\
 &= (\lambda - 1)^{B_r} \det(A_{r-1} + (\lambda - k)I - (\lambda - 1)^{-1}C_r C_r^T)
 \end{aligned} \tag{2.4.1}$$

The size of I is N_r or N_{r-1} or B_r , indicated by its position.

Recall from Section 2.2.1

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

So we have a recursive structure

$$\begin{aligned}\tilde{P}_r(\lambda) &= (\lambda - 1)^{B_r} \det(A_{r-1} + (\lambda - k)I - (\lambda - 1)^{-1}C_r C_r^T) \\ &= (\lambda - 1)^{B_r} \det \begin{bmatrix} A_{r-2} + (\lambda - k)I & C_{r-1} \\ C_{r-1}^T & \lambda - k - (k - 1)(\lambda - 1)^{-1}I \end{bmatrix} \end{aligned} \quad (2.4.2)$$

We see immediately that $\tilde{P}_r(\lambda)$ in equation (2.4.2) is the special case $f(r, k - \lambda, 1 - \lambda)$ with f defined in (2.2.3). So an explicit expression for $f(r, k - \lambda, 1 - \lambda)$ will give us the characteristic polynomial of L_r .

Using the recursive formula (2.2.4), we find that the third argument of $f(n, k - \lambda, \tilde{q}_{r+1-n})$ ($1 \leq n \leq r$) follows a recursive relation $\tilde{q}_n = k - \lambda - (k - 1)\tilde{q}_{n-1}^{-1}$, with $\tilde{q}_1 = 1 - \lambda$. And the backward recursion for f stops at radius $n = 1$, where

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

Now our characteristic polynomial $\tilde{P}_r(\lambda)$ is

$$\begin{aligned}f(r, k - \lambda, 1 - \lambda) &= (1 - \lambda)^{B_r} f(r - 1, k - \lambda, \tilde{q}_2(\lambda)) \\ &= \tilde{q}_1^{B_r} \tilde{q}_2^{-B_{r-1}} f(r - 2, k - \lambda, \tilde{q}_3(\lambda))\end{aligned}$$

Continuing the recursion we obtain

$$\begin{aligned}f(r, k - \lambda, 1 - \lambda) &= \tilde{q}_1^{B_r} \tilde{q}_2^{-B_{r-1}} \dots \tilde{q}_{r-1}^{-B_2} f(1, k - \lambda, \tilde{q}_r) \\ &= (-1)^{k-1} \tilde{q}_1^{B_r} \tilde{q}_2^{-B_{r-1}} \dots \tilde{q}_{r-1}^{-B_2} \tilde{q}_r^{k-1} ((k - \lambda)\tilde{q}_r - k)\end{aligned} \quad (2.4.3)$$

So if we could find an expression for \tilde{q}_n , then we have the characteristic polynomial.

To do this, we use the similar technique we used in section 2.2.1. Let $\tilde{p}_0 = 1$, $\tilde{p}_1 = 1 - \lambda$, and $\tilde{p}_2 = \tilde{q}_2 \tilde{p}_1 = (k - \lambda)(1 - \lambda) - (k - 1)$. The relation satisfied

by $\tilde{p}_n = \tilde{q}_n \tilde{p}_{n-1}$ is:

$$\begin{aligned}\tilde{p}_n &= (k - \lambda - (k - 1)\tilde{q}_{n-1}^{-1})\tilde{p}_{n-1} \\ &= (k - \lambda - (k - 1)\frac{\tilde{p}_{n-2}}{\tilde{p}_{n-1}})\tilde{p}_{n-1} \\ &= (k - \lambda)\tilde{p}_{n-1} - (k - 1)\tilde{p}_{n-2}\end{aligned}$$

These polynomials $\tilde{p}_n(\lambda)$ of degree n are the coefficients in the generating function

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

From the recursive relation, we have

$$\begin{aligned}\tilde{p}_{n+1}t^n &= (k - \lambda)\tilde{p}_n t^n - (k - 1)\tilde{p}_{n-1}t^n \\ \Rightarrow \frac{1}{t} \sum_{n=1}^{\infty} \tilde{p}_{n+1}t^{n+1} &= (k - \lambda) \sum_{n=1}^{\infty} \tilde{p}_n t^n - t(k - 1) \sum_{n=1}^{\infty} \tilde{p}_{n-1}t^{n-1} \\ \Rightarrow \frac{1}{t}(\tilde{g}(t, \lambda) - (1 - \lambda)t - 1) &= (k - \lambda)(\tilde{g}(t, \lambda) - 1) - (k - 1)t\tilde{g}(t, \lambda) \\ \Rightarrow \tilde{g}(t, \lambda) &= \frac{1 + (1 - k)t}{1 - (k - \lambda)t + (k - 1)t^2}\end{aligned}$$

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

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

So we have

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

The coefficient of t^n is

$$\tilde{p}_n(\lambda) = \frac{1}{(k - 1)(\alpha - \beta)} \left[\left(\frac{1}{\beta^{n+1}} - \frac{1}{\alpha^{n+1}} \right) + (1 - k) \left(\frac{1}{\beta^n} - \frac{1}{\alpha^n} \right) \right]$$

Returning to the characteristic polynomial,

$$\begin{aligned}
\tilde{P}_r(\lambda) &= f(r, k - \lambda, 1 - \lambda) = \tilde{p}_1^{B_r} \left(\frac{\tilde{p}_2}{\tilde{p}_1}\right)^{B_{r-1}} \left(\frac{\tilde{p}_3}{\tilde{p}_2}\right)^{B_{r-2}} \dots \left(\frac{\tilde{p}_r}{\tilde{p}_{r-1}}\right)^k \left(k - \lambda - \frac{k\tilde{p}_{r-1}}{\tilde{p}_r}\right) \\
&= \tilde{p}_1^{B_r - B_{r-1}} \tilde{p}_2^{B_{r-1} - B_{r-2}} \dots \tilde{p}_{r-1}^{k(k-2)} \tilde{p}_r^{k-1} ((k - \lambda)\tilde{p}_r - k\tilde{p}_{r-1})
\end{aligned} \tag{2.4.4}$$

So almost all the eigenvalues are roots of \tilde{p}_n ($1 \leq n \leq r$). A smaller set of eigenvalues, asymptotically a zero fraction, are roots of the extra factor $(k - \lambda)\tilde{p}_r - k\tilde{p}_{r-1}$.

We take a closer look at eigenvalue $\lambda = 1$ of the Laplacian matrix. By numerical experiment, 1 has the largest multiplicity among all the eigenvalues. Notice that when $\lambda = 1$, the recursion for $\tilde{p}_n(1)$ is $\tilde{p}_{n+1}(1) = (k - 1)(\tilde{p}_n(1) - \tilde{p}_{n-1}(1))$ with initial conditions $\tilde{p}_0(1) = 1$ and $\tilde{p}_1(1) = 0$. The sequence $\tilde{p}_n(1)$ then proceeds as

$$\begin{aligned}
&1 \quad 0 \quad -(k-1) \quad -(k-1)^2 \quad -(k-1)^2(k-2) \quad -(k-1)^3(k-3) \\
&\quad -(k-1)^3(k^2 - 5k + 5) \quad -(k-1)^4(k-2)(k-4) \quad \dots
\end{aligned}$$

For degree $k = 3$, we will hit the first zero after $\tilde{p}_1(1)$ at $\tilde{p}_5(1)$. Then the sequence repeats itself with a different constant factor and we hit additional zeros at $\tilde{p}_9(1)$ and every \tilde{p}_{4n+1} . Similarly, for $k = 4$, we will get zeros at $\tilde{p}_{6n+1}(1)$. For $k > 4$, it is easy to prove from the recursion that the magnitude of the sequence $\tilde{p}_n(1)$ will increase geometrically and there are no more zeros after $\tilde{p}_1(1)$.

Thus, when the degree is $k = 3$, the multiplicity of $\lambda = 1$ is

$$\begin{aligned}
h_1(r) &= (B_r - B_{r-1}) + (B_{r-4} - B_{r-5}) + \dots + (B_{r-4n} - B_{r-4n-1}) + \dots \\
&= 3(2^{r-2} + 2^{r-6} + 2^{r-10} + \dots)
\end{aligned} \tag{2.4.5}$$

As the trees grow, this is asymptotically

$$h_1(r) \approx \frac{4}{5}2^r \quad \text{as } r \rightarrow \infty$$

This accounts for a fraction $\frac{h_1(r)}{N_r} = \frac{4}{15}$ of all eigenvalues. Similarly, when $k = 4$, the multiplicity of $\lambda = 1$ is $\frac{81}{91}3^r$ asymptotically and this accounts for a fraction $\frac{81}{182}$ of all eigenvalues.

For $k > 4$, the multiplicity of $\lambda = 1$ is just $B_r - B_{r-1} = k(k-2)(k-1)^{r-2}$ and this accounts for a fraction $(\frac{k-2}{k-1})^2$ of all eigenvalues.

We turn now to the eigenvectors.

2.4.2 The eigenspace of the Laplacian matrix

We look first at the eigenvectors with eigenvalue $\lambda = 1$. Denote this space by $\tilde{E}_r(1)$. We solve $(I - L_r)x = 0$ to find the interior component x_i and boundary component x_b of these eigenvectors:

$$(I - L_r)x = \begin{bmatrix} A_{r-1} - (k-1)I & C_r \\ C_r^T & 0 \end{bmatrix} \begin{bmatrix} x_i \\ x_b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

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 the interior part $x_i = 0$, then we need $C_r x_b = 0$. This is exactly the same equation we studied in section 2.2.2, and we know from there that $B_r - B_{r-1} = k(k-2)(k-1)^{r-2}$ number of independent eigenvectors come from here.

For trees that have degree $k > 4$, the multiplicity of $\lambda = 1$ is $B_r - B_{r-1}$, and we have found all eigenvectors. For trees with degree $k = 3$ or 4 , there is an additional set of eigenvectors.

2. If $x_i \neq 0$ then the interior components x_i separate into x_{ii} (the interior of the interior) and x_{ib} (the interior that is adjacent to the boundary):

$$(A_{r-1} - (k-1)I)x_i + C_r x_b = \begin{bmatrix} A_{r-2} - (k-1)I & C_{r-1} \\ C_{r-1}^T & -(k-1)I \end{bmatrix} \begin{bmatrix} x_{ii} \\ x_{ib} \end{bmatrix} + \begin{bmatrix} 0 \\ D_r x_b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (2.4.6)$$

$$C_r^T x_i = \begin{bmatrix} 0 & D_r^T \end{bmatrix} \begin{bmatrix} x_{ii} \\ x_{ib} \end{bmatrix} = D_r^T x_{ib} = 0 \quad (2.4.7)$$

From the second equation, we have $x_{ib} = 0$:

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

The first equation in (2.4.6) now reduces to $(A_{r-2} - (k-1)I)x_{ii} = 0$ which means that x_{ii} is in the eigenspace of A_{r-2} with eigenvalue $k-1$, which we have studied in section 2.2.2. Then for each such x_{ii} , the second part of (2.4.6) becomes $C_{r-1}^T x_{ii} + D_r x_b = 0$. This produces a unique x_b that is orthogonal to the boundary eigenvectors.

For the eigenspace $\tilde{E}_r(\lambda)$, with eigenvalue $\lambda \neq 1$, we solve $(\lambda I - L_r)x = 0$ to find the eigenvectors:

$$(\lambda I - L_r)x = \begin{bmatrix} A_{r-1} + (\lambda - k)I & C_r \\ C_r^T & (\lambda - 1)I \end{bmatrix} \begin{bmatrix} x_i \\ x_b \end{bmatrix} = 0 \quad (2.4.8)$$

This gives us two equations:

$$(A_{r-1} + (\lambda - k)I)x_i + C_r x_b = 0 \quad (2.4.9)$$

$$C_r^T x_i + (\lambda - 1)x_b = 0 \quad (2.4.10)$$

Multiply (2.4.10) by C_r to find

$$\begin{aligned} C_r C_r^T x_i + (\lambda - 1)C_r x_b &= 0 \\ \Rightarrow C_r x_b &= -(\lambda - 1)^{-1} \begin{bmatrix} 0 & 0 \\ 0 & (k - 1)I \end{bmatrix} x_i \end{aligned} \quad (2.4.11)$$

Substitute (2.4.11) into (2.4.9):

$$\begin{aligned} &(A_{r-1} + (\lambda - k)I + \begin{bmatrix} 0 & 0 \\ 0 & -(k - 1)(\lambda - 1)^{-1}I \end{bmatrix})x_i \\ &= \begin{bmatrix} A_{r-2} + (\lambda - k)I & C_{r-1} \\ C_{r-1}^T & (\lambda - k) - (k - 1)(\lambda - 1)^{-1}I \end{bmatrix} x_i = 0 \end{aligned} \quad (2.4.12)$$

So x_i is the solution of (2.4.12) while x_b is uniquely decided by x_i through (2.4.11).

Not surprisingly, we see that the matrix in (2.4.12) 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 $\tilde{p}_n(\lambda) = 0$, we will hit a zero at the $(n - 1)$ th step of the backward recursion. At that point, the equation is

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

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 $y_i = [y_{ii} \ y_{ib}]^T$, Following the earlier steps in calculating the eigenspace $E_r(1)$, we have

$$y_{ib} = 0, (A_{r-n-1} + (\lambda - k)I)y_{ii} = 0 \text{ and } C_{r-n}y_{ii} + D_{r-n+1}y_b = 0$$

If $k - \lambda$ is an eigenvalue of A_{r-n-1} , y_{ii} will be in the eigenspace of A_{r-n-1} with eigenvalue $k - \lambda$. For each such y_{ii} , we can uniquely solve for a y_b that is orthogonal to the boundary eigenvectors. If $k - \lambda$ is not an eigenvalue of A_{r-n-1} , we have $y_{ii} = 0$ which reduces back to the boundary eigenvector case.

Our conclusion flows directly from our introduction: The spectrum associated with a growing family of trees can be remarkable. The Laplacian matrix shares the property of high multiplicities with the adjacency matrix, which was worked out earlier in full detail. It remains an open problem to describe the (perhaps generalized) infinite graph whose spectrum agrees with the limit from the sequence of finite graphs.

3 Effects of widely spaced modification on the spectrum

Let A be the adjacency matrix of an n -node linear chain, so A is a tridiagonal matrix with 1's on the first sub-diagonal and super-diagonal. The modification of A will be governed by an M by M matrix B , which needs not be symmetric. We choose M widely spaced indices $1 \ll r_1 \ll \dots \ll r_M \ll n$; the differences between these indices all exceed a number $L \gg 1$. Then the (i, j) entry of B is added to the (r_i, r_j) entry of A . By a terrible abuse of notation, we call the modified matrix $A + B$.

It is well known that the spectrum of A concentrates in the interval $[-2, 2]$ and all of its eigenvectors are widely spread in the sense that the \mathcal{L}^2 norm of any eigenvector with \mathcal{L}^∞ norm 1 diverges as n approaches infinity. We find that with a widely spaced modification of this form, new isolated eigenvalues with localized eigenvector emerge. Our problem is to estimate the “new” eigenvalues and eigenvectors after the modification:

$$(A + B)x = \lambda x \tag{3.0.13}$$

First, let's take a look at the simplest case when B is just a 1 by 1 matrix, i.e., a single real number.

3.1 Single point modification

Choose an index $1 \ll r \ll n$, modify the (r, r) entry of A by adding a real number b there, and let \tilde{A} be the resulted matrix. So $\tilde{A} = A + bE_{rr}$, where E_{ij} is the matrix with 1 at (i, j) entry and 0 elsewhere.

Figure 3.1 shows the spectrum and the localized eigenvector corresponding to the isolated eigenvalue. As we can see, this eigenvector decays very fast and centers at the position of the modification. By looking at the logplot of the

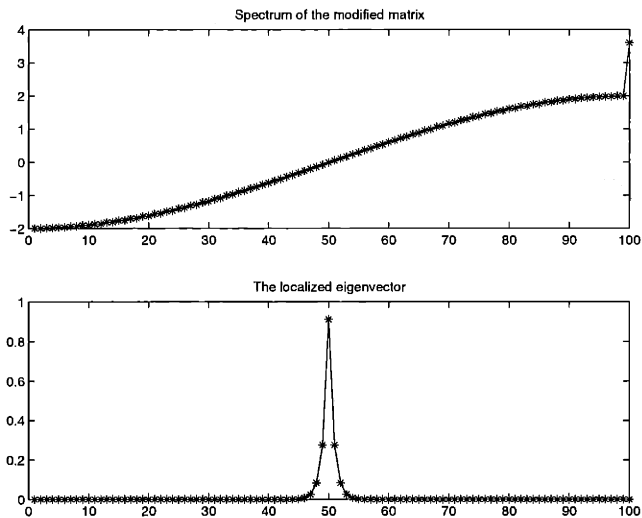


Figure 3.1: The spectrum of \tilde{A} and the eigenvector corresponding to the isolated eigenvalue. $n = 100, r = 50, b = 3$

eigenvector in figure 3.2, we can see that it is exponentially decaying with a constant exponent. The irregular curves at the two ends are due to round-off errors.

Following this observation, we assume the eigenvector is a spike centered at r with $x_r = 1$. The “spike ratio” between neighboring entries is denoted by t , with $|t| < 1$. Then the j -th component of this eigenvector is $t^{|j-r|}$. Substitute this form of x into equation (3.0.13), and let $R = \tilde{A}x - \lambda x$ be the residual. There are 3 cases for the entries of R :

1. For nodes other than 1, r and n , there is no contribution from B and it is not at the boundary,

$$R_j = x_{j-1} + x_{j+1} - \lambda x_j = t^{|j-r|} \left(t + \frac{1}{t} - \lambda \right).$$

2. For node r , the entry has an extra term from B ,

$$R_r = x_{r-1} + bx_r + x_{r+1} - \lambda x_r = 2t + b - \lambda.$$

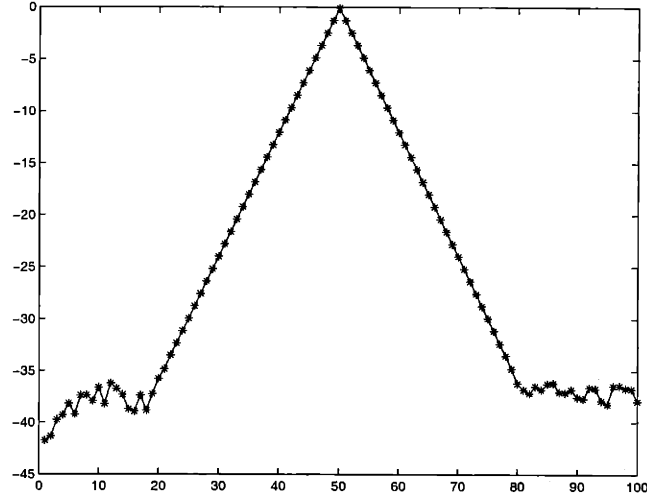


Figure 3.2: logplot of the localized eigenvector

3. For boundary nodes $j = 1, n$, the degrees of these two nodes are 1, and we have $R_1 = t^{r-2} - \lambda t^{r-1}$, $R_n = t^{n-r-1} - \lambda t^{n-r}$

For x to be an exact eigenvector, R has to be zero, which means that all the R_j 's in the cases above have to be zero. But there we have four equations with only two unknowns t and λ , which in general does not have a solution. To overcome this difficulty, we notice that since $|t| < 1$ and $1 \ll r \ll n$, the two boundary residuals will be of order t^L , $L = \min\{r-1, n-r\}$, which decays exponentially as L goes to infinity. Thus, for $L \gg 1$, we can treat those 2 terms as approximation errors and focus on annihilating other terms in the residual, this gives us a system of equations

$$\lambda = t + \frac{1}{t} \quad \text{and} \quad \lambda = 2t + b \quad (3.1.1)$$

with the constraint $|t| < 1$. Equation (3.1.1) has a unique solution

$$\begin{cases} t = \frac{1}{2}(-b + \text{sign}(b)\sqrt{4+b^2}) \\ \lambda = \text{sign}(b)\sqrt{4+b^2}. \end{cases} \quad (3.1.2)$$

Keep in mind that the vector x constructed this way is only an approximation to a real eigenvector since the residual terms are not zero at boundary nodes. But when L is large, the residual term will be very small, and we will prove later on that there is indeed a pair of eigenvalue and eigenvector that is very close to the ones we constructed. Going back to the numerical experiment we showed in figure 3.1, the magnitude of modification b is 3, the eigenvalue predicted by our construction is $\sqrt{13}$, and the actual eigenvalue calculated using MATLAB is the same as our prediction up to 15 digits.

If instead of a finite linear chain, we consider an infinite linear chain with nodes numbered from $-\infty$ to ∞ and a single point modification at $(0, 0)$ entry, then it is obvious from the arguments above that the same construction will produce an exact pair of eigenvalue and eigenvector. In this case, we can also show that the eigenvector we constructed is the only \mathcal{L}^2 -finite eigenvector for the system (the following approach is suggested by Prof. David Ingerman).

For any eigenvector x that is \mathcal{L}^2 -finite, let $f(y)$ be x 's Fourier transform,

$$f(y) = \sum_{n=-\infty}^{\infty} x_n e^{-iny}.$$

The eigenvector equation $\tilde{A}x = \lambda x$ can be rewritten as

$$x_{n-1} + x_{n+1} + b\delta(n)x_n = \lambda x_n, \quad (3.1.3)$$

where $\delta(n)$ is the discrete Dirac Delta function. Applying Fourier transform on both sides of (3.1.3), we get

$$f(y) = \frac{bx_0}{\lambda - e^{-iy} - e^{iy}}. \quad (3.1.4)$$

By the inverse Fourier transform formula, we know that

$$x_n = \frac{1}{2\pi} \int_0^{2\pi} f(y) e^{iny} dy. \quad (3.1.5)$$

Plugging (3.1.4) into (3.1.5), and setting $n = 0$, we get

$$x_0 = \frac{1}{2\pi} \int_0^{2\pi} \frac{bx_0 dy}{\lambda - e^{-iy} - e^{iy}}. \quad (3.1.6)$$

x_0 can't be zero since $f(y)$ will be zero otherwise. By cancelling out x_0 and making the variable substitution $z = e^{iy}$, (3.1.6) becomes

$$\frac{1}{2\pi i} \int_{S^1} \frac{b dz}{\lambda z - z^2 - 1} = 1. \quad (3.1.7)$$

The integral in (3.1.7) is the contour integral on the unit circle S^1 . The two poles of the integrand are $z_1 = (\lambda + \sqrt{\lambda^2 - 4})/2$ and $z_2 = (\lambda - \sqrt{\lambda^2 - 4})/2$. If $|\lambda| \leq 4$, the integral in (3.1.6) diverges. So we must have $|\lambda| > 4$. Notice that z_1 and z_2 are a pair of reciprocals, and only one of them is inside the unit circle. The pole that is inside the unit circle has the form

$$z = \frac{1}{2}(\lambda - \text{sign}(\lambda)\sqrt{\lambda^2 - 4}).$$

Using Cauchy's integral formula, we get

$$\frac{1}{2\pi i} \int_{S^1} \frac{b dz}{\lambda z - z^2 - 1} = \frac{b}{\text{sign}(\lambda)\sqrt{\lambda^2 - 4}}. \quad (3.1.8)$$

Substituting (3.1.8) into (3.1.7) and solving the equation, we get

$$\lambda = \text{sign}(b)\sqrt{4 + b^2} \quad (3.1.9)$$

Substituting (3.1.9) into the inverse Fourier transform formula (3.1.5), we get $x_n = x_0 t^{|n|}$ with t defined as in (3.1.2), which is the same as our construction in (3.2.1). This shows that the eigenvector we constructed is the unique localized eigenvector of \tilde{A} .

3.2 The general case: rank M modifications

Now let's turn to the general case. From what we have seen in the single point case, it is natural to expect that there will also be spiked eigenvectors here, and

indeed that is the case. But now, instead of one spike, we usually have several spikes of different heights. A typical localized eigenvector with three spikes and its logplot are shown in figure 3.3. Note that the logplot is the logplot of the absolute value of the original eigenvector.

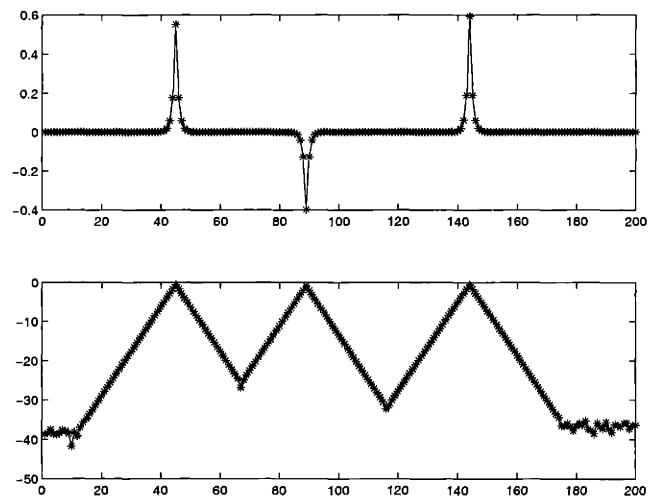


Figure 3.3: the localized eigenvector with 3 spikes and its logplot

To find out what the new eigenvalues and eigenvectors are, we construct a vector x that is now a sum of M spikes. Suppose the spike centered at the r_k -th entry of x has height h_k , and the spike ratio for all the spikes is denoted by t . Then the j -th component of x has the form

$$x_j = \sum_{k=1}^M t^{|j-r_k|} h_k. \quad (3.2.1)$$

Substitute (3.2.1) into equation (3.0.13) and let the residual $R = (A + B)x - \lambda x$. Intuitively, for x to be close to a real eigenvector, $\|R\|$ needs to be small. Following similar arguments as in section 3.1, we can divide the entries of R into three categories.

1. For nodes j other than r_1, r_2, \dots, r_M and the boundary nodes,

$$R_j = \left(t + \frac{1}{t}\right)x_j - \lambda x_j. \quad (3.2.2)$$

2. For nodes r_k , $1 \leq k \leq M$, the spike centered at r_k contributes $2th_k + (Bh)_k - \lambda h_k$ to the residual. All other spikes contribute a small number which is of order t^L to the residual, since by our assumption, they are all well separated with distance at least L . Thus, we have

$$R_{r_k} = 2th_k + (Bh)_k - \lambda h_k + O(t^L). \quad (3.2.3)$$

3. For boundary nodes $j = 1$ or n , every spike contributes $O(t^L)$ to the residual and we have

$$R_j = O(t^L), \quad j = 1, n. \quad (3.2.4)$$

Since $|t| < 1$, when $L \gg 1$, t^L is a very small number. Suppose we ignore all errors of order t^L and set all the R_j 's to be zero, then equation (3.2.3) says that the vector h of spike heights is an eigenvector of B . If that eigenvector has an eigenvalue μ , equations (3.2.2) and (3.2.3) become

$$2t + \mu = \lambda = t + \frac{1}{t}. \quad (3.2.5)$$

Equation (3.2.5) is exactly the same system of equations we have in (3.1.1) with b replaced by μ . From there, we know the unique solution to (3.2.5) is

$$\begin{cases} t = \frac{1}{2}(-\mu + \text{sign}(\mu) \sqrt{4 + \mu^2}) \\ \lambda = \text{sign}(\mu) \sqrt{4 + \mu^2}. \end{cases} \quad (3.2.6)$$

Equation (3.2.6) is the (approximate) relation between the new eigenvalue λ of $A + B$ and the eigenvalue μ of B . Our next goal is to prove that the error in (3.2.6) is of the same order t^L as the terms that were dropped.

First we will prove it for the easier case when B is a symmetric matrix. In this case, the modified matrix $\tilde{A} = A + B$ will also be symmetric and we can bound the eigenvalue using the following easy estimate:

Theorem 3.3.1 *Let A be an n by n hermitian matrix. For any real number λ_0 and any unit vector x_0 , let $R = Ax_0 - \lambda_0 x_0$, then there is an eigenvalue λ of A satisfying $|\lambda - \lambda_0| \leq \|R\|$.*

Proof: If λ_0 is an eigenvalue of A , then the theorem is proved. Assume λ_0 is not an eigenvalue of A . Let $\sigma = \|(A - \lambda_0 I)^{-1}\|$. We know that σ^{-1} is the smallest singular value of $A - \lambda_0 I$. Since A is hermitian, this means that σ^{-1} is the smallest distance between λ_0 and eigenvalues of A . We have

$$1 = \|x_0\| = \|(A - \lambda_0 I)^{-1}R\| \leq \sigma \|R\|.$$

Thus, $\sigma^{-1} \leq \|R\|$. □

In our problem, we already showed that for λ in (3.2.6) and x in (3.2.1), the norm of the residual $\|R\| = \|\tilde{A}x - \lambda x\|$ is of order t^L . So by Theorem 3.3.1, there is an actual eigenvalue of \tilde{A} that's within $O(t^L)$ distance of λ_0 .

Now we can state the result for the non-symmetric case.

Theorem 3.3.2 *If μ is a simple non-zero real eigenvalue of the M by M matrix B , with eigenvector h of norm one, then λ in (3.2.6) and x in (3.2.1) are within $O(t^L)$ distance of an exact eigenvalue-eigenvector pair for the modified matrix $A + B$, where t is defined in (3.2.6).*

To prove this theorem, we need the following lemma:

Lemma 3.3.1 *Let A and E be two n by n matrices, and let N_A and N_E be the maximum of the absolute values of the entries of A and E respectively. Assume $N_E < N_A$. Then for matrix $B = A + E$, we have $|\det(B) - \det(A)| \leq n!(2^n - 1)N_A^{n-1}N_E$.*

Proof: Using the formula for matrix determinants (see for example [12, p. 214]), we know that

$$\det(A + E) = \sum_{\pi} (-1)^{p(\pi)} (a_{1\pi(1)} + e_{1\pi(1)}) (a_{2\pi(2)} + e_{2\pi(2)}) \cdots (a_{n\pi(n)} + e_{n\pi(n)}), \quad (3.2.7)$$

where the summation here is taken over all $n!$ permutations of $\{1, 2, \dots, n\}$ and $p(\pi)$ denotes the parity of permutation π .

Each term in the summation in (3.2.7) can be expanded into the sum of 2^n products, with exactly one product that does not involve entries from E . The sum of this product gives the determinant of A . For all the other products, we can bound them by $N_A^{n-1} N_E$, and there are $n!(2^n - 1)$ of them. Thus, we have $|\det(B) - \det(A)| \leq n!(2^n - 1) N_A^{n-1} N_E$. \square

Now we can prove Theorem 3.3.2.

Proof of Theorem 3.3.2: To prove this theorem, let's study the eigenvector equation (3.0.13) carefully. Since we applied a modification matrix B to A at M widely spaced indices $1 \ll r_1 \ll r_2 \ll \cdots \ll r_M \ll n$, the eigenvector equation (3.0.13) can be divided naturally into $M + 2$ parts. The first $M + 1$ parts do not involve matrix B , each of which corresponds to an equation of the form

$$\begin{bmatrix} 1 & -\lambda & 1 & & & \\ & 1 & -\lambda & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -\lambda & 1 \end{bmatrix} \begin{bmatrix} x_{r_i} \\ x_{r_i+1} \\ \vdots \\ x_{r_{i+1}-1} \\ x_{r_{i+1}} \end{bmatrix} = 0, \quad (3.2.8)$$

where i varies from 0 to M . To simplify our discussion, we added two indices $r_0 = 0$ and $r_{M+1} = n + 1$. We also let the eigenvector x be 0 at those two imaginary indices r_0 and r_{M+1} , i.e., $x_0 = x_{n+1} = 0$ (x by itself is only a length n vector).

The only part that involves B is the following equation:

$$(B - \lambda I_M) \begin{bmatrix} x_{r_1} \\ x_{r_2} \\ \vdots \\ x_{r_M} \end{bmatrix} + \begin{bmatrix} x_{r_1-1} + x_{r_1+1} \\ x_{r_2-1} + x_{r_2+1} \\ \vdots \\ x_{r_M-1} + x_{r_M+1} \end{bmatrix} = 0. \quad (3.2.9)$$

If we can express x_{r_i-1} and x_{r_i+1} in terms of x_{r_1}, \dots, x_{r_M} and plug that in (3.2.9), this will effectively convert the problem of finding the eigenvalues of an n by n matrix to a root-finding problem based on an M by M matrix. Since M is fixed and is far smaller than n , this will help us to bound the actual eigenvalue.

To accomplish that, we will use the first $M + 1$ equations. Let A_i be the $(r_{i+1} - r_i - 1)$ by $(r_{i+1} - r_i + 1)$ matrix in (3.2.8). Simple calculation shows that A_i can be decomposed into the following form:

$$\begin{bmatrix} 1 & -\lambda & 1 & & & \\ & 1 & -\lambda & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -\lambda & 1 \end{bmatrix} = \begin{bmatrix} 1 & -t & & & & \\ & 1 & -t & & & \\ & & \ddots & \ddots & & \\ & & & 1 & -t & \end{bmatrix} \begin{bmatrix} 1 & -t^{-1} & & & & \\ & 1 & -t^{-1} & & & \\ & & \ddots & \ddots & & \\ & & & 1 & -t^{-1} & \end{bmatrix}, \quad (3.2.10)$$

where t satisfies the quadratic equation

$$t^2 - \lambda t + 1 = 0. \quad (3.2.11)$$

The first matrix on the righthand side of (3.2.10) is of size $(r_{i+1} - r_i - 1)$ by $(r_{i+1} - r_i)$ and the second matrix is of size $(r_{i+1} - r_i)$ by $(r_{i+1} - r_i + 1)$.

Substituting decomposition (3.2.10) into (3.2.8), we have

$$\begin{bmatrix} 1 & -t & & & & \\ & 1 & -t & & & \\ & & \ddots & \ddots & & \\ & & & 1 & -t & \end{bmatrix} \begin{bmatrix} x_{r_i} - t^{-1}x_{r_i+1} \\ x_{r_i+1} - t^{-1}x_{r_i+2} \\ \vdots \\ x_{r_{i+1}-1} - t^{-1}x_{r_{i+1}} \end{bmatrix} = 0. \quad (3.2.12)$$

Solving (3.2.12), we get

$$\begin{aligned}
x_{r_i+1} - t^{-1}x_{r_i+2} &= t^{-1}(x_{r_i} - t^{-1}x_{r_i+1}), \\
x_{r_i+2} - t^{-1}x_{r_i+3} &= t^{-2}(x_{r_i} - t^{-1}x_{r_i+1}), \\
&\dots, \\
x_{r_{i+1}-1} - t^{-1}x_{r_{i+1}} &= t^{-(r_{i+1}-r_i-1)}(x_{r_i} - t^{-1}x_{r_i+1}).
\end{aligned} \tag{3.2.13}$$

Multiplying the k -th equation in (3.2.13) by $t^{r_{i+1}-r_i-1-k}$ and adding all of them up, we get

$$t^{r_{i+1}-r_i-2}x_{r_{i+1}} - t^{-1}x_{r_{i+1}} = t^{r_{i+1}-r_i-3}(x_{r_i} - t^{-1}x_{r_i+1}) \sum_{k=0}^{r_{i+1}-r_i-2} t^{-2k} \tag{3.2.14}$$

We can solve $x_{r_{i+1}}$ from (3.2.14),

$$x_{r_{i+1}} = \frac{t^{r_{i+1}-r_i-1} - t^{-(r_{i+1}-r_i-1)}}{t^{r_{i+1}-r_i} - t^{-(r_{i+1}-r_i)}}x_{r_i} + \frac{t - t^{-1}}{t^{r_{i+1}-r_i} - t^{-(r_{i+1}-r_i)}}x_{r_{i+1}}. \tag{3.2.15}$$

Substituting (3.2.15) into the last equation in (3.2.13) and solving for $x_{r_{i+1}-1}$, we get

$$x_{r_{i+1}-1} = \frac{t - t^{-1}}{t^{r_{i+1}-r_i} - t^{-(r_{i+1}-r_i)}}x_{r_i} + \frac{t^{r_{i+1}-r_i-1} - t^{-(r_{i+1}-r_i-1)}}{t^{r_{i+1}-r_i} - t^{-(r_{i+1}-r_i)}}x_{r_{i+1}}. \tag{3.2.16}$$

To simplify our notation, let $\psi(t, n) \equiv t^{-n} - t^n$. Using this new notation, (3.2.15) and (3.2.16) can be written as

$$x_{r_{i+1}} = \frac{\psi(t, r_{i+1} - r_i - 1)}{\psi(t, r_{i+1} - r_i)}x_{r_i} + \frac{\psi(t, 1)}{\psi(t, r_{i+1} - r_i)}x_{r_{i+1}} \tag{3.2.17}$$

and

$$x_{r_{i+1}-1} = \frac{\psi(t, 1)}{\psi(t, r_{i+1} - r_i)}x_{r_i} + \frac{\psi(t, r_{i+1} - r_i - 1)}{\psi(t, r_{i+1} - r_i)}x_{r_{i+1}} \tag{3.2.18}$$

Before proceeding to study (3.2.9), we make some observations here. The quadratic equation (3.2.11) has two roots which are a pair of reciprocals. Since $\psi(t, n) = -\psi(t^{-1}, n)$ and all the terms in (3.2.17) and (3.2.18) involve pairs of

ψ 's, it makes no difference which root we choose. Without loss of generality, we choose the root

$$t = \frac{1}{2}(\lambda - \text{sign}(\lambda)\sqrt{\lambda^2 - 4}). \quad (3.2.19)$$

Notice that when λ is real with $|\lambda| > 2$, t will be a real number that lies in $(-1, 1)$, and as n gets big, $\psi(1, n) = t^{-n}(1 - t^{2n})$ approaches t^{-n} . Using this approximation, we have

$$\begin{aligned} \frac{\psi(t, n-1)}{\psi(t, n)} &= \frac{t^{-(n-1)}(1 - t^{2(n-1)})}{t^{-n}(1 - t^{2n})} \\ &= t(1 - t^{2(n-1)})(1 + t^{2n} + t^{4n} + \dots) \\ &= t - (1 - t^2)t^{2n-1} + O(t^{4n}) \end{aligned} \quad (3.2.20)$$

and

$$\begin{aligned} \frac{\psi(t, 1)}{\psi(t, n)} &= \frac{t^{-1} - t}{t^{-n}(1 - t^{2n})} \\ &= t^n(t^{-1} - t)(1 + t^{2n} + t^{4n} + \dots) \\ &= t^n(t^{-1} - t) + O(t^{3n}). \end{aligned} \quad (3.2.21)$$

So when $|t| < 1$ and $n \gg 1$, $\psi(t, n-1)/\psi(t, n)$ is approximately t with error $O(t^{2n})$ and $\psi(t, 1)/\psi(t, n)$ is approximately 0 with error $O(t^n)$.

Let's return to (3.2.9). Substituting (3.2.17) and (3.2.18) into (3.2.9), we get

$$(B - \lambda I + \Delta(\lambda))x_r = 0, \quad (3.2.22)$$

where $x_r = (x_{r_1}, \dots, x_{r_M})^T$ is a subvector of eigenvector x and $\Delta(\lambda)$ is a symmetric tridiagonal M by M matrix of the following form:

$$\Delta(\lambda) = \begin{bmatrix} \frac{\psi(t, r_1-1)}{\psi(t, r_1)} + \frac{\psi(t, r_2-r_1-1)}{\psi(t, r_2-r_1)} & & \frac{\psi(t, 1)}{\psi(t, r_2-r_1)} & & \\ & \frac{\psi(t, 1)}{\psi(t, r_2-r_1)} & & & \\ \frac{\psi(t, 1)}{\psi(t, r_2-r_1)} & & \frac{\psi(t, r_2-r_1-1)}{\psi(t, r_2-r_1)} + \frac{\psi(t, r_3-r_2-1)}{\psi(t, r_3-r_2)} & & \frac{\psi(t, 1)}{\psi(t, r_3-r_2)} \\ & & \ddots & & \ddots \\ & & & & \ddots & \ddots \end{bmatrix}. \quad (3.2.23)$$

Δ is a function of λ because t is a function of λ defined as in (3.2.19). When $|\lambda| > 2$, we have $|t(\lambda)| < 1$. Recall that we assumed all the indices to be widely separated, i.e., the minimum distance between any two adjacent indices, L , is far greater than one. Using the approximations (3.2.20) and (3.2.21), we get

$$\Delta(\lambda) = \begin{bmatrix} 2t & & & & \\ & 2t & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 2t \end{bmatrix} + \begin{bmatrix} O(t^{2L}) & O(t^L) & & & \\ O(t^L) & O(t^{2L}) & O(t^L) & & \\ & \ddots & \ddots & \ddots & \\ & & & O(t^L) & O(t^{2L}) \end{bmatrix}. \quad (3.2.24)$$

So when $|\lambda| > 2$, the difference between $\Delta(\lambda)$ and $2tI$ is an M by M symmetric tridiagonal matrix $\Omega(\lambda) = \Delta(\lambda) - 2tI$ whose non-zero entries are all of order t^L or lower.

Let's consider the M by M matrix $B - \lambda I + \Delta(\lambda)$ in (3.2.22). The determinant of this matrix, $\rho(\lambda) = \det(B - \lambda I + \Delta(\lambda))$, is a function of λ , and the roots of $\rho(\lambda)$ correspond to the eigenvalues of the matrix \tilde{A} . Let λ_0 and t_0 be defined by (3.2.6). To prove that there is an eigenvalue of \tilde{A} within $O(t_0^L)$ distance of λ_0 is equivalent to proving that one root of $\rho(\lambda)$ is within $O(t_0^L)$ distance of λ_0 for sufficiently large L . To simplify our discussion, from now on, we will assume μ is a positive simple eigenvalue of B . The case when μ is a negative simple eigenvalue of B is exactly the same.

From (3.2.5) we know that $\lambda_0 - 2t(\lambda_0) = \mu$. Since we assumed μ is a simple eigenvalue of B , μ is separated from other eigenvalues of B . Let δ_1 be the minimal distance between μ and any other eigenvalue of B . Let $\delta_2 = 1 - |t(\lambda_0)|$. Since both $t(\lambda)$ and $\lambda - 2t(\lambda) = \sqrt{\lambda^2 - 4}$ are continuous functions of λ , we can always choose a small enough positive constant δ such that for $\lambda \in (\lambda_0 - \delta, \lambda_0 + \delta)$, the distance between $\sqrt{\lambda^2 - 4}$ and any other eigenvalue of B is at least $\delta_1/2$, and $|t(\lambda)| \leq 1 - \delta_2/2$.

Recall that all the entries of $\Omega(\lambda)$ are of order $t(\lambda)^L$ or lower, using this fact and Lemma 3.3.1, and since $M!(2^M - 1)N_B^{M-1}$ is a fixed constant once B

is chosen, we know that there exist two constants C and L_1 such that for any $\lambda \in (\lambda_0 - \delta, \lambda_0 + \delta)$ and for all $L > L_1$,

$$|\rho(\lambda) - \det(B - \sqrt{\lambda^2 - 4}I)| < Ct(\lambda)^L. \quad (3.2.25)$$

Since $\lambda_0 = \sqrt{\mu^2 + 4}$, and μ is an eigenvalue of B , $\det(B - \sqrt{\lambda_0^2 - 4}I) = 0$. Substituting this into (3.2.25), we have $|\rho(\lambda_0)| < Ct_0^L$ which is arbitrarily close to 0 as L gets large.

Rewrite (3.2.25) as

$$\det(B - \sqrt{\lambda^2 - 4}I) - Ct(\lambda)^L < \rho(\lambda) < \det(B - \sqrt{\lambda^2 - 4}I) + Ct(\lambda)^L. \quad (3.2.26)$$

Consider the function $\rho_1(\lambda) = \det(B - \sqrt{\lambda^2 - 4}I)$. Let $\{\mu_1, \mu_2, \dots, \mu_M\}$ be the set of eigenvalues of B with $\mu_1 = \mu$. We know that

$$\rho_1(\lambda) = \prod_{i=1}^M (\mu_i - \sqrt{\lambda^2 - 4}).$$

Let $\nu = \sqrt{\lambda^2 - 4}$, then $\nu(\lambda_0) = \mu$. Since μ is a simple eigenvalue of B ,

$$\frac{\partial \rho_1}{\partial \nu} = - \prod_{i=2}^M (\mu_i - \nu) + (\mu_1 - \nu) \frac{\partial \prod_{i=2}^M (\mu_i - \nu)}{\partial \nu}$$

is non-zero at $\nu(\lambda_0) = \mu$.

$$\frac{\partial \nu}{\partial \lambda} = \frac{\lambda}{\sqrt{\lambda^2 - 4}}$$

is also non-zero at λ_0 . By the chain rule of differentiation, $\rho_1'(\lambda)$ is non-zero at λ_0 . Without loss of generality, assume $\rho_1'(\lambda_0) > 0$. Recall that $t(\lambda)$ is defined in (3.2.19), so

$$t'(\lambda) = \frac{1}{2} - \frac{\lambda}{\sqrt{\lambda^2 - 4}} \leq -\frac{1}{2}$$

is also non-zero at λ_0 . Since $\rho_1(\lambda)$ and $t'(\lambda)$ are smooth functions, there exists a $\delta_3 < \delta$ such that for λ in $(\lambda_0 - \delta_3, \lambda_0 + \delta_3)$, $\rho_1'(\lambda)$ is bounded from below by a positive constant θ , and $|t'(\lambda)|$ is bounded from above by a positive constant ξ .

Let $\gamma = \sup\{t(\lambda) \mid \lambda \in (\lambda_0 - \delta_3, \lambda_0 + \delta_3)\}$. Since $\delta_3 < \delta$ and from the way δ is chosen, we know $\gamma \in (0, 1)$. Function $L\gamma^{L-1}$ and t_0^L approach 0 as L goes to infinity. Thus, there exists a constant $L_2 > L_1$ such that for any $L > L_2$,

$$|L\gamma^{L-1}| < \frac{\theta}{2\xi C}$$

and

$$t_0^L < \frac{\theta\delta_3}{2C}.$$

For any $L > L_2$, Let $\epsilon = 2Ct_0^L/\theta < \delta_3$. Let $f_1(\lambda) = \rho_1(\lambda) + Ct(\lambda)^L$, then $f_1(\lambda_0) = Ct_0^L > 0$. For λ in $(\lambda_0 - \delta_3, \lambda_0 + \delta_3)$ and $L > L_2$,

$$\begin{aligned} f_1'(\lambda) &= \rho_1'(\lambda) - CLt(\lambda)^{L-1}t'(\lambda) \\ &> \theta - \xi CL\gamma^{L-1} \\ &> \theta - \frac{\theta}{2} = \frac{\theta}{2}. \end{aligned} \tag{3.2.27}$$

So

$$\begin{aligned} f_1(\lambda_0 - \epsilon) &= f_1(\lambda_0) - \int_{\lambda_0 - \epsilon}^{\lambda_0} f_1'(\lambda) d\lambda \\ &< Ct_0^L - \frac{\theta}{2}\epsilon = 0 \end{aligned}$$

Since $f_1(\lambda_0) > 0$ and $f_1(\lambda_0 - \epsilon) < 0$, By the continuity of f_1 , there exists a $\lambda_1 \in (\lambda_0 - \epsilon, \lambda_0)$ such that $f_1(\lambda_1) = 0$. Similar argument shows that for $f_2(\lambda) = \rho_1(\lambda) - Ct(\lambda)^L$, there exists a $\lambda_2 \in (\lambda_0, \lambda_0 + \epsilon)$ such that $f_2(\lambda_2) = 0$. From (3.2.26), we know $\rho(\lambda_1) < 0$ and $\rho(\lambda_2) > 0$, so there exists a $\tilde{\lambda}$ in $(\lambda_1, \lambda_2) \subset (\lambda_0 - \epsilon, \lambda_0 + \epsilon)$ such that $\rho(\tilde{\lambda}) = 0$. This is the eigenvalue we are looking for. Since $|\tilde{\lambda} - \lambda_0| < \epsilon$, which is of order t_0^L , we conclude that for sufficiently large L , the distance of λ_0 from a real eigenvalue of \tilde{A} is of order t_0^L .

The other part of the theorem is to prove that there is an eigenvector \tilde{x} corresponding to the actual eigenvalue $\tilde{\lambda}$ such that \tilde{x} is within $O(t_0^L)$ distance of x defined by (3.2.1). Let H be the one dimensional eigenspace of B corresponding

to eigenvalue μ , and let H^\perp be the orthogonal complement of H . Since μ is a simple eigenvalue of B , we know that for any non-zero vector β in H^\perp , $(B - \mu)\beta \neq 0$. Let

$$\delta_4 = \min\{\|(B - \mu)\beta\| \mid \beta \in H^\perp, \|\beta\| = 1\}. \quad (3.2.28)$$

Note that δ_4 is a positive constant.

Let \tilde{x} be an eigenvector of \tilde{A} corresponding to eigenvalue $\tilde{\lambda}$, and let \tilde{h} be the subvector $\{\tilde{x}_{r_1}, \dots, \tilde{x}_{r_M}\}^T$ of \tilde{x} . We normalize \tilde{x} by letting $\|\tilde{h}\| = 1$. Let $\tilde{\mu} = \sqrt{\tilde{\lambda}^2 - 4}$ and $\tilde{t} = t(\tilde{\lambda})$. Since the difference between λ_0 and $\tilde{\lambda}$ is of order t_0^L and the derivatives of $t(\lambda)$ and $\sqrt{\lambda^2 - 4}$ do not vanish at λ_0 , it is clear that $\tilde{\mu}$ and \tilde{t} are within $O(t_0^L)$ distance of μ and t_0 respectively. Recall that all the non-zero entries of the tridiagonal matrix $\Omega(\lambda) = \Delta(\lambda) - 2t(\lambda)I$ are of order $t(\lambda)^L$ or lower, so $\|\Omega(\lambda)\|$ is of order $t(\lambda)^L$. Thus there exist two constants C_1 and $L_3 > L_2$ such that for any $L > L_3$, $|\tilde{\mu} - \mu| < C_1 t_0^L$, $|\tilde{t} - t_0| < C_1 t_0^L$, $L\gamma^L < 1$ and $\|\Omega(\tilde{\lambda})\| < C_1 \tilde{t}^L$.

For any $L > L_3$,

$$\begin{aligned} |\tilde{t}^L - t_0^L| &= |\tilde{t} - t_0| \sum_{i=0}^{L-1} \tilde{t}^i t_0^{L-i-1} \leq |\tilde{t} - t_0| L \gamma^L \\ &< |\tilde{t} - t_0| \leq C_1 t_0^L. \end{aligned} \quad (3.2.29)$$

This implies that $\tilde{t}^L < (C_1 + 1)t_0^L$ for $L > L_3$. Let $C_2 = C_1(C_1 + 1)$, then for $L > L_3$, $\|\Omega(\tilde{\lambda})\| < C_1 \tilde{t}^L < C_2 t_0^L$.

There exist two unique vectors $\alpha \in H$ and $\beta \in H^\perp$ such that $\tilde{h} = \alpha + \beta$. For any $L > L_3$, from (3.2.22), we have

$$\begin{aligned} 0 &= \|(B - \tilde{\lambda} + \Delta(\tilde{\lambda}))\tilde{h}\| = \|(B - \tilde{\mu})\tilde{h} + \Omega(\tilde{\lambda})\tilde{h}\| \\ &= \|(B - \mu)\alpha + (B - \mu)\beta + (\mu - \tilde{\mu})\tilde{h} - \Omega(\tilde{\lambda})\tilde{h}\| \\ &\geq \delta_4 \|\beta\| - |\mu - \tilde{\mu}| - \|\Omega(\tilde{\lambda})\| \\ &> \delta_4 \|\beta\| - (C_1 + C_2)t_0^L. \end{aligned} \quad (3.2.30)$$

From (3.2.30) we know

$$\|\beta\| < \frac{(C_1 + C_2)t_0^L}{\delta_4}. \quad (3.2.31)$$

Recall that x 's construction in (3.2.1) is based on a norm 1 eigenvector of B corresponding to eigenvalue μ . Since the eigenspace H is of dimension 1, without loss of generality, we can always assume $\alpha/\|\alpha\| = h$ (otherwise just multiply \tilde{x} by -1 to make that true). Thus,

$$\begin{aligned} \|h - \tilde{h}\| &\leq \|h - \alpha\| + \|\beta\| \\ &= (1 - \|\alpha\|) + \|\beta\| \\ &\leq 2\|\beta\| < \frac{2(C_1 + C_2)t_0^L}{\delta_4}. \end{aligned} \quad (3.2.32)$$

Denote the constant $2(C_1 + C_2)/\delta_4$ by C_3 .

Recall that we computed in (3.2.17) that

$$\tilde{x}_{r_{i+1}} = \frac{\psi(t, r_{i+1} - r_i - 1)}{\psi(t, r_{i+1} - r_i)} \tilde{x}_{r_i} + \frac{\psi(t, 1)}{\psi(t, r_{i+1} - r_i)} \tilde{x}_{r_{i+1}}.$$

In the same way, we can solve for other terms between indices r_i and r_{i+1} , and the result is

$$\tilde{x}_{r_i+k} = \frac{\psi(t, r_{i+1} - r_i - k)}{\psi(t, r_{i+1} - r_i)} \tilde{x}_{r_i} + \frac{\psi(t, k)}{\psi(t, r_{i+1} - r_i)} \tilde{x}_{r_{i+1}}, \quad (3.2.33)$$

where $0 \leq k \leq r_{i+1} - r_i$.

The eigenvector we constructed in (3.2.1) is a combination of M spikes, i.e.,

$$x = \sum_{i=1}^M u_i, \quad (3.2.34)$$

where the j -th entry of spike u_i is

$$u_{i,j} = h_i t_0^{|j-r_i|}. \quad (3.2.35)$$

From (3.2.33), we know that the actual eigenvector \tilde{x} can also be written as a combination of M spikes:

$$\tilde{x} = \sum_{i=1}^M w_i, \quad (3.2.36)$$

where the j -th entry of w_i has the following form:

$$w_{i,j} = \begin{cases} \frac{\psi(\tilde{t}, r_i - r_{i-1} - |j - r_i|) \tilde{h}_i}{\psi(\tilde{t}, r_i - r_{i-1})} \tilde{h}_i, & r_{i-1} \leq j \leq r_i \\ \frac{\psi(\tilde{t}, r_{i+1} - r_i - |j - r_i|) \tilde{h}_i}{\psi(\tilde{t}, r_{i+1} - r_i)} \tilde{h}_i, & r_i \leq j \leq r_{i+1} \\ 0. & \text{Otherwise} \end{cases} \quad (3.2.37)$$

Since

$$\|x - \tilde{x}\| = \left\| \sum_{i=1}^M u_i - \sum_{i=1}^M w_i \right\| \leq \sum_{i=1}^M \|u_i - w_i\|, \quad (3.2.38)$$

it is clear that if each of the $\|u_i - w_i\|$ is of order t_0^L , then $\|x - \tilde{x}\|$ is of order t_0^L . Without loss of generality, we look at $\|u_1 - w_1\|$. Substituting (3.2.35) and (3.2.37) into vector norm formula, we get

$$\begin{aligned} & \|u_1 - w_1\|^2 \\ &= \sum_{i=1}^{r_1} (t_0^{r_1-i} h_1 - \frac{\psi(\tilde{t}, i)}{\psi(\tilde{t}, r_1)} \tilde{h}_1)^2 + \sum_{i=r_1+1}^{r_2} (t_0^{i-r_1} h_1 - \frac{\psi(\tilde{t}, r_2-i)}{\psi(\tilde{t}, r_2-r_1)} \tilde{h}_1)^2 + \sum_{i=r_2+1}^n (t_0^{i-r_1} h_1)^2. \end{aligned} \quad (3.2.39)$$

From (3.2.32), we know that

$$|h_1 - \tilde{h}_1| \leq \|h - \tilde{h}\| < C_3 t_0^L \quad (3.2.40)$$

for $L > L_3$. Also notice that for sufficiently large n and for any $0 \leq k \leq n$,

$$\begin{aligned} \left| \tilde{t}^{n-k} - \frac{\psi(\tilde{t}, k)}{\psi(\tilde{t}, n)} \right| &= \frac{\tilde{t}^{n+k} - \tilde{t}^{3n-k}}{1 - \tilde{t}^{2n}} \\ &\leq \frac{\tilde{t}^{n+k}}{1 - \tilde{t}^{2n}} \leq 2\tilde{t}^{n+k}, \end{aligned} \quad (3.2.41)$$

Using (3.2.29), (3.2.40) and (3.2.41), the first term in the righthand side of (3.2.39) can be bounded in the following way for some constant C_4 and all $L > L_3$:

$$\begin{aligned}
& \sum_{i=1}^{r_1} \left(t_0^{r_1-i} h_1 - \frac{\psi(\tilde{t}, i)}{\psi(\tilde{t}, r_1)} \tilde{h}_1 \right)^2 \\
& \leq 2 \sum_{i=1}^{r_1} \left[(t_0^{r_1-i} h_1 - \tilde{t}^{r_1-i} h_1)^2 + (\tilde{t}^{r_1-i} h_1 - \tilde{t}^{r_1-i} \tilde{h}_1)^2 + (\tilde{t}^{r_1-i} \tilde{h}_1 - \frac{\psi(\tilde{t}, i)}{\psi(\tilde{t}, r_1)} \tilde{h}_1)^2 \right] \\
& < 2C_1^2 t_0^{2L} \sum_{i=0}^{r_1-1} (i\gamma^i)^2 + 2C_3^2 t_0^{2L} \sum_{i=0}^{r_1-1} \tilde{t}^{2i} + 8\tilde{t}^{2r_1} \sum_{i=1}^{r_1} \tilde{t}^{2i} \\
& < 2C_1^2 t_0^{2L} \sum_{i=0}^{\infty} (i\gamma^i)^2 + 2C_3^2 t_0^{2L} \sum_{i=0}^{\infty} \gamma^{2i} + 8(C_2 + 1)^2 t_0^{2L} \sum_{i=0}^{\infty} \gamma^{2i} \\
& = C_4 t_0^{2L}.
\end{aligned} \tag{3.2.42}$$

The second term in the righthand side of (3.2.39) can be bounded in exactly the same way, and we have

$$\sum_{i=r_1+1}^{r_2} \left(t_0^{i-r_1} h_1 - \frac{\psi(\tilde{t}, r_2-i)}{\psi(\tilde{t}, r_2-r_1)} \tilde{h}_1 \right)^2 < C_5 t_0^{2L}. \tag{3.2.43}$$

For the third term in the righthand side of (3.2.39), we get

$$\sum_{i=r_2+1}^n \left(t_0^{i-r_1} h_1 \right)^2 < t_0^{2L} \sum_{i=0}^{\infty} t_0^{2i} = C_6 t_0^{2L} \tag{3.2.44}$$

for a constant $C_6 = 1/(1 - t_0^2)$. Combining (3.2.42), (3.2.43) and (3.2.44), we get

$$\|u_1 - w_1\|^2 < (C_4 + C_5 + C_6) t_0^{2L}. \tag{3.2.45}$$

This implies that $\|u_1 - w_1\|$ is of order t_0^L . The same is true for all the $\|u_i - w_i\|$, $i = 1, \dots, M$. Thus, we conclude that $\|\tilde{x} - x\|$ is of order t_0^L . \square

Remark 1: When B is a diagonal matrix, simple arguments show that the bound in (3.2.25) can be improved to $O(t(\lambda)^{2L})$. This in turn will translate to

a $O(t_0^{2L})$ bound for the eigenvalue. The eigenvector bound will remain to be $O(t_0^L)$ due to some $O(t_0^L)$ terms in (3.2.39).

Remark 2: The condition that μ is a real number is not necessary. Our construction and estimation bound remain valid as long as the spike ratio t has norm less than one. This is true for any μ outside the $[-2i, 2i]$ line segment in the complex plane. The formulas for t and λ still apply. Take $B = \begin{bmatrix} 0 & 3 \\ -3 & 0 \end{bmatrix}$ as an example. The two eigenvalues of B are $\pm 3i$. If we apply a widely spaced modification governed by matrix B to A , experiments show that \tilde{A} will have two isolated eigenvalues that are approximately $\pm\sqrt{5}i$. One of the two localized eigenvectors is also very close to our construction with $h = [1, i]$ and $t = (\sqrt{5} - 3)i/2$ (the other localized eigenvector is just this one's complex conjugate).

In Theorem 3.3.2, the underlying matrix is the adjacency matrix of an n -node linear chain. Similar conclusions can be drawn when the underlying matrix is the adjacency matrix of an n -node circle. The difference between these two cases are that in the n -node circle case, the $\Delta(\lambda)$ in (3.2.22) has the form

$$\Delta(\lambda) = \begin{bmatrix} \frac{\psi(t, n+r_1-r_M)}{\psi(t, n+r_1-r_M+1)} + \frac{\psi(t, r_2-r_1-1)}{\psi(t, r_2-r_1)} & \frac{\psi(t, 1)}{\psi(t, r_2-r_1)} & 0 & \dots & 0 & \frac{\psi(t, 1)}{\psi(t, n+r_1-r_M+1)} \\ \frac{\psi(t, 1)}{\psi(t, r_2-r_1)} & \frac{\psi(t, r_2-r_1-1)}{\psi(t, r_2-r_1)} + \frac{\psi(t, r_3-r_2-1)}{\psi(t, r_3-r_2)} & \frac{\psi(t, 1)}{\psi(t, r_3-r_2)} & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix},$$

i.e., it has a similar circular structure as the adjacency matrix of an n -node circle.

Repeat the arguments in the proof of Theorem (3.3.2) with this new $\Delta(\lambda)$, and in the same way, we can prove that the λ and x in (3.2.6) and (3.2.1) are within $O(t^L)$ distance of a pair of eigenvalue and eigenvector of the modified matrix.

3.3 Beyond tridiagonal matrices

Let's now turn to some other cases where the original matrix is no longer a tridiagonal matrix.

First, let's consider the case when the original matrix is an n by n symmetric toeplitz matrix $A = \text{Toeplitz}\{0, a_1, \dots, a_q, 0, \dots, 0\}$, i.e., a toeplitz matrix with $(0, a_1, \dots, a_q, 0, \dots, 0)$ as its first row. We apply a rank one modification to A by choosing an index $1 \ll r \ll n$ and changing the (r, r) entry of A from 0 to b , and denote the modified matrix by \tilde{A} . Numerical experiments tell us that with a rank one modification like this, one isolated eigenvalue will appear in \tilde{A} 's spectrum together with a localized eigenvector. Figure 3.4 shows a typical example of the localized eigenvector of a modified toeplitz matrix. In this example,

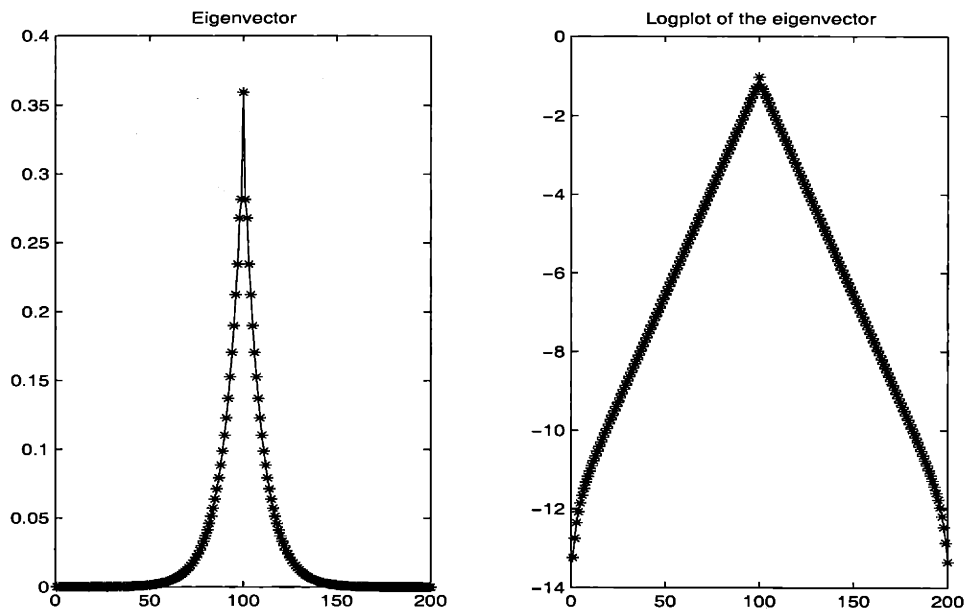


Figure 3.4: Localized eigenvector of a modified toeplitz matrix

the underlying matrix is a 200 by 200 toeplitz matrix $\text{Toeplitz}\{0, 1, 1, 0, \dots, 0\}$, $r = 100$ and $b = 1$. Using MATLAB, we computed the new isolated eigenvalue

to be

$$\lambda = 4.05956284882943. \quad (3.3.1)$$

In figure 3.4, the plot on the left is the plot of the localized eigenvector and the plot on the right is the logplot of that localized eigenvector. Comparing to figure 3.2, we notice here that even though the eigenvector still has the shape of a spike, the spike ratio is no longer a constant near the position of the modification. As it turns out, for $q \geq 2$, the localized eigenvector of a modified symmetric toeplitz matrix of this form is approximately the sum of q different spikes with different weights and different spike ratios.

Take $q = 2$ as an example, and to simplify our discussion, assume our matrix is an infinite matrix with index numbered from $-\infty$ to ∞ (as we will see, if the matrix is finite, by our construction, the boundary terms will be of order t^L or lower, and are of little importance to us). Suppose the infinite matrix A has all ones on the first and second sub-diagonal and super-diagonal, and all zeros on the main diagonal. We apply a unit modification ($b = 1$) on the $(0, 0)$ entry of A , and denote the localized eigenvector and the corresponding eigenvalue of the modified matrix \tilde{A} by x and λ respectively. Based on numerical experiment results, we assume x is the sum of two different spikes both centered at 0. So

$$x_k = c_1 t_1^{|k|} + c_2 t_2^{|k|}, \quad (3.3.2)$$

where t_1 and t_2 are the spike ratios of the two spikes respectively, c_1 and c_2 represent the weights on the two spikes. We normalize x by letting $x_0 = 1$, which is equivalent to

$$c_1 + c_2 = 1. \quad (3.3.3)$$

Now consider the eigenvector equation (3.0.13). When considered entry-wisely, equation (3.0.13) can be written as

$$(Ax)_k = \lambda x_k \quad (3.3.4)$$

for arbitrary integer k . Substituting (3.3.2) into (3.3.4), we get the following three cases corresponding to different values of k (since both Ax and x are symmetric with respect to $k = 0$, we only considered the cases when $k \geq 0$):

1. For $k \geq 2$, we have

$$\begin{aligned} & c_1 t_1^{k-2} + c_2 t_2^{k-2} + c_1 t_1^{k-1} + c_2 t_2^{k-1} + c_1 t_1^{k+1} + c_2 t_2^{k+1} + c_1 t_1^{k+2} + c_2 t_2^{k+2} \\ & = \lambda(c_1 t_1^k + c_2 t_2^k). \end{aligned} \tag{3.3.5}$$

Rewrite (3.3.5) into the following form:

$$c_1 t_1^{k-2}(1 + t_1 + t_1^3 + t_1^4 - \lambda t_1^2) + c_2 t_2^{k-2}(1 + t_2 + t_2^3 + t_2^4 - \lambda t_2^2) = 0. \tag{3.3.6}$$

It is clear that (3.3.6) will be satisfied if

$$1 + t_1 + t_1^3 + t_1^4 - \lambda t_1^2 = 0 \tag{3.3.7}$$

and

$$1 + t_2 + t_2^3 + t_2^4 - \lambda t_2^2 = 0. \tag{3.3.8}$$

2. For $k = 1$, we have

$$c_1 t_1 + c_2 t_2 + 1 + c_1 t_1^2 + c_2 t_2^2 + c_1 t_1^3 + c_2 t_2^3 = \lambda(c_1 t_1 + c_2 t_2). \tag{3.3.9}$$

3. For $k = 0$, we have

$$2(c_1 t_1 + c_2 t_2 + c_1 t_1^2 + c_2 t_2^2) + 1 = \lambda. \tag{3.3.10}$$

These are all the cases. Notice that in order to satisfy them, we need to satisfy the four equations (3.3.7), (3.3.8), (3.3.9) and (3.3.10). Those four equations together with the normality constraint (3.3.3) form a system of five equations.

There are exactly five unknowns here which are λ , t_1 , t_2 , c_1 and c_2 . So this system of equations can be solved. Using MATLAB, we get the following solution to this system:

$$\begin{aligned} \lambda &= 4.05956284889808, & t_1 &= -0.37994846989306, & t_2 &= 0.89676509565825 \\ c_1 &= 0.088390260956474, & c_2 &= 0.91160973904353 \end{aligned} \tag{3.3.11}$$

Comparing with (3.3.1), we can see that the λ we computed here agrees with the numerical experiment results up to ten digits. This shows that our conjecture (3.3.2) about the structure of the localized eigenvector is correct.

Notice that since $|t_2| > |t_1|$, when k is big, $c_2 t_2^k$ will dominate $c_1 t_1^k$. This explains the seemingly single spike appearance in the logplot in figure 3.4.

Now we consider the general case where the underlying matrix A is an infinite symmetric toeplitz matrix with a_1, a_2, \dots, a_q on the first q sub and super diagonals and zero elsewhere. Based on our experiment results, we conjecture that in this case, the localized eigenvector x of \tilde{A} is the sum of q spikes with different weights and spike ratios, i.e.,

$$x_k = \sum_{j=1}^q c_j t_j^{|k|} \tag{3.3.12}$$

with the normality constraint

$$\sum_{j=1}^q c_j = 1. \tag{3.3.13}$$

To see that, let's again consider the entry-wise eigenvector equation (3.3.4). For $k \geq q$, substituting (3.3.12) into (3.3.4), we get

$$\sum_{i=1}^q \sum_{j=1}^q a_i c_j (t_j^{k-i} + t_j^{k+i}) = \lambda \sum_{j=1}^q c_j t_j^k. \tag{3.3.14}$$

Equation (3.3.14) will be satisfied if the following q equations can all be satisfied:

$$\sum_{i=1}^q a_i(t_j^i + t_j^{-i}) - \lambda = 0, \quad (3.3.15)$$

where j varies from 1 to q .

We get q more equations by substituting (3.3.12) into (3.3.4) for $k = 0, 1, \dots, q - 1$.

The $2q$ equations here together with the normality constraint equation (3.3.13) provide us with a system of $2q + 1$ equations. This matches with the number of unknowns we have: $t_1, \dots, t_q, c_1, \dots, c_q, \lambda$. Thus, except some degenerate cases, this system can be solved. This proves that our conjecture about the structure of the localized eigenvector is correct.

Remark 1: Even though the system of equations can be solved numerically given values of (a_1, \dots, a_q) , in general there is no closed form solution since that will involve solving a polynomial equation of degree higher than five.

Remark 2: A vector constructed this way (sum of spikes) is an exact eigenvector when A is an infinite matrix. When A is finite, it will only be an approximation to an actual eigenvector with a residual error of order t^L , where t is the largest of the absolute values of spike ratios.

Now that we know the structure of the localized eigenvector for a single point modification, it is not hard to generalize it to an arbitrary widely spaced modification. Let's consider the infinite symmetric toeplitz matrix $A = \text{Toeplitz}\{0, a_1, \dots, a_q, 0, \dots\}$. Denote the localized eigenvector of A after a single point modification of magnitude b at index r by $x_{r,b}$, assume $x_{r,b}$ is normalized in the sense that the r -th entry of $x_{r,b}$ is 1. From what we have shown, we know that $x_{r,b}$ is the sum of q spikes that are all centered at r . Let the eigenvalue corresponding to $x_{r,b}$ be λ_b and the largest of the absolute values of spike ratios

of $x_{r,b}$ be t_b . Pick M widely spaced indices $r_1 \ll r_2 \ll \dots \ll r_M$. The minimal distance between two adjacent indices, L , satisfies $L \gg q \geq 1$. Modify matrix A at the selected indices by an M by M matrix B to get matrix \tilde{A} . Let μ be a simple eigenvalue of B with corresponding eigenvector h . We will show that when $x = \sum_{i=1}^M h_i x_{r_i, \mu}$, $\|\tilde{A}x - \lambda_\mu x\|$ is of order t_μ^L . Since $|t_\mu| < 1$ and $L \gg 1$, t_μ^L is a very small number. This suggests that (λ_μ, x) is close to a pair of eigenvalue and eigenvector of \tilde{A} .

To see this, notice that for k not equal to one of the selected indices, the entry-wise eigenvector equation (3.3.4) is satisfied exactly by the definition of $x_{r, \mu}$. For k equals to one of the indices r_i , equation (3.3.4) becomes

$$h_i (Ax_{r_i, \mu})_{r_i} + (Bh)_i = \lambda_\mu h_i + O(t_\mu^L). \quad (3.3.16)$$

The $O(t_\mu^L)$ term comes from the other $M - 1$ vectors $x_{r_j, \mu}$ with $j \neq i$, since their contributions at index r_i are all of order t_μ^L . Recall from the definition of h that $(Bh)_i = \mu h_i$. Substituting this into (3.3.16) and cancelling out h_i , we get the following equation

$$(Ax_{r_i, \mu})_{r_i} + \mu = \lambda_\mu + O(t_\mu^L). \quad (3.3.17)$$

By the definition of $x_{r_i, b}$ we know that $(Ax_{r_i, \mu})_{r_i} + \mu = \lambda_\mu$. So (3.3.17) is satisfied up to an error term of $O(t_\mu^L)$. This proved what we wanted to show.

Figure 3.5 shows a localized eigenvector of a modified 400 by 400 toeplitz matrix $A = \text{Toeplitz}\{0, 1, 1, 1, 0, \dots, 0\}$. The modification matrix B is a 3 by 3 random matrix. As we can see, the plot shows clearly three spikes centered at different positions. We also know now that each spike in the figure is a combination of three spikes centered at the same position with different weights and spike ratios.

Let's go back to the single point modification case. Another way to calculate the new isolated eigenvalue is to again use the Fourier transform technique. Without loss of generality, let's assume the magnitude of the modification $b = 1$.

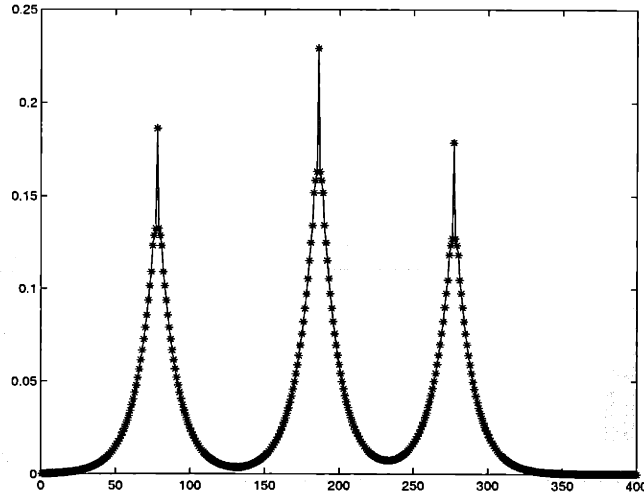


Figure 3.5: Localized eigenvector of a modified Toeplitz matrix with 3 spikes

Let x be an \mathcal{L}^2 -finite eigenvector of the modified matrix \tilde{A} , and let λ be the corresponding eigenvalue.

The eigenvector equation (3.0.13) can be written as

$$\lambda x_n = \sum_{k=1}^q a_k (x_{n-k} + x_{n+k}) + \delta(n)x_n. \quad (3.3.18)$$

Let $f(y)$ be x 's Fourier transform,

$$f(y) = \sum_{n=-\infty}^{\infty} x_n e^{-iny}.$$

Applying Fourier transform to (3.3.18), we get

$$\lambda f(y) = \sum_{k=1}^q a_k f(y) (e^{-iky} + e^{iky}) + x_0, \quad (3.3.19)$$

which is equivalent to

$$f(y) = \frac{x_0}{\lambda - \sum_{k=1}^q a_k (e^{-iky} + e^{iky})}. \quad (3.3.20)$$

Using the inverse Fourier transform formula (3.1.5), and applying it to x_0 , we get

$$x_0 = \frac{1}{2\pi} \int_0^{2\pi} \frac{x_0 dy}{\lambda - \sum_{k=1}^q a_k (e^{-iky} + e^{iky})}. \quad (3.3.21)$$

Note that x_0 can't be zero, otherwise x will be a zero vector by (3.1.5). Cancelling out x_0 and using the substitution $z = e^{iy}$, we get the following integral equation

$$\frac{1}{2\pi i} \int_{S^1} \frac{z^{q-1} dz}{\lambda z^q - \sum_{k=1}^q a_k (z^{q+k} + z^{q-k})} = 1. \quad (3.3.22)$$

The solutions of the integral equation (3.3.22) correspond to the eigenvalues of \tilde{A} whose corresponding eigenvectors are localized.

In general, there is no closed form solution to (3.3.22) for $q \geq 2$. The simplest case is $q = 2$. In this case, the contour integral in (3.3.22) can be computed and (3.3.22) can be simplified to

$$\frac{2}{v\sqrt{v^2 - 2a_1v + a_1^2 - 16a_2^2}} + \frac{2}{v\sqrt{v^2 + 2a_1v + a_1^2 - 16a_2^2}} - 1 = 0, \quad (3.3.23)$$

where $v = \sqrt{4a_2\lambda + a_1^2 + 8a_2^2}$.

This can be further converted to a 6-th order polynomial which does not have a closed form solution. If we apply (3.3.23) to our example with $a_1 = a_2 = 1$, using MATLAB, we find the numerical solution to be $\lambda = 4.05956284889808$, which, not surprisingly, is exactly the same as the solution in (3.3.11).

Another type of structured matrices that we considered is the adjacency matrix of a regular 2D grid. Suppose we have an M by N 2D regular grid G , with an edge connecting node (i, j) with node (k, l) if and only if $i = k$ and $|j - l| = 1$ or $|i - k| = 1$ and $j = l$. The adjacency matrix A is an MN by MN symmetric matrix such that node (i, j) in G is represented by the $((i - 1)N + j)$ -th row and column in A . Numerical experiment tells us that a single point modification, when applied to a node (i, j) with $1 \ll i \ll M$ and

$1 \ll j \ll N$, also produces localized eigenvector which doesn't exist previously. Figure 3.6 shows one example of this. In this example, the dimension of the grid is 30 by 30. A single point modification of magnitude 1 is applied to the node (16, 15) (so for the adjacency matrix A , $A(465, 465)$ was changed from 0 to 1). The 3D-plot is drawn using MATLAB's "surf" function. The eigenvector shown in figure 3.6 corresponds to the largest eigenvalue of the modified matrix \tilde{A} . As we can see, this is a localized eigenvector in the shape of a 2D-spike. From the logplot on the right, it is clear that the spike ratio is no longer a constant.

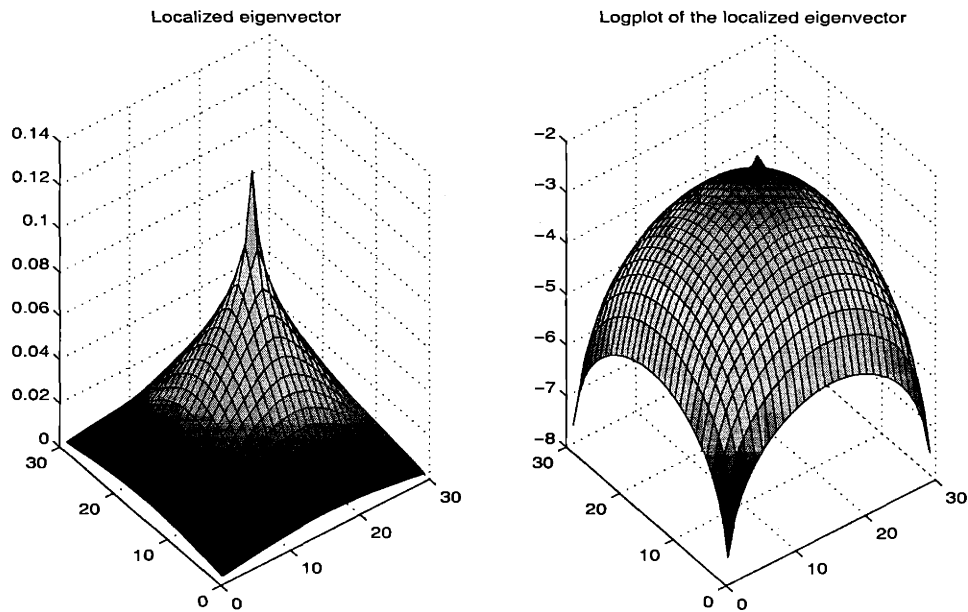


Figure 3.6: Localized eigenvector of the modified adjacency matrix of a 2D grid

For this case, we don't have a conjecture on the structure of the localized eigenvector, but we can still estimate the eigenvalue that corresponds to any localized eigenvector. To do that, we once again use the Fourier transform technique. Consider the case when G is an infinite 2D grid. Define the vector space V_G to be the space of all mappings from nodes of G to \mathbb{R} , and let $u_{i,j}$ be the value of node (i, j) under mapping (vector) u . Note that our previous

way of defining the adjacency matrix for G does not work any more since N is now infinite. So we will use the operator definition of the adjacency matrix of a graph (see for example [1]), i.e., A is seen as an operator that maps V_G to V_G , $Au = v$, such that $v_{i,j}$ is the weighted sum of all $u_{k,l}$'s, where the weight is the weight of the edge connecting node (i, j) to (k, l) . In our case, the weight is either one or zero depending on whether the two nodes are connected or not. Apply a unit modification on G by adding a weight one edge connecting node $(0, 0)$ to itself. Let x be a localized eigenvector of the modified adjacency matrix \tilde{A} with eigenvalue λ . By definition, x and λ satisfies the following difference equation

$$x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1} + \delta(i, j)x_{i,j} = \lambda x_{i,j}, \quad (3.3.24)$$

where $\delta(i, j)$ is a two-variable delta function that equals one if and only if $i = j = 0$ and zero otherwise.

Let $f(y, z)$ be the two dimensional Fourier transform of x , so

$$f(y, z) = \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} x_{k,l} e^{-i(ky+lz)}. \quad (3.3.25)$$

Applying Fourier transform on both sides of (3.3.24), we get

$$f(y, z) = \frac{x_{0,0}}{\lambda - e^{-iy} - e^{iy} - e^{-iz} - e^{iz}}. \quad (3.3.26)$$

Using the inverse 2D Fourier transform formula

$$x_{k,l} = \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} f(y, z) e^{i(yk+zl)} dy dz \quad (3.3.27)$$

on $x_{0,0}$ and cancelling out $x_{0,0}$, we get the following integral equation for the eigenvalue λ :

$$\frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \frac{1}{\lambda - e^{-iy} - e^{iy} - e^{-iz} - e^{iz}} dy dz = 1. \quad (3.3.28)$$

By using the result in (3.1.8), (3.3.28) can be simplified to

$$\frac{1}{2\pi} \int_0^{2\pi} \frac{1}{\sqrt{(\lambda - e^{-iy} - e^{iy})^2 - 4}} dy = 1. \quad (3.3.29)$$

Notice that $e^{iy} + e^{-iy} = 2 \cos y$. Let $u = \cos y$ and we get

$$\frac{1}{\pi} \int_{-1}^1 \frac{du}{\sqrt{(1-u^2)((\lambda-2u)^2-4)}} = 1 \quad (3.3.30)$$

Equation (3.3.30) is an integral equation that involves an elliptic integral which in general does not have a closed form solution. Using the software package PARI/GP (see [2]), we are able to calculate numerically the integral in (3.3.29). A plot of the integral is shown in figure 3.7. The dashed horizontal line in

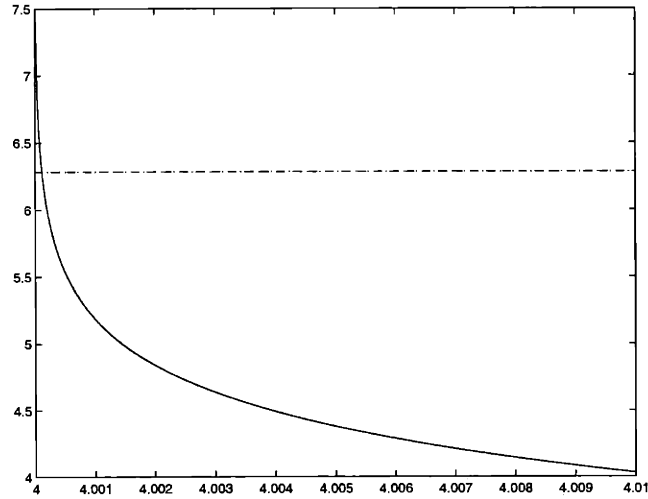


Figure 3.7: Plot of the integral in (3.3.29)

figure 3.7 is the $y = 2\pi$ line whose intersection with the main curve is the solution to (3.3.29). Using PARI/GP, we calculated the solution to be $\lambda = 4.00011576954677619$.

From the numerical result of the integral in (3.3.20), we can also extrapolate out the special eigenvalue corresponding to each magnitude of modifications. Figure 3.8 shows a plot of their relationship.

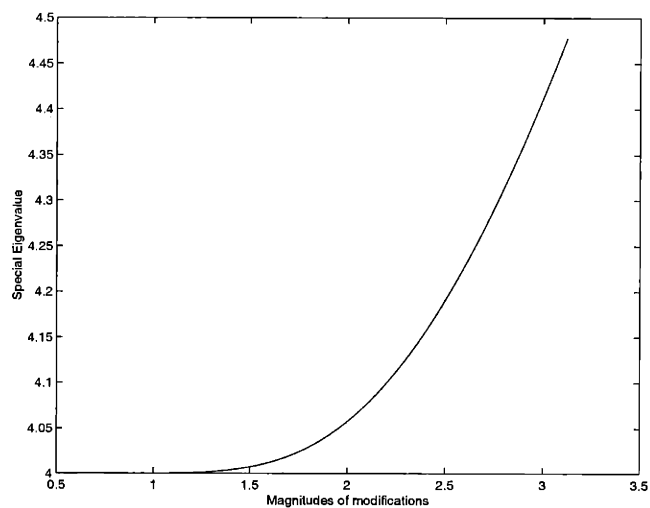


Figure 3.8: Localized eigenvalue of an infinite 2D grid under different magnitudes of modifications

Similar reasonings also apply to the adjacency matrix of higher-dimensional grids or other types of structured regular graphs. In all the cases we investigated, with widely spaced modifications, new localized eigenvectors appear. But in general there is no closed form solution for the special eigenvalues corresponding to those localized eigenvectors.

References

- [1] F. Chung, *Spectral Graph Theory*, CBMS Conference Series 92, American Math. Soc., Providence, 1997.
- [2] H. Cohen and K. Belabas, PARI-GP Software. <http://www.parigp-home.de>.
- [3] A. Edelman, H. Eriksson, and G. Strang, The eigenvalues for a cycle plus a random cycle. In preparation.
- [4] A. Figa-Talamanca, *Harmonic analysis and representation theory for groups acting on homogeneous trees*. Cambridge University Press, Cambridge, 1991.
- [5] C.D. Godsil, *Algebraic combinatorics*. Chapman and Hall, New York and London, 1993.
- [6] I. Gutman, Characteristic and matching polynomials of some compound graphs. *Publ. Inst. Math. Beograd* **27 (41)**:61–66, 1980.
- [7] O. J. Heilmann and E. H. Lieb, Theory of monomer-dimer systems. *Comm. Math. Phys.* **25**:190–232, 1972.
- [8] C.R. Johnson and A. Leal Duarte, The maximum multiplicity of an eigenvalue in a matrix whose graph is a tree. *Linear and Multilinear Algebra*, **46**:139–144, 1999.
- [9] L. He, X. Liu and G. Strang, Trees with Cantor eigenvalue distribution. Submitted to *Journal of Combinatorial Theory*.
- [10] L. He, X. Liu and G. Strang, Laplacian eigenvalues of growing trees. *Proc. Conf. on Math. Theory of Networks and Systems*, Perpignan (2000).

- [11] B. McKay, On the spectral characterisation of trees. *Combinatorica*, **3**:219–232, 1977.
- [12] G. Strang, *Introduction to Linear Algebra*. Wellesley-Cambridge Press, Wellesley, 1993.
- [13] G. Strang, X. Liu and S. Ott, Localized eigenvectors from widely spaced matrix modifications. In preparation.
- [14] S. Strogatz, Exploring complex networks. *Nature*, **410**: 268–276, 2001.
- [15] D. Watts, *Small Worlds: The Dynamics of Networks Between Order and Randomness*. Princeton University Press, Princeton, 1999.
- [16] D. Watts and S. Strogatz, Collective dynamics of ‘small-world’ networks. *Nature*, **393**:440–442, 1998.