Mysteries around the graph Laplacian eigenvalue 4

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Abstract

We describe our current understanding on the phase transition phenomenon associated with the graph Laplacian eigenvalue $\lambda = 4$ on trees: eigenvectors for $\lambda < 4$ oscillate *semi-globally* while those for $\lambda > 4$ are *concentrated* around junctions. For starlike trees, we obtain a complete understanding of this phenomenon. For general graphs, we prove the number of $\lambda > 4$ is bounded from above by the number of vertices with degrees higher than 2; and if a graph contains a branching path, then the eigencomponents for $\lambda > 4$ decay exponentially from the branching vertex toward the leaf.

Keywords: graph Laplacian; localization of eigenvectors; phase transition phenomena; starlike trees; dendritic trees; Gerschgorin's disks
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1. Introduction

In our previous report [11], we proposed a method to characterize dendrites of neurons, more specifically retinal ganglion cells (RGCs) of a mouse, and cluster them into different cell types using their morphological features, which are derived from the eigenvalues of the graph Laplacians when such dendrites are represented as graphs (in fact literally as "trees"). For the details on the data acquisition and the conversion of dendrites to graphs, see [11] and the references therein. While analyzing the eigenvalues and eigenvectors of those graph Laplacians, we observed a very peculiar *phase transition phenomenon* as shown in Figure 1.1. The

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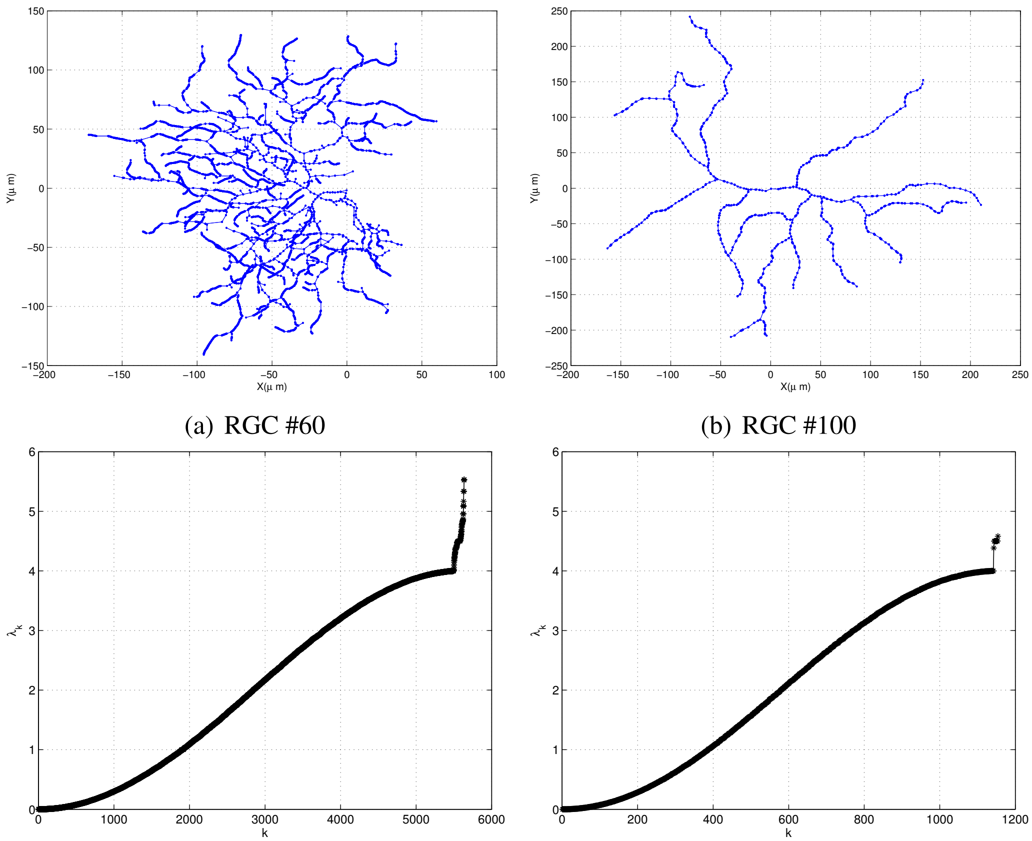
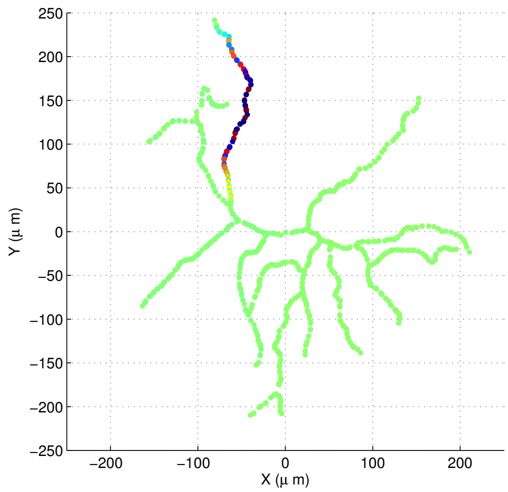


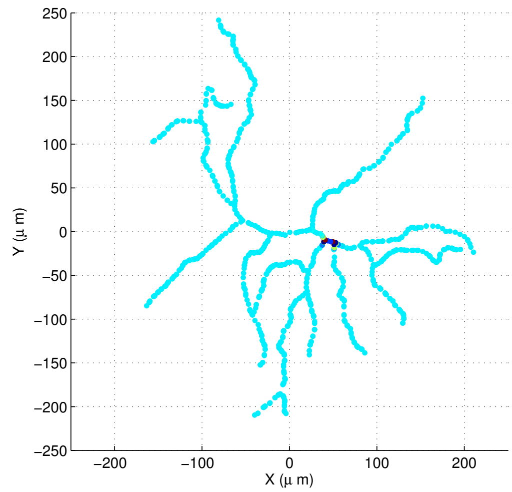
(a) RGC #60 (b) RGC #100

(c) Eigenvalues of (a) (d) Eigenvalues of (b)

Figure 1.1: Typical dendrites of Retinal Ganglion Cells (RGCs) of a mouse and the graph Laplacian eigenvalue distributions. (a) 2D projection of dendrites of an RGC of a mouse; (b) that of another RGC revealing different morphology; (c) the eigenvalue distribution of the RGC shown in (a); (d) that of the RGC shown in (b). Regardless of their morphological features, a phase transition occurs at the eigenvalue 4.



(a) RGC #100; $\lambda_{1141} = 3.9994$



(b) RGC #100; $\lambda_{1142} = 4.3829$

Figure 1.2: The graph Laplacian eigenvectors of RGC #100. (a) The one corresponding to the eigenvalue $\lambda_{1141} = 3.9994$, immediately below the value 4; (b) the one corresponding to the eigenvalue $\lambda_{1142} = 4.3829$, immediately above the value 4.

eigenvalue distribution for each dendritic tree is a smooth bell-shaped curve starting from the eigenvalue 0 up to 4. Then, at the eigenvalue 4, there is a sudden jump as shown in Figure 1.1(c, d). Interestingly, the eigenvectors corresponding to the eigenvalues below 4 are *semi-global* oscillations (like Fourier cosines/sines) over the entire dendrites or one of the dendrite arbors (or branches); on the other hand, those corresponding to the eigenvalues above 4 are much more *localized* and *concentrated* (like wavelets) around junctions/branching vertices, as shown in Figure 1.2.

We want to answer the following questions:

Q1 Why does such a phase transition phenomenon occur?

Q2 What is the significance of the eigenvalue 4?

Q3 Is there any tree that possesses an eigenvalue exactly equal to 4?

Q4 What about more general graphs that possess eigenvalues exactly equal to 4?

As for Q1 and Q2, which are closely related, we have a complete answer for a specific and simple class of trees called *starlike trees* as described in Section 3,

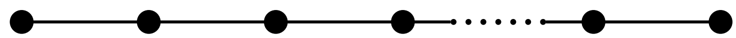


Figure 2.3: A path graph P_n provides a simple yet important example.

and a partial answer for more general trees and graphs such as those representing neuronal dendrites, which we discuss in Section 4. For Q3, we identify two classes of trees that have an eigenvalue exactly equal to 4, which is necessarily a simple eigenvalue, in Section 5.

In Section 6, we will prove that the existence of a long path between two subgraphs implies that the eigenvalues of either of the subgraphs that are larger than 4 are actually very close to some eigenvalues of the whole graph. Then, in Section 7, we will give a counterexample to the conjecture that the largest component in the eigenvector corresponding to the largest eigenvalue (which is larger than 4) lies on the vertex of the highest degree. Finally, we describe our investigation on Q4 in Section 8. But let us first start by fixing our notation and reviewing the basics of graph Laplacians in Section 2.

2. Definitions and Notation

Let $G = (V, E)$ be a graph where $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ is a set of vertices in G and $E = E(G) = \{e_1, e_2, \ldots, e_m\}$ is a set of edges where e_k connects two vertices v_i, v_j for some $1 \le i, j \le n$, and we write $e_k = (v_i, v_j)$. Let $d_k = d(v_k)$ be the degree of the vertex v_k. If a graph G is a *tree*, i.e., a connected graph without cycles, then it has $m = n - 1$ edges. Let $L(G) := D(G) - A(G)$ be the *Laplacian matrix* where $D(G) := \operatorname{diag}(d_1, \ldots, d_n)$ is called the *degree matrix* of G, i.e., the diagonal matrix of vertex degrees, and $A(G) = (a_{ij})$ is the *adjacency matrix* of G, i.e., $a_{ij} = 1$ if v_i and v_j are adjacent; otherwise it is 0. Furthermore, let $0 = \lambda_0(G) \le \lambda_1(G) \le \cdots \le \lambda_{n-1}(G)$ be the eigenvalues of $L(G)$, and $m_G(\lambda)$ be the multiplicity of the eigenvalue λ. More generally, if $I \subset \mathbb{R}$ is an interval of the real line, then we define $m_G(I) := \#\{\lambda_k(G) \in I\}$.

At this point we would like to give a simple yet important example of a tree and its graph Laplacian: a *path* graph P_n consisting of n vertices shown in Figure 2.3. The graph Laplacian of such a path graph can be easily obtained and is instructive.

$$
\underbrace{\begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{bmatrix}}_{L(G)} = \underbrace{\begin{bmatrix} 1 & & & & \\ & 2 & & & \\ & & \ddots & & \\ & & & 2 & \\ & & & & 1 \end{bmatrix}}_{D(G)} - \underbrace{\begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ & & & 1 & 0 \end{bmatrix}}_{A(G)}.
$$

The eigenvectors of this matrix are nothing but the *DCT Type II* basis vectors used for the JPEG image compression standard; see e.g., [14]. In fact, we have

$$
\lambda_k = 4\sin^2\left(\frac{\pi k}{2n}\right); \tag{2.1}
$$

$$
\phi_{j,k} = \cos\left(\frac{\pi k}{n}\left(j - \frac{1}{2}\right)\right), \quad j = 1, \ldots, n \tag{2.2}
$$

for $k = 0, 1, \ldots, n-1$, where $\boldsymbol{\phi}_k = (\phi_{1,k}, \cdots, \phi_{n,k})^{\mathsf{T}}$ is the eigenvector corresponding to λ_k. From these, it is clear that for any finite $n \in \mathbb{N}$, $\lambda_{\max} = \lambda_{n-1} < 4$, and no localization/concentration occurs in the eigenvector $\boldsymbol{\phi}_{n-1}$ (or any eigenvector), which is simply a global oscillation with the highest possible (i.e., the Nyquist) frequency, i.e., $\boldsymbol{\phi}_{n-1} = \left((-1)^{j-1}\sin\left(\frac{\pi}{n}\left(j - \frac{1}{2}\right)\right)\right)^{\mathsf{T}}_{1 \le j \le n}$.

3. Analysis of Starlike Trees

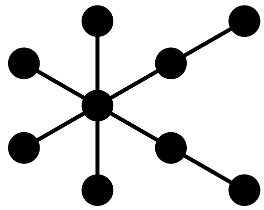
As one can imagine, analyzing this phase transition phenomenon for complicated dendritic trees turns out to be rather formidable. Hence, we start our analysis on a simpler class of trees called *starlike trees*. A starlike tree is a tree that has exactly one vertex of degree higher than 2. Examples are shown in Figure 3.4.

We use the following notation. Let $S(n_1, n_2, \ldots, n_k)$ be a starlike tree that has $k(\geq 3)$ paths (i.e., branches) emanating from the central vertex v_1. Let the ith branch have n_i vertices excluding v_1. Let $n_1 \geq n_2 \geq \cdots \geq n_k$. Hence, the total number of vertices is $n = 1 + \sum_{i=1}^{k} n_i$.

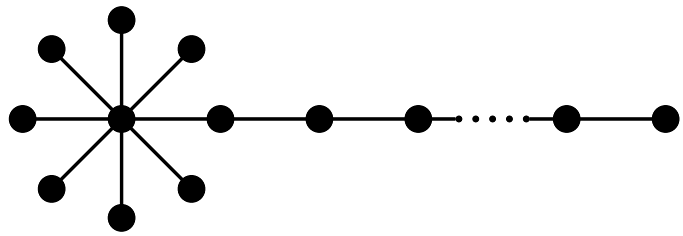
Das proved the following results for a starlike tree $S(n_1, \ldots, n_k)$ in [3]:

$$
\lambda_{\max} = \lambda_{n-1} < k + 1 + \frac{1}{k-1};
$$

$$
2 + 2\cos\left(\frac{2\pi}{2n_k + 1}\right) \leq \lambda_{n-2} \leq 2 + 2\cos\left(\frac{2\pi}{2n_1 + 1}\right). \tag{3.3}
$$



(a) $S(2, 2, 1, 1, 1, 1)$



(b) $S(n_1, 1, 1, 1, 1, 1, 1, 1)$ a.k.a. comet

Figure 3.4: Typical examples of a starlike tree.

On the other hand, Grone and Merris [7] proved the following lower bound for a general graph G with at least one edge:

$$\lambda_{\max} \geq \max_{1 \leq j \leq n} d(v_j) + 1. \tag{3.4}$$

Hence we have the following

Corollary 3.1. *A starlike tree has exactly one graph Laplacian eigenvalue greater than or equal to 4. The equality holds if and only if the starlike tree is* $K_{1,3} = S(1, 1, 1)$*, which is also known as a* claw.

Proof. The first statement is easy to show. The lower bound in (3.4) is larger than or equal to 4 for any starlike tree since $\max_{1 \leq j \leq n} d(v_j) = d(v_1) \geq 3$. On the other hand, the second largest eigenvalue λ_{n-2} is clearly strictly smaller than 4 due to (3.3).

To prove the second statement about the necessary condition on the equality (the sufficiency is easily verified), first note that by (3.4), $d(v_1) = 3$ is a necessary condition for $\lambda_{\max} = 4$. Let d_1 denote the highest degree of such a starlike tree, i.e., $d_1 = d(v_1)$. Since we only consider starlike trees, the second highest degree d_2 must be either 2 or 1. Now, we use the following

Theorem 3.1 (Das 2004, [4])**.** *Let* $G = (V, E)$ *be a connected graph and* $d_1 \neq d_2$ *where* d_1 *and* d_2 *are the highest and the second highest degree, respectively. Then,* $\lambda_{\max}(G) = d_1 + d_2$ *if and only if* G *is a star graph.*

If $\lambda_{\max}(G) = 4$ and $d_1 = 3$, then using this theorem, we must have $d_2 = 1$. Hence, G must be a star graph with $d_1 = 3$ and $d_2 = 1$, i.e., $G = K_{1,3}$. □

As for the concentration/localization of the eigenvector $\boldsymbol{\phi}_{n-1}$ corresponding to the largest eigenvalue λ_{n-1}, we prove the following

Theorem 3.2. *Let* $\boldsymbol{\phi}_{n-1} = (\phi_{1,n-1}, \cdots, \phi_{n,n-1})^{\mathsf{T}}$*, where* $\phi_{j,n-1}$ *is the value of the eigenvector corresponding to the largest eigenvalue* λ_{n-1} *at the vertex* v_j*,* $j = 1, \ldots, n$*. Then, the absolute value of this eigenvector at the central vertex* v_1 *cannot be exceeded by those at the other vertices, i.e.,*

$$|\phi_{1,n-1}| > |\phi_{j,n-1}|, \quad j = 2, \ldots, n.$$

To prove this theorem, we use the following lemma, which is simply a corollary of Gerschgorin's theorem [15, Theorem 1.1]:

Lemma 3.1. *Let* A *be a square matrix of size* $n \times n$*,* $\lambda_k(A)$ *be any eigenvalue of* A*, and* $\boldsymbol{\phi}_k = (\phi_{1,k}, \ldots, \phi_{n,k})^{\mathsf{T}}$ *be the corresponding eigenvector. Let* k^* *denote the index of the largest eigenvector component in* $\boldsymbol{\phi}_k$*, i.e.,* $\left|\phi_{k^*,k}\right| = \max_{j\in N}\left|\phi_{j,k}\right|$ *where* $N := \{1, \ldots, n\}$*. Then, we must have* $\lambda_k(A) \in \Gamma_{k^*}(A)$*, where* $\Gamma_i(A) := \left\{z \in \mathbb{C} : |z - a_{ii}| \leq \sum_{j\in N\setminus\{i\}} |a_{ij}|\right\}$ *is the ith Gerschgorin disk of* A*. In other words, for the index of the largest eigenvector component, the corresponding Gerschgorin disk must contain the eigenvalue.*

Proof. Recall the proof of Gerschgorin's theorem. The k^*th row of $A\boldsymbol{\phi}_k = \lambda_k\boldsymbol{\phi}_k$ yields

$$|\lambda_k - a_{k^*k^*}| \leq \sum_{j\in N\setminus\{k^*\}} \left|a_{k^*j}\right| \frac{\left|\phi_{j,k}\right|}{\left|\phi_{k^*,k}\right|} \leq \sum_{j\in N\setminus\{k^*\}} \left|a_{k^*j}\right|.$$

This implies $\lambda_k \in \Gamma_{k^*}(A)$, which proves the lemma. □

Proof of Theorem 3.2. First of all, by Corollary 3.1 we have $\lambda_{n-1} \geq 4$. However, $\lambda_{n-1} = 4$ happens only for $K_{1,3}$. In that case, it is easy to see that this theorem holds by directly examining the eigenvector $\boldsymbol{\phi}_{n-1} = \boldsymbol{\phi}_3 \propto (3, -1, -1, -1)^{\mathsf{T}}$. Hence, let us examine the case $\lambda_{n-1} > 4$. In this case, Lemma 3.1 indicates $4 < \lambda_{n-1} \in \Gamma_{(n-1)^*}(L)$ where $(n-1)^* \in N$ is the index of the largest component in $\boldsymbol{\phi}_{n-1}$. Now, note that the disk $\Gamma_i(L)$ for any vertex v_i that has degree 2 is $\{z \in \mathbb{C} : |z - 2| \leq 2\}$ (and $\{z \in \mathbb{C} : |z - 1| \leq 1\}$ for a degree 1 vertex). This means that the Gerschgorin disk $\Gamma_{(n-1)^*}$ containing the eigenvalue $\lambda_{n-1} > 4$ cannot be in the union of the Gerschgorin disks corresponding to the vertices whose degrees are 2 or lower. Hence the index of the largest eigenvector component in $\boldsymbol{\phi}_{n-1}$ must correspond to an index for which the vertex has degree 3 or higher. In our starlike-tree case, there is only one such vertex, v_1, i.e., $(n-1)^* = 1$. □

For different proofs without using Gerschgorin's theorem, see Das [3, Lemma 4.2] and E. Woei's dissertation [16]. We note that our proof using Gerschgorin's disks is more powerful than those other proofs and can be used for more general situations than the starlike trees as we will see in Section 4.

REMARK **3.1.** *Let $\boldsymbol{\phi} = (\phi_1, \phi_2, \dots, \phi_n)^{\mathsf{T}}$ be an eigenvector of a starlike tree $S(n_1, \dots, n_k)$ corresponding to the Laplacian eigenvalue λ. Without loss of generality, let $v_2, \dots, v_{n_1+1}$ be the n_1 vertices along a branch emanating from the central vertex v_1 with v_{n_1+1} being the leaf (or pendant) vertex. Then, along this branch, the eigenvector components satisfy the following equations:*

$$\begin{aligned} \lambda\phi_{n_1+1} &= \phi_{n_1+1} - \phi_{n_1}, && (3.5) \\ \lambda\phi_j &= 2\phi_j - \phi_{j-1} - \phi_{j+1} \quad 2 \le j \le n_1. && (3.6) \end{aligned}$$

From Eq. (3.6)*, we have the following recursion relation:*

$$\phi_{j+1} + (\lambda - 2)\phi_j + \phi_{j-1} = 0, \quad j = 2, \dots, n_1.$$

This recursion can be explicitly solved using the roots of the characteristic equation

$$r^2 + (\lambda - 2)r + 1 = 0, \tag{3.7}$$

and when (3.7) *has distinct roots r_1, r_2, the general solution can be written as*

$$\phi_j = Ar_1^{j-2} + Br_2^{j-2}, \quad j = 2, \dots, n_1 + 1, \tag{3.8}$$

where A, B are appropriate constants derived from the boundary condition (3.5)*. Now, let us consider these roots of* (3.7) *in detail. The discriminant of* (3.7) *is*

$$\mathcal{D}(\lambda) := (\lambda - 2)^2 - 4 = \lambda(\lambda - 4).$$

Since we know that $\lambda \ge 0$, this discriminant changes its sign depending on $\lambda < 4$ or $\lambda > 4$. (Note that $\lambda = 4$ occurs only for the claw $K_{1,3}$ on which we explicitly know everything; hence we will not discuss this case further in this remark.) If $\lambda < 4$, then $\mathcal{D}(\lambda) < 0$ and it is easy to show that the roots are complex valued with magnitude 1. This implies that (3.8) *becomes*

$$\phi_j = A' \cos(\omega(j - 2)) + B' \sin(\omega(j - 2)), \quad j = 2, \dots, n_1 + 1,$$

where ω satisfies $\tan\omega = \sqrt{\lambda(4 - \lambda)}/(2 - \lambda)$, and A', B' are appropriate constants. In other words, if $\lambda < 4$, the eigenvector along this branch is of oscillatory nature. On the other hand, if $\lambda > 4$, then $\mathcal{D}(\lambda) > 0$ and it is easy to show that both r_1 and r_2 are real valued with $-1 < r_1 = \left(2 - \lambda + \sqrt{\lambda(\lambda - 4)}\right)/2 < 0$ while

$r_2 = \left(2 - \lambda - \sqrt{\lambda(\lambda-4)}\right)/2 < -1$. *On the surface, the term* Br_2^{j-2} *looks like a dominating part in* (3.8)*; however, we see from* (3.5) *that* $|\phi_{n_1}| > |\phi_{n_1+1}|$*, which means the real dominating part in* (3.8) *for* $j = 2, \ldots, n_1 + 1$ *is the term* Ar_1^{j-2}*. Hence we conclude that* $|\phi_j|$ *decays exponentially with* j*, that is, the eigenvector component decays rapidly towards the leaves. The siuation is the same for the other branches.*

In summary, we have shown that a starlike tree has only one eigenvalue ≥ 4, and its eigenvector is localized at the central vertex in the sense of Theorem 3.1. Furthermore, the other eigenvectors are of oscillatory nature. Therefore the phase transition phenomenon for a starlike tree (with the eigenvalue 4 as its threshold) is completely understood.

4. The Localization Phenomena on General Graphs

Unfortunately, actual dendritic trees are not exactly starlike. However, our numerical computations and data analysis on totally 179 RGCs indicate that:

$$0 \leq \frac{\#\{j \in N \mid d(v_j) > 2\} - m_G([4, \infty))}{n} \leq 0.047$$

for each RGC. Hence, we can define the *starlikeliness* $S\ell(T)$ of a given tree T as

$$S\ell(T) := 1 - \frac{\#\{j \in N \mid d(v_j) > 2\} - m_T([4, \infty))}{n}$$

We note that $S\ell(T) \equiv 1$ for a certain class of RGCs whose dendrites are sparsely spread (see [11] for the characterization). This means that dendrites in that class are all close to a starlike tree or a concatenation of several starlike trees. We show some examples of dendritic trees with $S\ell(T) \equiv 1$ and with $S\ell(T) < 1$ in Figure 4.5.

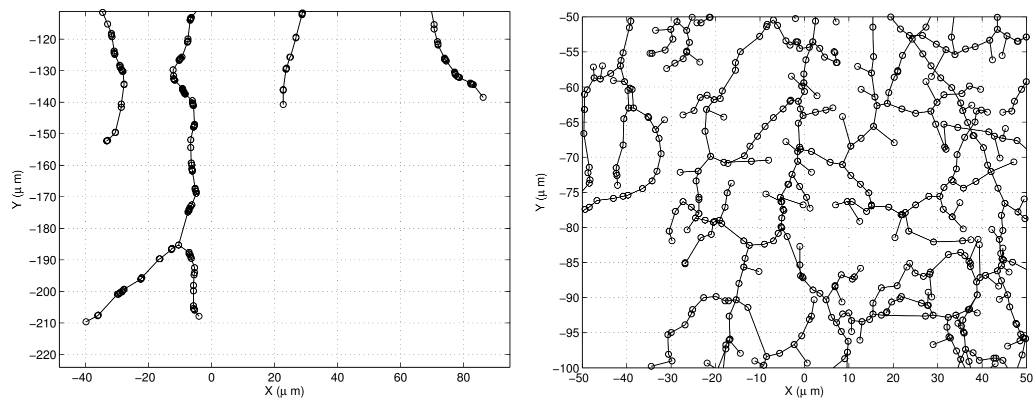
The above observation has led us to prove the following

Theorem 4.1. *For any graph* G *of finite volume, i.e.,* $\sum_{j=1}^{n} d(v_j) < \infty$*, we have*

$$0 \leq m_G([4, \infty)) \leq \#\{j \in N \mid d(v_j) > 2\}$$

and each eigenvector corresponding to $\lambda \geq 4$ *has its largest component (in absolute value) on the vertex whose degree is higher than 2.*

We refer the interested readers to [10, Sec. 2] that reviews various relationships between the multiplicity of certain eigenvalues and the graph structural properties different from our Theorem 4.1.



(a) RGC #100; $S\ell(T) \equiv 1$

(b) RGC #155; $S\ell(T) = 0.953 < 1$

Figure 4.5: Zoomed-up versions of parts of some dendritic trees.

Proof. The second statement follows from Lemma 3.1, because the Gerschgorin disks corresponding to vertices of degree 1 or 2 do not include $\lambda > 4$.

We next prove the first statement. Let L be a Laplacian matrix of G. We can apply a permutation P such that

$$P^{\mathsf{T}} L P = \begin{bmatrix} L_1 & E^{\mathsf{T}} \\ E & L_2 \end{bmatrix}, \tag{4.9}$$

where the diagonals of L_1 are 3 or larger (correspond to vertices of degree > 2), and the diagonals of L_2 are 2 or 1. Suppose L_2 is ℓ-by-ℓ. By Gerschgorin's theorem all the eigenvalues of L_2 must be 4 or below.

In fact, we can prove the eigenvalues of L_2 are strictly below 4. By [15, Theorem 1.12], for an irreducible matrix (a Laplacian of a connected graph is irreducible) an eigenvalue can exist on the boundary of the union of the Gerschgorin disks only if it is the boundary of *all* the disks. Furthermore, if there is such an eigenvalue, then the corresponding eigenvector has the property that all its components have the same absolute value.

Suppose on the contrary that $L_2 \boldsymbol{x} = 4\boldsymbol{x}$. Suppose without loss of generality that L_2 is irreducible; if not, we can apply a permutation so that $P L_2 P^{\mathsf{T}}$ is block diagonal and treat each block separately.

Now if L_2 has a diagonal 1, then the corresponding Gerschgorin disk lies on $[0, 2]$, which does not pass 4. Hence by [15, Theorem 1.12] this case is ruled out. It follows that all the diagonals of L_2 are 2, and the sum of the absolute values of the rows of L_2 are all 4 (this happens only if L_2 is disjoint from L_1). So we need $\ell \geq 3$ (for example when $\ell = 3$, $L_2 = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}$). Now the ith ($1 \leq i \leq \ell$) row of $L_2\boldsymbol{x} = 4\boldsymbol{x}$ and the fact $|x_1| = |x_2| = \cdots = |x_\ell|$ force $x_i = -x_j$ for all $j \neq i$. This needs to hold for all i, which clearly cannot happen for $\ell \geq 3$. Therefore the eigenvalues of L_2 must be strictly below 4.

By the min-max characterization of the eigenvalues of $P^\mathsf{T}LP$, denoting by $\lambda_\ell(P^\mathsf{T}LP)$ the ℓth smallest eigenvalue, we have

$$\lambda_\ell(P^\mathsf{T}LP) = \min_{\dim S = \ell} \max_{\boldsymbol{y} \in \mathrm{span}(S), \|\boldsymbol{y}\|_2 = 1} \boldsymbol{y}^\mathsf{T}(P^\mathsf{T}LP)\boldsymbol{y}.$$

Hence letting S_0 be the last ℓ column vectors of the identity I_n and noting $S_0^\mathsf{T}P^\mathsf{T}LPS_0 = L_2$, we have

$$\begin{aligned} \lambda_\ell(P^\mathsf{T}LP) \leq \max_{\boldsymbol{y} \in S_0, \|\boldsymbol{y}\|_2 = 1} \boldsymbol{y}^\mathsf{T}(P^\mathsf{T}LP)\boldsymbol{y} &= \lambda_{\max}(S_0^\mathsf{T}P^\mathsf{T}LPS_0) \\ &= \lambda_{\max}(L_2). \end{aligned}$$

Since $\lambda_{\max}(L_2) < 4$, we conclude that $P^\mathsf{T}LP$ (and hence L) has at least ℓ eigenvalues smaller than 4, i.e., $m_G([0,4)) \geq \ell$. Hence, $m_G([4,\infty)) = n - m_G([0,4)) \leq n - \ell = \#\{j \in N \mid d(v_j) > 2\}$, which proves the first statement. □

To give a further explanation for the eigenvector localization behavior observed in Introduction, we next show that eigenvector components of $\lambda > 4$ must decay exponentially along a branching path.

Theorem 4.2. *Suppose that a graph G has a branch that consists of a path of length k, whose indices are $\{i_1, i_2, \ldots, i_k\}$ where i_1 is connected to the rest of the graph and i_k is the leaf of that branch. Then for any eigenvalue λ greater than 4, the corresponding eigenvector $\boldsymbol{\phi} = (\phi_1, \cdots, \phi_n)^\mathsf{T}$ satisfies*

$$|\phi_{i_{j+1}}| \leq \gamma |\phi_{i_j}| \quad \textit{for } j = 1, 2, \ldots, k-1, \tag{4.10}$$

where

$$\gamma := \frac{2}{\lambda - 2} < 1. \tag{4.11}$$

Hence $|\phi_{i_j}| \leq \gamma^{j-1}|\phi_{i_1}|$ for $j = 1, \ldots, k$, that is, the magnitude of the components of an eigenvector corresponding to any $\lambda > 4$ along such a branch decays exponentially toward its leaf with rate at least γ.

Proof. There exists a permutation P such that

$$\widehat{L} := P^{\mathsf{T}} L P = \begin{bmatrix} L_1 & E^{\mathsf{T}} \\ E & L_2 \end{bmatrix},$$

where

$$L_2 = \begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix} \in \mathbb{R}^{k \times k}$$

and E has a -1 in the top-right corner and 0 elsewhere. The diagonals of L_2 correspond to the vertices $v_{i_1}, \ldots, v_{i_k}$ of the branch under consideration.

Let $L\boldsymbol{\phi} = \lambda\boldsymbol{\phi}$ with $\lambda > 4$. We have $\widehat{L}\boldsymbol{y} = \lambda\boldsymbol{y}$ where $\boldsymbol{y} = (y_1, y_2, \cdots, y_n)^{\mathsf{T}} = P^{\mathsf{T}}\boldsymbol{\phi}$. Note that $(y_{n-k+1}, y_{n-k+2}, \cdots, y_n) = (\phi_{i_1}, \phi_{i_2}, \ldots, \phi_{i_k})$. The last row of $\widehat{L}\boldsymbol{y} = \lambda\boldsymbol{y}$ gives

$$-y_{n-1} + y_n = \lambda y_n,$$

hence

$$|y_n| = \frac{1}{\lambda - 1}|y_{n-1}| \leq \gamma |y_{n-1}|. \tag{4.12}$$

The $(n-1)$st row of $\widehat{L}\boldsymbol{y} = \lambda\boldsymbol{y}$ gives

$$-y_{n-2} + 2y_{n-1} - y_n = \lambda y_{n-1}.$$

Using $|y_n| \leq |y_{n-1}|$ we get

$$|y_{n-1}| = \frac{|y_{n-2} + y_n|}{\lambda - 2} \leq \frac{|y_{n-2}| + |y_{n-1}|}{\lambda - 2}, \tag{4.13}$$

from which we get $|y_{n-1}| \leq |y_{n-2}|$. Therefore $|y_n| \leq |y_{n-1}| \leq |y_{n-2}|$, and so

$$|y_{n-1}| = \frac{|y_{n-2} + y_n|}{\lambda - 2} \leq \frac{2|y_{n-2}|}{\lambda - 2} = \gamma |y_{n-2}|.$$

Repeating this argument $k - 1$ times we obtain (4.10). □

We note that the inequalities (4.12) and (4.13) include considerable overestimates, and tighter bounds can be obtained at the cost of simplicity. Hence in practice the decay rate is much smaller than γ defined in (4.11). We also note that the larger the eigenvalue $\lambda > 4$, the smaller the decay rate γ is, i.e., the faster the amplitude decays along the branching path.

Also note that the above result holds for any branching path of a tree. In particular, if a tree has k branches consisting of paths, they must all have the exponential decay in eigenvector components if $\lambda > 4$. This gives a partial explanation for the eigenvector localization behavior observed in Introduction. However, the theorem cannot compare the eigenvector components corresponding to branches emanating from different vertices of degrees higher than 2, so a complete explanation remains an open problem.

Remark **4.1.** *Let us briefly consider the case $\lambda = 4$. In this case we have $\gamma = \frac{2}{\lambda-2} = 1$, suggesting the corresponding eigenvector components along a branching path may not decay. However, we can still prove that unless $\phi_{i_1} = \phi_{i_2} = \cdots = \phi_{i_k} = 0$, we must have*

$$|\phi_{i_k}| < |\phi_{i_{k-1}}| < \cdots < |\phi_{i_1}|. \tag{4.14}$$

In other words, the eigenvector components must decay along the branch, although not necessarily exponentially. To see this, we first note that if $y_n = 0$, then the last row of $\widehat{L}\boldsymbol{y} = \lambda\boldsymbol{y}$ forces $y_{n-1} = 0$. Then, $y_n = y_{n-1} = 0$ together with the $(n-1)$st row gives $y_{n-2} = 0$. Repeating this argument we conclude that y_j must be zero for all $j = n-k+1, \ldots, n$. Now suppose that $|y_n| > 0$. Following the above arguments we see that the inequality in (4.12) *with $\gamma = 1$ must be strict, that is, $|y_n| < |y_{n-1}|$. Using this we see that the inequality in* (4.13) *must also be strict, hence $|y_{n-1}| < |y_{n-2}|$. Repeating this argument proves* (4.14).

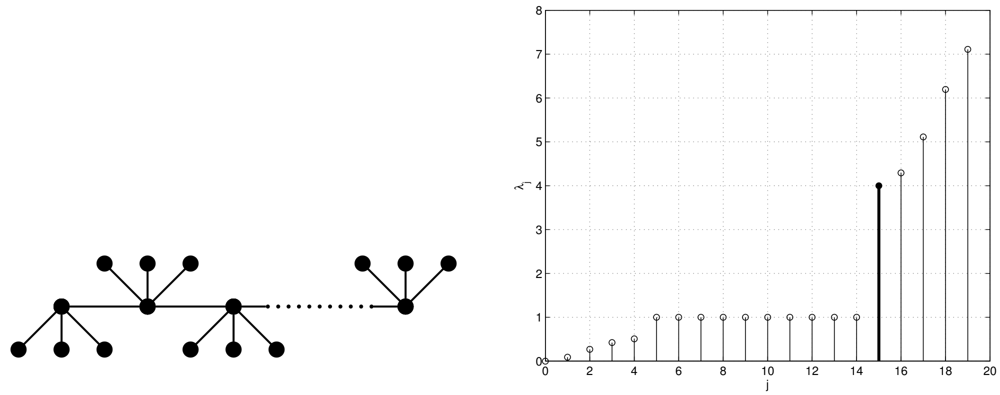
5. A Class of Trees Having the Eigenvalue 4

As raised in Introduction, we are interested in answering Q3: Is there any tree that possesses an eigenvalue exactly equal to 4? To answer this question, we use the following result of Guo [9] (written in our own notation).

Theorem 5.1 (Guo 2006, [9])**.** *Let T be a tree with n vertices. Then,*

$$\lambda_j(T) \le \left\lceil \frac{n}{n-j} \right\rceil, \quad j = 0, \ldots, n-1,$$

and the equality holds if and only if all of the following hold: a) $j \neq 0$; b) $n-j$ divides n; and c) T is spanned by $n-j$ vertex disjoint copies of $K_{1,\frac{j}{n-j}}$.



(a) (b)

Figure 5.6: (a) A tree spanned by multiple copies of $K_{1,3}$ connected via their central vertices. This tree has an eigenvalue equal to 4 with multiplicity 1. (b) The eigenvalue distribution of such a tree spanned by 5 copies of $K_{1,3}$. We note that $S\ell(T) = 1$ for this tree.

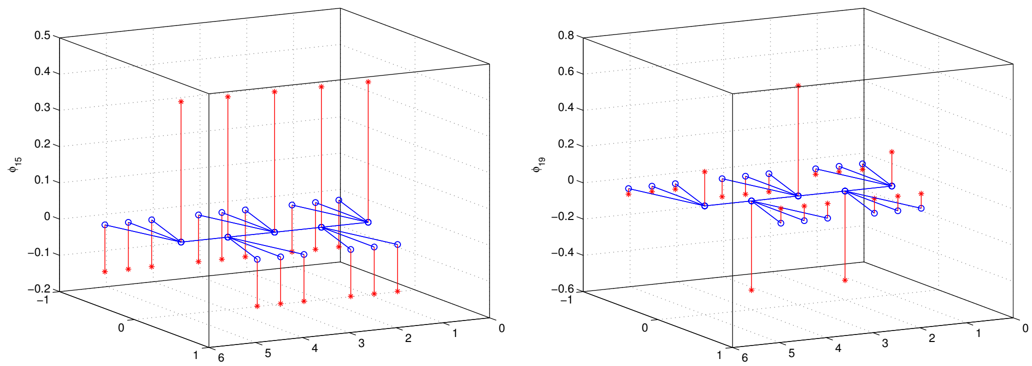
Here, a tree $T = T(V, E)$ is said to be spanned by ℓ *vertex disjoint copies* of identical graphs $K_i(V_i, E_i)$ for $i = 1, \ldots, \ell$ if $V = \bigcup_{i=1}^{\ell} V_i$ and $V_i \cap V_j = \emptyset$ for all $i \neq j$. Figure 5.6(a) shows an example of such vertex disjoint copies for $K_i = K_{1,3}$ by connecting their central vertices. We note that there are many other ways to form disjoint vertex copies of $K_{1,3}$.

This theorem implies the following

Corollary 5.1. *A tree has an eigenvalue exactly equal to 4 if it is spanned by* $m(= n/4 \in \mathbb{N})$ *vertex disjoint copies of* $K_{1,3} \equiv S(1, 1, 1)$.

Figure 5.6(b) shows the eigenvalue distribution of a tree spanned by $m = 5$ copies of $K_{1,3}$ as shown in Figure 5.6(a). Regardless of m, the eigenvector corresponding to the eigenvalue 4 has only two values: one constant value at the central vertices, and the other constant value of the opposite sign at the leaves, as shown in Figure 5.7(a). By contrast, the eigenvector corresponding to the largest eigenvalue is again concentrated around the central vertex as shown in Figure 5.7(b).

Theorem 5.1 asserts that a general tree T with n vertices can have *at most* $\lfloor n/4 \rfloor$ Laplacian eigenvalues ≥ 4. We also know by Theorem 2.1 of [8] that any tree T possessing the eigenvalue 4 must have multiplicity $m_T(4) = 1$ and $n = 4m$ for some $m \in \mathbb{N}$. Hence, Theorem 5.1 also asserts that trees spanned by m vertex disjoint copies of $K_{1,3}$ form the only class of trees for which 4 is the $3n/4(= 3m)$th



(a) $\boldsymbol{\phi}_{15}$ (b) $\boldsymbol{\phi}_{19}$

Figure 5.7: (a) The eigenvector $\boldsymbol{\phi}_{15}$ corresponding to $\lambda_{15} = 4$ in the 3D perspective view. (b) The eigenvector $\boldsymbol{\phi}_{19}$ corresponding to the maximum eigenvalue $\lambda_{19} = 7.1091$, which concentrates around the central vertex.

eigenvalue of T; in other words, trees in this class are the only ones that have *exactly* $n/4 (= m)$ eigenvalues ≥ 4.

Trees spanned by vertex disjoint copies of $K_{1,3}$, however, are not the only ones that have an eigenvalue exactly equal to 4. For instance, Example 2.9 of [8], which has $n = 36 = 4 \cdot 9$ vertices and is called Z_4 as shown in Figure 5.8, is *non-isomorphic* to any tree spanned by 9 vertex disjoint copies of $K_{1,3}$; yet it has $\lambda_{30} = 4$ (but $\lambda_{27} = 1 \neq 4$).

On the other hand, we have the following

Proposition 5.1. *If $n \leq 11$, any tree possessing an eigenvalue exactly equal to 4 must be spanned by vertex disjoint copies of $K_{1,3}$.*

Proof. First of all, 4 must divide n, hence $n = 4m$ with $m = 1$ or $m = 2$. If $m = 1$, then we know from Theorem 5.1 that $\lambda_{max} = \lambda_3 \leq 4$ and $\lambda_2 \leq 2$. Hence, $\lambda_3 = 4$ is the only possibility, and consequently $T = K_{1,3}$ using the same theorem. If $m = 2$, then Theorem 5.1 states that $\lambda_{max} = \lambda_7 \leq 8$; $\lambda_6 \leq 4$; and $\lambda_5 \leq 3$; ... If $\lambda_6 = 4$, then the necessary and sufficient conditions for the equality in Theorem 5.1 state that T must be spanned by two vertex disjoint copies of $K_{1,3}$, so we are done. Now we still need to show that λ_7 cannot be 4. Let d_1 be the degree of the highest degree vertex of a tree T under consideration. Then, we have

$$d_1 + 1 \leq \lambda_7 < d_1 + 2\sqrt{d_1 - 1}. \tag{5.15}$$

Here, the lower bound is due to Grone and Merris [7] and the upper bound is due to Stevanović [13]. Now, we need to check a few cases of the values of d_1.

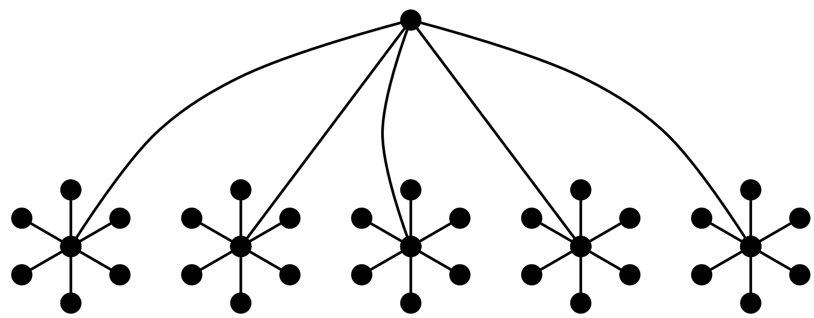


Figure 5.8: Yet another tree Z_4 (Example 2.9 of [8] with $k = 4$) that has an eigenvalue exactly equal to 4. This is non-isomorphic to any tree spanned by vertex disjoint copies of $K_{1,3}$ such as the one shown in Figure 5.6(a).

- If $d_1 = 2$, then the upper bound in (5.15) is 4. Hence, $\lambda_7 = 4$ cannot happen. (This includes the case of a path graph that cannot reach the eigenvalue 4). So, we must have $d_1 \geq 3$.
- If $d_1 > 3$, of course, the lower bound in (5.15) is greater than 4. Hence, λ_7 cannot be 4 either.
- Finally, if $d_1 = 3$, then the above bounds are: $4 \leq \lambda_7 < 5.8284\cdots$. Can $\lambda_7 = 4$ in this case? According to Zhang and Luo [17], the equality in that lower bound holds if and only if there exists a vertex that is adjacent to all the other vertices in T. That is, the degree of that vertex is $n - 1 = 7$. Since $d_1 = 3$, this cannot happen.

Hence, for $n = 8$, the only possibility for a tree T to have an eigenvalue exactly equal to 4 is the case when $\lambda_6 = 4$, which happens if and only if T is spanned by two vertex disjoint copies of $K_{1,3}$. $\square$

It turns out, however, that proving the necessity for $n > 11$ using similar arguments quickly becomes cumbersome, even for the next step $n = 12$. At this point, we do not know whether there are other classes of trees than Z_4 discussed above or those spanned by vertex disjoint copies of $K_{1,3}$ that can have an eigenvalue exactly equal to 4. Hence, identifying every possible tree that has an eigenvalue exactly equal to 4 is an open problem.

6. Implication of a Long Path on Eigenvalues

In Section 4 we saw that for a graph that has a branch consisting of a long path, its Laplacian eigenvalue greater than 4 has the property that the corresponding eigenvector components along the branch must decay exponentially.

Here we discuss a consequence of such a structure in terms of the eigenvalues. We consider a graph G formed by connecting two graphs G_1 and G_3 with a path G_2. Note that this is a more general graph than in Section 4 (which can be regarded as the case without G_3). We show that if G_2 is a long path then any eigenvalue greater than 4 of the Laplacian of either of the two subgraphs $G_1 \cup G_2$ and $G_2 \cup G_3$ must be nearly the same as an eigenvalue of the Laplacian of the whole graph G.

Theorem 6.1. *Let G be a graph obtained by connecting two graphs with a path, whose Laplacian L can be expressed as*

$$L = \begin{bmatrix} L_1 & E_1^\mathsf{T} & 0 \\ E_1 & L_2 & E_2^\mathsf{T} \\ 0 & E_2 & L_3 \end{bmatrix},$$

where E_1 and E_2 have -1 in the top-right corner and 0 elsewhere. L_i is $\ell_i \times \ell_i$ for $i = 1, 2, 3$ and L_2 represents the path G_2, that is, a tridiagonal matrix with 2 on the diagonals and -1 on the off-diagonals.

Let $\widetilde{\lambda} > 4$ be any eigenvalue of the top-left $(\ell_1+\ell_2)\times(\ell_1+\ell_2)$ (or bottom-right $(\ell_2+\ell_3)\times(\ell_2+\ell_3)$) submatrix of L. Then there exists an eigenvalue λ of L such that

$$|\lambda - \widetilde{\lambda}| \le \widetilde{\gamma}^{\ell_2}, \tag{6.16}$$

where $\widetilde{\gamma} := \frac{2}{\widetilde{\lambda}-2} < 1$.

Proof. We treat the case where $\widetilde{\lambda}$ is an eigenvalue of the top-left $(\ell_1+\ell_2)\times(\ell_1+\ell_2)$ part of L, which we denote by L_{12}. The other case is analogous.

As in Theorem 4.2, we can show that any eigenvalue $\widetilde{\lambda} > 4$ of L_{12} has its corresponding eigenvector components decay exponentially along the path G_2. This means that the bottom eigenvector component is smaller than $\widetilde{\gamma}^{\ell_2}$ in absolute value (we normalize the eigenvector so that it has unit norm) where $\widetilde{\gamma} := \frac{2}{\widetilde{\lambda}-2} < 1$ as in (4.11).

Let $L_{12} = Q\Lambda Q^\mathsf{T}$ be an eigendecomposition where $Q^\mathsf{T}Q = I$ and the eigenvalues are arranged so that $\widetilde{\lambda}$ appears in the top diagonal of Λ. For notational convenience let $\ell_{12} := \ell_1 + \ell_2$. Then, consider the matrix

$$\widehat{L} = \begin{bmatrix} Q^\mathsf{T} & 0 \\ 0 & I \end{bmatrix} L \begin{bmatrix} Q & 0 \\ 0 & I \end{bmatrix} = \begin{bmatrix} \Lambda & \boldsymbol{v}\boldsymbol{e}_1^\mathsf{T} \\ \boldsymbol{e}_1\boldsymbol{v}^\mathsf{T} & L_3 \end{bmatrix}, \tag{6.17}$$

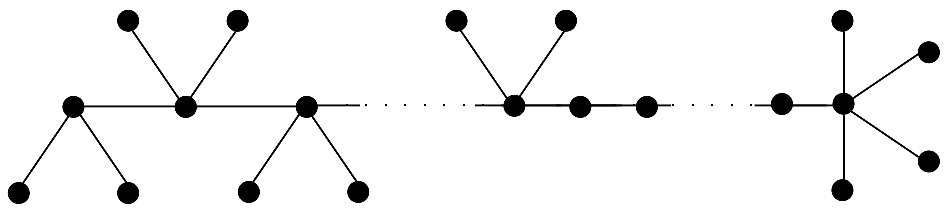


Figure 7.9: Counterexample graph for the conjecture.

where $\boldsymbol{e}_1 = (1, 0, \ldots, 0)^\top \in \mathbb{R}^{\ell_3}$ and $\boldsymbol{v} = (v_1, \ldots, v_{\ell_{12}})^\top \in \mathbb{R}^{\ell_{12}}$. Direct calculations show that $v_i = -q_{\ell_{12},i}$ where $q_{\ell_{12},i}$ is the bottom component of the eigenvector $\boldsymbol{q}_i$ of L_{12} corresponding to the ith eigenvalue. In particular, by the above argument we have $|q_{\ell_{12},1}| = |v_1| \le \widetilde{\gamma}^{\ell_2} (\ll 1)$.

Note that in the first row and column of $\widehat{L}$, the only nonzeros are the diagonal (which is $\widetilde{\lambda}$), and the $(1, \ell_{12} + 1)$ and $(\ell_{12} + 1, 1)$ entries, both of which are equal to v_1. Now, viewing the $(1, \ell_{12}+1)$ and $(\ell_{12}+1, 1)$ entries of $\widehat{L}$ as perturbations (write $\widehat{L} = \widehat{L_1} + \widehat{L_2}$ where $\widehat{L_1}$ is obtained by setting the $(1, \ell_{12} + 1)$ and $(\ell_{12} + 1, 1)$ entries of $\widehat{L}$ to 0) and using Weyl's theorem [6, Theorem 8.1.5] we see that there exists an eigenvalue λ of $\widehat{L}$ (and hence of L) that lies in the interval $[\widetilde{\lambda} - \|\widehat{L_2}\|_2, \widetilde{\lambda} + \|\widehat{L_2}\|_2] = [\widetilde{\lambda} - |v_1|, \widetilde{\lambda} + |v_1|]$. Together with $|v_1| \le \widetilde{\gamma}^{\ell_2}$ we obtain (6.16). $\square$

Recall that $\widetilde{\gamma}^{\ell_2}$ decays exponentially with ℓ_2, and it can be negligibly small for moderate ℓ_2; for example, for $(\lambda, \ell_2) = (5, 30)$ we have $\widetilde{\gamma}^{\ell_2} = 5.2 \times 10^{-6}$. We conclude that the existence of a subgraph consisting of a long path implies that the eigenvalues $\lambda > 4$ of a subgraph must match those of the whole graph to high accuracy.

7. On the Eigenvector of the Largest Eigenvalue

In view of the results in Section 4 it is natural to ask whether it is always true that the largest component of the eigenvector corresponding to the largest eigenvalue of a Laplacian matrix of a graph lies on the vertex of the highest degree. Here we show by a counterexample that this is not necessarily true.

Consider for example a tree as in Figure 7.9, which is generated as follows: first we connect m copies of $K_{1,2}$ (equal to P_3) as shown in Figure 5.6(a); then add to the right a comet $S(\ell, 1, 1, 1, 1)$ as in Figure 3.4(b).

Now for sufficiently large m and ℓ ($m, \ell \ge 5$ is sufficient), the largest component in the eigenvector $\boldsymbol{\phi}$ corresponding to the largest eigenvalue of the resulting

Laplacian L occurs at one of the central vertices of $K_{1,2}$, not at the vertex of degree 5 belonging to the comet.

Let us explain how we came up with this counterexample. The idea is based on two facts. The first is the discussion in Section 6, where we noted that a long path G_2 implies any eigenvalue larger than 4 must be close to an eigenvalue of a subgraph $G_1 \cup G_2$ or $G_2 \cup G_3$. Therefore, in the notation of Section 6, by connecting two graphs ($G_1 = mK_{1,2}$ and $G_3 = K_{1,5}$, a star) with a path G_2 such that the largest eigenvalue $\widetilde{\lambda}$ of L_{12} is larger than that of L_{23}, we ensure that the largest eigenvalue λ of L is very close to $\widetilde{\lambda}$. The second is the Davis-Kahan $\sin\theta$ theorem [5], which states that a small perturbation of size $\widetilde{\gamma}^{\ell_2}$ in the matrix $\widehat{L_1}$ (recall the proof of Theorem 6.1) can only induce small perturbation also in the eigenvector: its angular perturbation is bounded by $\widetilde{\gamma}^{\ell_2}/\delta$, where δ is the distance between λ and the eigenvalues of $\widehat{L}$ after removing its first row and column. Furthermore, the eigenpair $(\widetilde{\lambda}, \widetilde{\boldsymbol{\phi}})$ of $\widehat{L_1}$ satisfies $\widetilde{\boldsymbol{\phi}} = (1, 0, \ldots, 0)^{\mathsf{T}}$, and the eigenvectors $\widehat{\boldsymbol{\phi}}$ ($\simeq \widetilde{\boldsymbol{\phi}}$ by Davis-Kahan) of $\widehat{L}$ and $\boldsymbol{\phi}$ of L corresponding to λ are related by $\boldsymbol{\phi} = \left[\begin{smallmatrix} Q & 0 \\ 0 & I \end{smallmatrix}\right] \widehat{\boldsymbol{\phi}}$, which follows from (6.17). Therefore, $\boldsymbol{\phi}$ has its large components at the vertices belonging to G_1. In view of these our approach was to find two graphs G_1 and G_3 such that the highest degrees of the vertices of G_1 and G_3 are 4 and 5, respectively, and the largest eigenvalue of the Laplacian of G_1 is larger than that of G_3.

8. Discussion

In this paper, we obtained precise understanding of the phase transition phenomenon of the combinatorial graph Laplacian eigenvalues and eigenvectors for starlike trees. For a more complicated class of graphs including those representing dendritic trees of RGCs, we proved in Theorem 4.1 that the number of the eigenvalues greater than or equal to 4 is bounded from above by the number of vertices whose degrees are strictly higher than 2. In Theorem 4.2, we proved that if a graph has a branching path, the magnitude of the components of an eigenvector corresponding to any eigenvalue greater than 4 along such a branching path decays exponentially toward its leaf. In Remark 4.1, we also extended Theorem 4.2 for the case of $\lambda = 4$ although the decay may not be exponential.

As for Q3 raised in Introduction—"Is there any tree that possesses an eigenvalue exactly equal to 4?"—we showed that any tree with n vertices ($n = 4m$ for some $m \in \mathbb{N}$) spanned by m vertex disjoint copies of $K_{1,3}$ possesses an eigenvalue exactly equal to 4 in Corollary 5.1, and that such class of trees are the only ones that can have an eigenvalue exactly equal to 4 if $n \leq 11$ in Proposition 5.1. On the other hand, for larger n, we pointed out that not only those spanned by vertex disjoint copies of $K_{1,3}$, but also a tree called Z_4 discovered in [8] and shown in Figure 5.8 have an eigenvalue exactly equal to 4. A challenging yet interesting question is whether or not one can identify every possible tree that has an eigenvalue 4.

Another quite interesting question is Q4 raised in Introduction: "Can a simple and connected graph, not necessarily a tree, have eigenvalues equal to 4?" The answer is a clear "Yes." For example, the d-cube ($d > 1$), i.e., the d-fold Cartesian product of K_2 with itself is known to have the Laplacian eigenvalue 4 with multiplicity $d(d-1)/2$; see e.g., [1, Sec. 4.3.1].

Another interesting example is a regular finite lattice graph in $\mathbb{R}^d$, $d > 1$, which is simply the d-fold Cartesian product of a path P_n shown in Figure 2.3 with itself. Such a lattice graph has repeated eigenvalue 4. In fact, each eigenvalue and the corresponding eigenvector of such a lattice graph can be written as

$$\lambda_{j_1,\dots,j_d} = 4\sum_{i=1}^{d} \sin^2\left(\frac{j_i\pi}{2n}\right) \tag{8.18}$$

$$\phi_{j_1,\dots,j_d}(x_1,\dots,x_d) = \prod_{i=1}^{d} \cos\left(\frac{j_i\pi(x_i+\frac{1}{2})}{n}\right), \tag{8.19}$$

where $j_i, x_i \in \mathbb{Z}/n\mathbb{Z}$ for each i, as shown by Burden and Hedstrom [2]. Note that (8.18) and (8.19) are also valid for $d = 1$. In that case these reduce to (2.2) that we already examined in Section 2.

Now, determining $m_G(4)$, i.e., the multiplicity of the eigenvalue 4 of this lattice graph, is equivalent to finding the number of the integer solutions $(j_1,\dots,j_d) \in (\mathbb{Z}/n\mathbb{Z})^d$ to the following equation:

$$\sum_{i=1}^{d} \sin^2\left(\frac{j_i\pi}{2n}\right) = 1. \tag{8.20}$$

For $d = 1$, there is no solution as we mentioned in Section 2. For $d = 2$, it is easy to show that $m_G(4) = n-1$ by direct examination of (8.20) using some trigonometric identities. For $d = 3$, $m_G(4)$ behaves in a much more complicated manner, which is deeply related to number theory. We expect that more complicated situations occur for $d > 3$. We are currently investigating this on regular finite lattices. On the other hand, it is clear from (8.19) that the eigenvectors corresponding to the eigenvalues greater than or equal to 4 on such lattice graphs cannot be localized or concentrated on those vertices whose degree is higher than 2 unlike the tree case.

Theorem 4.2 and Remark 4.1 do not apply either since such a finite lattice graph do not have branching paths.

Finally, we would like to note that even a simple path, such as the one shown in Figure 2.3, exhibits the eigenfunction localization phenomena *if it has nonuniform edge weights*, which we recently observed numerically. We will report our progress on investigation of localization phenomena on such weighted graphs at a later date.

Acknowledgments

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