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April 3, 2021

Diameter Bounds on the Spectral Gap of Quantum Graphs

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An abstract of
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of Emory University in partial fulfillment
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Mathematics

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Abstract

Diameter Bounds on the Spectral Gap of Quantum Graphs

By Tianlang Luo

A quantum graph is a metric graph equipped with a differential operator. The spectrum of a compact quantum graph is real and discrete, where its first positive eigenvalue is referred to as the spectral gap. We present a method to study the upper bound on the spectral gap of quantum graphs in terms of the diameter (and possibly of the total length and the total number of vertices) by reduction to a Sturm-Liouville problem.

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1 Introduction

1.1 Background on quantum graphs

Quantum graph is a rapidly growing mathematical field which can be extensively applied as a simple but non-trivial model to study complex physical systems. In chemistry, the complex band structures of carbon can be calculated by studying their quantum graph models [1]. In photonic crystal theory, spectral problems arising from the theory of classical waves in periodic high contrast photonic and acoustic media can be translated to spectral problems on quantum graphs [9]. In quantum mechanics, quantum graphs offer a simple setting to study various phenomena, such as Anderson localization [4,6], and quantum chaos [5,7].

One of the most important parameters of quantum graphs is the first positive eigenvalue λ_1 , also called the spectral gap. For example, in quantum many-body physics, it is the energy difference between the ground state and the first excited state of the system [3]. Estimation of the spectral gap in terms of geometric properties of the quantum graphs has been vastly explored. For example, in the early years Nicaise and Serge [10] proved the most fundamental lower bound in terms of the total length L of the graph

$$\lambda_1(G) \geq \frac{\pi^2}{L^2}.$$

The minimizer is the interval of length L , which is often considered as the trivial graph. Recently, Kennedy et al. [8] proved that the spectral gap cannot be bounded from above in terms of the diameter of the quantum graph alone. Rohleder and Jonathan [11] determined the maximizer of all eigenvalues (including the spectral gap) for tree graphs.

1.2 Spectral theory of quantum graphs

A metric graph is a graph where each edge e is assigned with length $\ell_e > 0$ and can be identified with the interval $[0, \ell_e] \subset \mathbb{R}$. A quantum graph G is a metric graph equipped

with a differential operator acting on the H^2 space of functions defined on the edges of G . In this paper, we will focus on the one-dimensional Laplacian operator $-\Delta = -\frac{d^2}{dx^2}$, which computes the second derivative. Here, x is the coordinate along the edge. By gluing all these operators on different edges together at vertices connecting them, we will assume the following vertex condition: functions in the domain of $-\Delta$

1. are continuous across the vertices (continuity condition).
2. their normal derivatives (outward first derivatives in one-dimension) on each vertex sum up to zero (Kirchhoff condition).

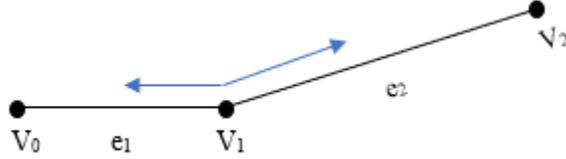


Figure 1: Vertex condition at v_1 and v_0 . The arrows indicates the outward direction of the first derivatives of functions defined on e_1, e_2 at v_1 .

For example, consider the graph with three vertices and two edges as shown in Figure 1.

1. Let $[0, \ell_{e_1}], [0, \ell_{e_2}]$ be the intervals associated to edges e_1, e_2 , where 0 corresponds to v_0 and ℓ_{e_1} corresponds to v_1 on e_1 , while 0 corresponds to v_1 and ℓ_{e_2} corresponds to v_2 on e_2 . Define φ_1, φ_2 on these intervals respectively. To satisfy the vertex condition at v_1 , we need $\varphi_1(v_1) = \varphi_2(v_1)$ and $-\varphi_1'(v_1) + \varphi_2'(v_1) = 0$. Furthermore, since v_1 is a vertex of degree 2, meaning there are exactly two edges connecting to it, we can freely remove v_1 and combine e_1, e_2 to form a single edge. Similarly, we can choose an interior point of an edge to be an artificial vertex, and this vertex clearly satisfies the vertex conditions above. For v_0 , however, since e_1 is the only edge connected to v_0 , we only need $\varphi_1'(v_0) = 0$ to satisfy the vertex conditions at v_0 . This is the same for v_2 .

We will also assume that G is compact, meaning that it has a finite number of edges with finite lengths; and G is connected, so that the first eigenvalue $\lambda_0 = 0$ has multiplicity

one with eigenfunction $\psi_0 \equiv 1$. Based on these assumptions, Theorem 1.4.4 in [2] shows that $-\Delta$ is self-adjoint, and [2, §3.1] suggests that eigenvalues of compact quantum graphs are real and discrete with finite multiplicity and converge to infinity. Therefore, the set of eigenvalues of G , denoted by $\{\lambda_j\}_{j=0}^\infty$, are real numbers which satisfy $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots$ and $\lambda_j \rightarrow \infty$ as $j \rightarrow \infty$. The spectral gap of G is the lowest non-trivial eigenvalue λ_1 .

1.3 Summary of results

In this paper we will review the methods and techniques to estimate the spectral gap λ_1 on the quantum graph in terms of geometric properties of the graph developed in [8]. Our goal is to present a comprehensive and detailed demonstration, and also correct the flaws in some of the proofs in the original literature. In section 2, an exact formula of λ_1 is derived by minimizing the Rayleigh quotient. In section 3, the reaction of λ_1 to the topology and metric change of the graph is carefully investigated as an application of the formula of λ_1 obtained in section 2. These changes are called “surgeries” on the graph. In section 4, first, the algorithm which reduces any graph to a pumpkin chain (a special type of graph) without decreasing λ_1 by surgeries on the graph is reviewed. We then present a correct proof of how to transform the eigenvalue problem on a pumpkin chain to a one-dimensional Sturm-Liouville problem. The difference compared to the original literature lies in the part to prove the existence of a first eigenfunction which does not vanish on at least one vertex. The original literature involves an invalid assumption on the eigenfunction, but the same results can be achieved even without it. In the final section, we apply the upper estimate of the spectral gap in terms of both diameter and total length of the graph, which is obtained in Theorem 7.1 of [8], as an application of the reduction to one-dimensional problem method, to a special type of pumpkin chain. A numerical investigation of the example justifies the comment in [8] which says that the upper estimate is far from optimal. An improvement on this estimate may involve construction of a new test function which suggests more information on the configuration of the maximizer graph.

2 Rayleigh Quotient

For any quantum graph G which satisfies the assumptions in section 1.2, we shall first derive a formula for the spectral gap $\lambda_1(G)$ by the min-max principle. Since $\lambda_1(G)$ is the first non-trivial eigenvalue, it can be obtained by minimizing the Rayleigh quotient subject to the constraint of L^2 -orthogonality to the eigensubspace corresponding to $\lambda_0 = 0$. Note that λ_0 is associated with the eigenfunction $\psi_0 \equiv 1$.

Theorem 2.1 (Equation (2.3) in [8]).

$$\lambda_1(G) = \inf \left\{ \frac{\int_G |u'(x)|^2 dx}{\int_G |u(x)|^2 dx} : u \in H^1(G), \int_G u(x) dx = 0 \right\},$$

where $H^1(G)$ is the space consisting of functions defined on the intervals associated with the edges of the graph, belonging to the first Sobolev space, and satisfying the continuity condition on each vertex, cf. [2, §1.3].

Proof. Let $\{\lambda_j\}_{j=0}^\infty$ be the set of eigenvalues of G , where $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots$. Let ψ_1 be an eigenfunction of λ_1 . Note that ψ_1 may not be unique. These satisfy

$$-\Delta\psi_j = \lambda_j\psi_j.$$

Choose the eigenfunction set which forms an orthonormal basis for $L^2(G)$. Then we have

$$\langle \psi_j, \psi_k \rangle = \int_G \psi_j \psi_k dx = \begin{cases} 1 & j = k, \\ 0 & j \neq k. \end{cases}$$

For $u \in H^1(G)$, $u \in L^2(G)$ and $u' \in L^2(G)$. Expanding u in terms of the orthonormal basis, we have

$$u = \sum_{j=0}^{\infty} c_j \psi_j.$$

Since we want to find the lowest non-trivial eigenvalue $\lambda_1 > 0$, we will only consider the sub-

space of $H^1(G)$ which is orthogonal to the eigensubspace corresponding to $\lambda_0 = 0$. Therefore, we have,

$$\begin{aligned} \int_G u \cdot 1 \, dx = 0 &\implies \langle u, \psi_0 \rangle = 0 \\ &\implies c_0 = 0. \end{aligned}$$

For any ψ_j , we know that $\langle \psi_j, \psi_j \rangle = \|\psi_j\|^2 = 1$. Then

$$\begin{aligned} \langle \psi'_j, \psi'_j \rangle &= \|\psi'_j\|^2 = \int_G \psi_j'^2 \, dx \\ &= - \int_G \psi_j \Delta \psi_j \, dx \\ &= \lambda_j \|\psi_j\|^2 \\ &= \lambda_j. \end{aligned}$$

Thus, we obtain

$$\begin{aligned} \|u\|^2 &= \sum_{j=1}^{\infty} \langle c_j \psi_j, c_j \psi_j \rangle = \sum_{j=1}^{\infty} |c_j|^2 \\ \|u'\|^2 &= \sum_{j=1}^{\infty} \langle c_j \psi'_j, c_j \psi'_j \rangle = \sum_{j=1}^{\infty} |c_j|^2 \lambda_j. \end{aligned}$$

Now we write out the Rayleigh quotient

$$\begin{aligned} \text{Rayleigh quotient} &= \frac{\|u'\|^2}{\|u\|^2} \\ &= \frac{\sum_{j=1}^{\infty} |c_j|^2 \lambda_j}{\sum_{j=1}^{\infty} |c_j|^2}, \end{aligned}$$

Note that $\{c_j\}_{j=1}^{\infty}$ cannot all be identically zero or the function $u \equiv 0$. Taking the infimum of the Rayleigh quotient, we have to set c_1 to be nonzero, for example $c_1 = 1$, while all $\{c_j\}_{j=2}^{\infty}$ equal to zero since the set of eigenvalues $\{\lambda_j\}_{j=0}^{\infty}$ is listed in an ascending order. Therefore,

the infimum of the Rayleigh quotient is

$$\begin{aligned} & \inf \left\{ \frac{\|u'\|^2}{\|u\|^2} : u \in H^1(G), \int_G u(x) dx = 0 \right\} \\ &= \inf \left\{ \frac{\int_G |u'(x)|^2 dx}{\int_G |u(x)|^2 dx} : u \in H^1(G), \int_G u(x) dx = 0 \right\} \\ &= \lambda_1(G). \end{aligned}$$

□

Remark 2.2. 1. Take arbitrary test function $u \in H^1$ which is perpendicular to the constant eigenfunction (usually C^1 on each edge and continuous on each vertex, but does not need to satisfy Kirchhoff condition), we have the inequality

$$\lambda_1(G) \leq \frac{\|u'\|^2}{\|u\|^2},$$

where equality is achieved when $u = \psi_1$.

2. We can further apply the min-max method to the Rayleigh quotient to derive a general formula for eigenvalues of any order. Specifically,

$$\lambda_k = \max_{\substack{W \subset H^1 \\ \dim(W)=k}} \min_{u \in W^\perp} \frac{\|u'\|^2}{\|u\|^2}.$$

Since we want to compute the k -th lowest eigenvalue, we will disregard the eigensubspaces that correspond to the eigenvalues smaller than λ_k , namely $\{\lambda_j\}_{j=0}^{k-1}$. Therefore,

$$W = \text{span}\{\psi_0, \dots, \psi_{k-1}\}.$$

Theorem 2.1 provides the exact formula for the spectral gap. However, it is often difficult to find test functions which attain or converge to the infimum, especially for complicated graphs. One usually needs to simplify the graphs depending on the problem.

3 Surgery on Quantum Graphs

Theorem 2.1 reveals a surprising relation between the spectral gap and both the topology and the geometry of the quantum graph. In this section, we will study how the spectral gap reacts to the alteration on the structure of the quantum graph.

Lemma 3.1 (Lemma 2.3 of [8]). *Suppose G and G' are connected compact quantum graphs with operators defined in the introduction.*

1. *If G' is formed by attaching a pendant edge, or more generally a pendant graph, to one vertex of G , then $\lambda_1(G) \geq \lambda_1(G')$. By “pendant graph” (or edge) we mean that the graph to be added, i.e. $G' \setminus G$, is attached to G only at one vertex. This covers the case of adding a loop. (Figure 2)*
2. *If G' is formed from G by identifying two vertices of G (say, v_1, v_2 are replaced with a new vertex v_0 and each edge having v_1 or v_2 as an endpoint is replaced with a new edge having v_0 as an endpoint, and in particular the edges between v_1 and v_2 are replaced with loops around v_0), then $\lambda_1(G) \leq \lambda_1(G')$. (Figure 3)*
3. *If we add an edge $e = v_1v_2$ between two already existing vertices of a quantum graph G , producing the new quantum graph G' , then $\lambda_1(G) \geq \lambda_1(G')$ provided there is an eigenfunction corresponding to $\lambda_1(G)$ attaining the same value on both v_1, v_2 . (Figure 4)*
4. *If G' is formed from G by lengthening a given edge, then $\lambda_1(G) \geq \lambda_1(G')$.*
5. *If G' is obtained from G by scaling each edge with the factor $\frac{1}{c} \in \mathbb{R}$, then the corresponding eigenvalues scale as c^2 , that is,*

$$\lambda_1(G) = c^{-2}\lambda_1(G').$$

Since the original literature includes only incomplete proofs and also contains minor

errors (incorrect test functions in parts 1, 4), we shall present a correct and detailed proof here.

Proof. 1. Let ψ_1 be any eigenfunction associated with $\lambda_1(G)$. We know that

$$\int_G \psi_1 dx = 0.$$

We assume G' is obtained by attaching a pendant edge to the vertex $v \in G$. We extend ψ_1 to a function $\tilde{\psi} \in H^1(G')$ by defining $\tilde{\psi} = \psi_1(v)$ on $G' \setminus G$. Then define another function $\varphi \in H^1(G')$ by

$$\varphi := \tilde{\psi} - \frac{L(G' \setminus G)}{L(G')} \psi_1(v).$$

We check that

$$\begin{aligned} \int_{G'} \left(\tilde{\psi} - \frac{L(G' \setminus G)}{L(G')} \psi_1(v) \right) dx &= \int_{G'} \tilde{\psi} dx - \int_{G'} \frac{L(G' \setminus G)}{L(G')} \psi_1(v) dx \\ &= \int_G \psi_1 dx + \int_{G' \setminus G} \psi_1(v) dx - \int_{G'} \frac{L(G' \setminus G)}{L(G')} \psi_1(v) dx \\ &= L(G' \setminus G) \psi_1(v) - L(G') \frac{L(G' \setminus G)}{L(G')} \psi_1(v) \\ &= 0. \end{aligned}$$

Hence, φ is a valid test function for $\lambda_1(G')$. First, consider

$$\begin{aligned}
\int_{G'} |\varphi'|^2 dx &= \int_{G'} \left| \tilde{\psi} - \frac{L(G' \setminus G)}{L(G')} \psi_1(v) \right|^2 dx \\
&= \int_{G'} |\tilde{\psi}'|^2 dx \\
&= \int_G |\psi_1'|^2 dx + \int_{G' \setminus G} |(\psi_1(v))'|^2 dx \\
&= \int_G |\psi_1'|^2 dx.
\end{aligned}$$

Next, consider

$$\begin{aligned}
\int_{G'} |\varphi|^2 dx &= \int_G \left(\psi_1(x) - \frac{L(G' \setminus G)}{L(G')} \psi_1(v) \right)^2 dx + \int_{G' \setminus G} \left(\psi_1(v) - \frac{L(G' \setminus G)}{L(G')} \psi_1(v) \right)^2 dx \\
&= \int_G \left((\psi_1(x))^2 + \left(\frac{L(G' \setminus G)}{L(G')} \psi_1(v) \right)^2 - 2\psi_1(x) \frac{L(G' \setminus G)}{L(G')} \psi_1(v) \right) dx \\
&\quad + \int_{G' \setminus G} \left(\frac{L(G)}{L(G')} \psi_1(v) \right)^2 dx \\
&= \int_G (\psi_1(x))^2 dx + \frac{L^2(G' \setminus G)L(G)}{L^2(G')} \psi_1^2(v) + \frac{L(G' \setminus G)L^2(G)}{L^2(G')} \psi_1^2(v) \\
&\geq \int_G |\psi_1(x)|^2 dx.
\end{aligned}$$

Hence, the Rayleigh quotient

$$\frac{\|\varphi'\|^2}{\|\varphi\|^2} = \frac{\int_{G'} |\varphi'|^2 dx}{\int_{G'} |\varphi|^2 dx} \leq \frac{\int_G |\psi_1'|^2 dx}{\int_G |\psi_1(x)|^2 dx} = \lambda_1(G).$$

By Theorem 2.1, we conclude that $\lambda_1(G) \geq \lambda_1(G')$. The more general pendant graph case can be shown by continuously adding pendant edges.

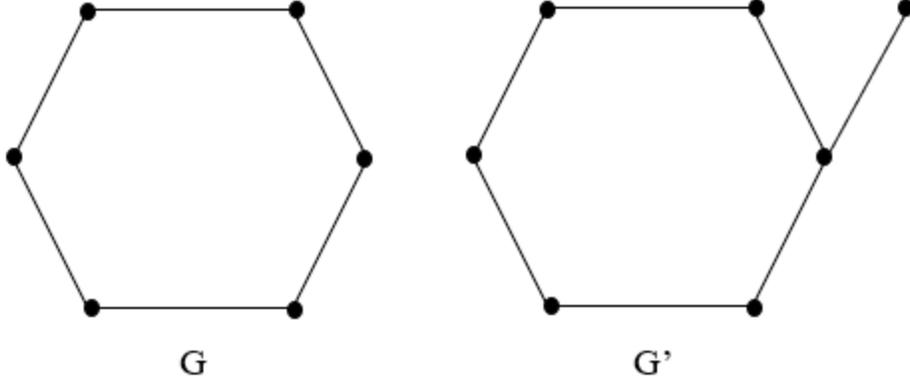


Figure 2: (Lemma 3.1-1) G' is formed by attaching a pendent edge to G .

2. Claim: $H^1(G') \subset H^1(G)$.

Since G' is obtained from G by identifying $v_1, v_2 \in G$ and all the other parts are identical, it suffices to consider the edges connecting to these two vertices. Take an arbitrary test function $u \in H^1(G')$. Let $\{e_j\}_{j=1}^n$ be the set of edges connected to v_0 , and the test function u restricted on intervals associated to each of them is denoted by $\{f_j\}_{j=1}^n$. The continuity condition from $H^1(G')$ ensures that $f_j(v_0) = f_k(v_0)$ for all j, k from 1 to n . However, in G , the set of edges connected to v_1, v_2 is also $\{e_j\}_{j=1}^n$. We can assume that $\{e_j\}_{j \in J_1}$ is the set of edges connected to v_1 , while $\{e_j\}_{j \in J_2}$ is the set of edges connected to v_2 . Since $f_j(v_0) = f_k(v_0)$ for all j, k from 1 to n in G' , we have $f_j(v_1) = f_k(v_1)$ for all $j, k \in J_1$, and $f_j(v_2) = f_k(v_2)$ for all $j, k \in J_2$ in G . Clearly, u also satisfies the continuity condition from $H^1(G)$. We can conclude that $u \in H^1(G)$, and thus $H^1(G') \subset H^1(G)$.

Since $H^1(G') \subset H^1(G)$, the search domain for the infimum in the Rayleigh quotient shrinks while all the other conditions remain unchanged, the infimum of the Rayleigh quotient cannot be smaller. Therefore, $\lambda_1(G) \leq \lambda_1(G')$.

3. The idea is similar to part 1. Extending the eigenfunction ψ_1 associated with $\lambda_1(G)$ by the constant value $\psi_1(v_1) = \psi_1(v_2)$ on the new edge yields a new function $\tilde{\psi} \in H^1(G')$.

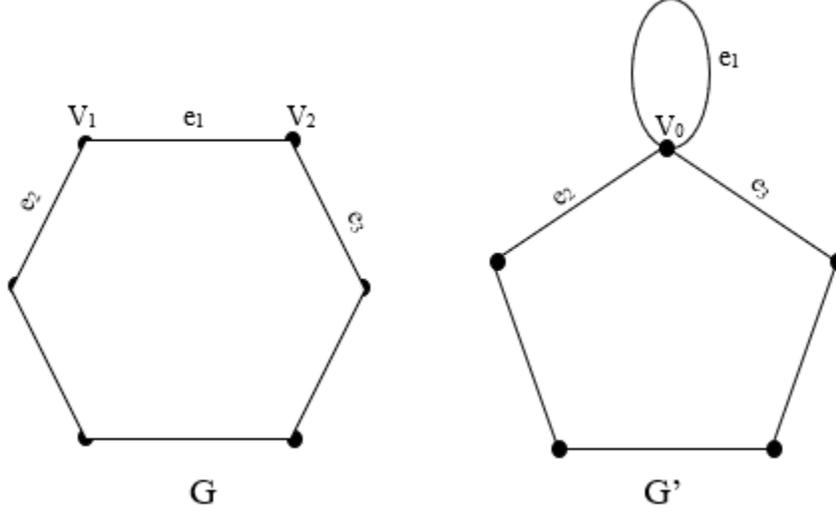


Figure 3: (Lemma 3.1-2) G' is formed by identifying v_1, v_2 of G .

Define the test function φ by

$$\varphi := \tilde{\psi} - \frac{L(G' \setminus G)}{L(G')} \psi_1(v_1).$$

Since

$$\int_{G'} \varphi \, dx = 0,$$

φ is a valid test function for $\lambda_1(G')$. And a similar analysis as in part 1 shows that $\lambda_1(G) \geq \lambda_1(G')$.

4. Assume $e \in G$ is lengthened. Denote its associated interval by $[0, a]$. Let the lengthened interval be $[0, a']$ with $a' > a$. Again, extending the eigenfunction ψ_1 associated with $\lambda_1(G)$ by the constant value $\psi_1(a)$ on $[a, a']$ yields a new function $\tilde{\psi} \in H^1(G')$. Define the valid test function φ for $\lambda_1(G')$ by

$$\varphi := \tilde{\psi} - \frac{a' - a}{L(G')} \psi_1(a).$$

Following a similar analysis as in part 1 we conclude that $\lambda_1(G) \geq \lambda_1(G')$.

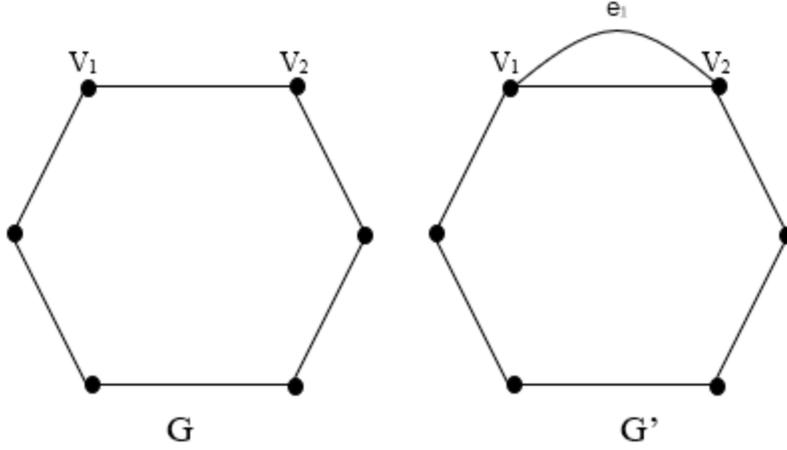


Figure 4: (Lemma 3.1-3) G' is formed by adding a new edge e_1 connecting v_1, v_2 of G , provided $\psi(v_1) = \psi(v_2)$ for some eigenfunction ψ corresponding to $\lambda_1(G)$.

5. Let ψ_1 be any eigenfunction associated with $\lambda_1(G)$. We know that

$$-\Delta\psi_1(x) = \lambda_1(G)\psi_1(x)$$

for all $x \in G$. If we scale each edge with a factor $\frac{1}{c} \in \mathbb{R}$ to obtain G' , by a change of variable we have

$$-\Delta\psi_1\left(\frac{x}{c}\right) = c^2\lambda_1(G)\psi_1\left(\frac{x}{c}\right)$$

for $\frac{x}{c} \in G$. Therefore, $c^2\lambda_1(G)$ is a non-trivial eigenvalue of G' with eigenfunction $\psi_1\left(\frac{x}{c}\right)$.

Claim: $c^2\lambda_1(G) = \lambda_1(G')$.

If not, let $\lambda_1(G') = \lambda' \in (0, c^2\lambda_1(G))$, and denote the eigenfunction associated to λ' by ψ' . We have

$$-\Delta\psi'(x) = \lambda'\psi'(x)$$

for all $x \in G'$. Again, by a change of variable we have

$$-\Delta\psi'(cx) = c^{-2}\lambda'\psi'(cx)$$

for $cx \in G$. Therefore $c^{-2}\lambda'$ is a non-trivial eigenvalue of G with eigenfunction $\psi'(cx)$. By construction, $0 < \lambda' < c^2\lambda_1(G)$, and thus $0 < c^{-2}\lambda' < \lambda_1(G)$. Since $\lambda_1(G)$ is the lowest non-trivial eigenvalue by definition, this is a contradiction. Therefore, $c^2\lambda_1(G) = \lambda_1(G')$, and this is equivalent to $\lambda_1(G) = c^{-2}\lambda_1(G')$.

□

Lemma 3.1 suggests that, when estimating the spectral gap of a particular quantum graph G , we can perform surgeries, such as adding or removing pendants, identifying vertices, and scaling edges, to transform G into a simpler graph G' without losing track of the spectral gap.

4 Reduction to One-dimensional Problem

In this section, we will show that, to study the upper bound on the spectral gap in terms of the diameter of the graph D (coupled with the number of vertices of the graph V and the total length of the graph L), it suffices to consider the upper bound of the spectral gap of a special quantum graph called a pumpkin chain. We can even further simplify the problem on the pumpkin chain to a one-dimensional Sturm-Liouville problem.

First, we will introduce the pumpkin graph and the pumpkin chain.

Definition 4.1.

1. A pumpkin graph consists of a pair of vertices connected by a set of parallel edges.
2. A pumpkin chain is a linear arrangement of equilateral pumpkin graphs joined at vertices. (Figure 5)

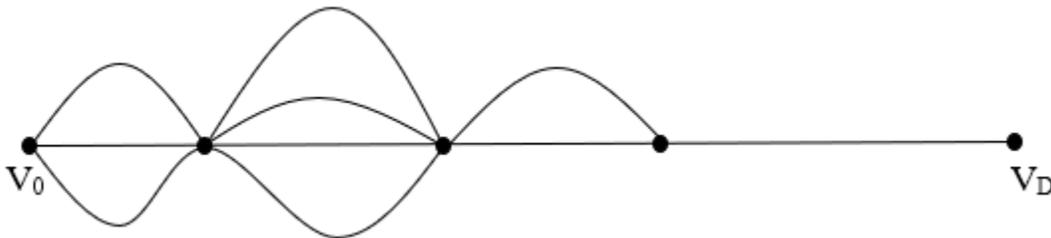


Figure 5: A pumpkin chain with 4 pumpkins.

In a pumpkin chain, we denote the two end vertices as v_0, v_D . All the $V - 2$ interior vertices connect to exactly two pumpkins on their sides, and every path from v_0 to v_D must pass through all of them. Since the edges on the same pumpkin of a pumpkin chain are equilateral, we observe that the diameter of a pumpkin chain is the distance between v_0 and v_D , which is also the length of any path connecting v_0 and v_D . For any pumpkin chain G , we are able to define a level function $S : G \rightarrow [0, D]$ by

$$S(z) = \text{dist}(v_0, z).$$

For example, $S(v_0) = 0$ and $S(v_D) = D$. $S(z)$ is called the level of z in G .

Kennedy et al. [8] introduced an algorithm to reduce a general quantum graph to a pumpkin chain without decreasing the spectral gap by the surgeries in Lemma 3.1.

Lemma 4.2 (Lemma 5.4 of [8]). *Given any compact, connected and non-empty quantum graph G , there exists a pumpkin chain G' such that*

1. $D(G') = D(G), L(G') \leq L(G), V(G') \leq V(G) + 2$.
2. $\lambda_1(G') \geq \lambda_1(G)$.

Proof. We will produce the pumpkin chain G' from G in the following steps, and the resulting graph after each step satisfies the above conditions.

Step 1. Choose any two points $x, y \in G$ such that $\text{dist}(x, y) = D := D(G)$. If x, y are not vertices of G , we will make them artificial vertices of G . This process potentially raises the upper bound of $V(G')$ by 2. If x, y are original vertices of G , then the upper bound of $V(G')$ remains unchanged. Relabel x, y as v_0, v_D (endpoints of the resulting pumpkin chain). (Figure 6)

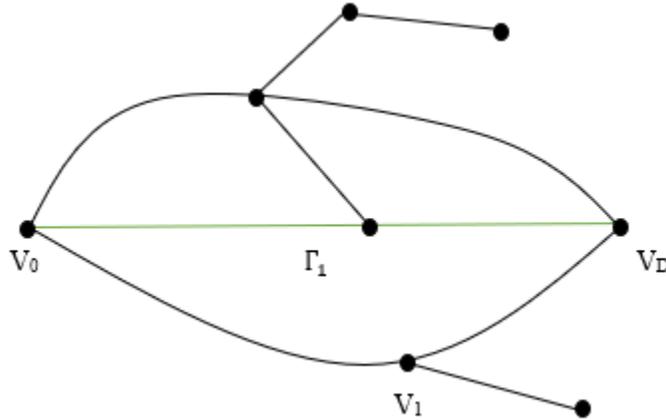


Figure 6: An arbitrary quantum graph G . Γ_1 is the path from v_0 to v_D which achieves the diameter D of the graph

Step 2. Find a path in G connecting v_0 and v_D . Since G is compact, we can find such a path with minimal length, denote it as Γ_1 , and thus $\ell(\Gamma_1) = D$. Observe that Γ_1 contains

no loop and traverses all of its vertices and edges only once. Similarly, choose the second shortest path $\Gamma_2 \not\subseteq \Gamma_1$ connecting v_0 and v_D such that Γ_2 also traverses all of its vertices and edges only once. Continue this process by finding the next shortest path Γ_j connecting v_0 and v_D such that Γ_j traverses all of its vertices and edges only once and

$$\Gamma_j \not\subseteq \sum_{k=1}^{j-1} \Gamma_k.$$

By compactness of G , this process must terminate in finitely many steps. Denote the last such path as Γ_n . We have $D = \ell(\Gamma_1) \leq \ell(\Gamma_2) \leq \dots \leq \ell(\Gamma_n)$.

Step 3. Let $G_1 := \cup_{j=1}^n \Gamma_j$. Observe that any connected component of $G \setminus G_1$ is attached to G_1 at a single vertex and hence is a pendant. Otherwise, we can find a path connecting v_0 and v_D such that it traverses all of its vertices and edges only once, but passes through $G \setminus G_1$. However, this path-finding process already terminates in step 2 and thus we cannot find such a path. Therefore, it is enough to consider G_1 instead of G . (Figure 7)

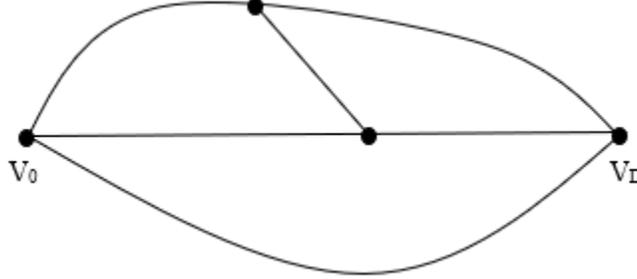


Figure 7: The graph G_1 is produced by removing all pendants, or as union of paths from v_0 to v_D . The vertex v_1 is removed since it is of degree 2.

Step 4. We will produce another graph G_2 out of G_1 by shortening $\Gamma_2, \dots, \Gamma_n$ to the same length as $\ell(\Gamma_1) = D$. Let $\Gamma_1 = \Gamma'_1$. To shorten Γ_2 without changing Γ'_1 , we shorten $\Gamma_2 \setminus \Gamma'_1$ by $\ell(\Gamma_2) - D$ and get Γ'_2 with $\ell(\Gamma'_2) = D$. Note that this may also shorten the other path $\Gamma_3, \dots, \Gamma_n$. However, by construction they still have length at least D and are still ordered in increasing length. Continue to shorten every $\Gamma_j \setminus \cup_{k=1}^{j-1} \Gamma'_k$ and

get Γ'_j with $\ell(\Gamma'_j) = D$. Note that the resulting path may be overlapping, and we only consider the $m \leq n$ distinct paths. Set $G_2 := \cup_{j=1}^m \Gamma'_j$. (Figure 8)

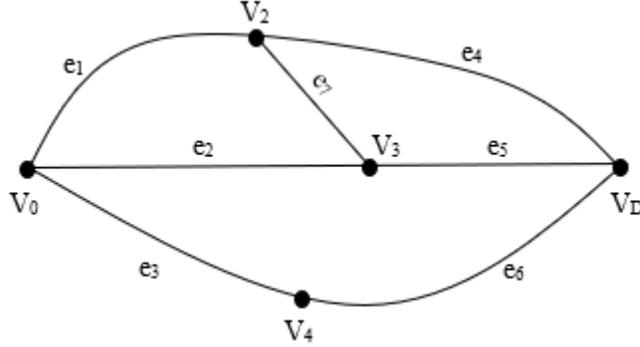


Figure 8: The graph G_2 produced by shortening paths from G_1 . The artificial vertex v_4 has been added with the same level as v_2 and v_3 , and the set of edges $\{e_1, e_2, e_3\}$ and $\{e_4, e_5, e_6\}$ are equilateral within their own sets.

Step 5. For each $\Gamma'_j \subset G_2$, define the level function restricted on Γ'_j as $S_j : \Gamma'_j \rightarrow [0, D]$. For each vertex $v_i \in \Gamma'_1$, make $S_k^{-1}(S_1(v_i))$ an artificial vertex of Γ'_k if it is not an original vertex for all $k \neq 1$. Continue this process for $\Gamma'_2, \dots, \Gamma'_m$. In the end, at each level of G_2 , if there exists a vertex on some paths, then each path has a vertex at this level. Finally, identifying all the vertices at the same level yields the desired pumpkin chain G' . Note that the $V(G')$ can be no larger than $V(G_2)$, with equality only if all vertices reside at different levels. (Figure 9)

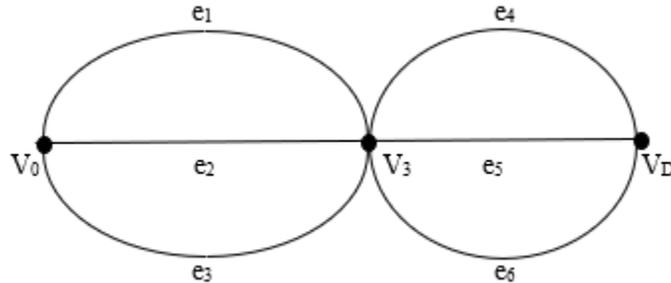


Figure 9: The graph G' produced by identifying v_2, v_3, v_4 and the edge e_7 has degraded to a point.

The algorithm involves removing pendants, shortening edges, and identifying vertices, which, by Lemma 3.1, can only potentially raise the spectral gap. \square

Therefore, for any quantum graph G with given geometric properties D, V, L , we can construct a pumpkin chain G' by Lemma 4.2, such that the diameter is preserved, and the length and number of vertices are bounded by those of G' , while $\lambda_1(G') \geq \lambda_1(G)$. Hence, we can solely study the upper bound on the spectral gap of pumpkin chains.

The next result introduced in [8] will reduce the study on a pumpkin chain G to a one-dimensional Sturm-Liouville problem, as we can find an eigenfunction ψ_1 corresponding to $\lambda_1(G)$ which only depends on the level of points in G . However, the original proof contains a flaw by assuming that the eigenfunction cannot vanish identically on any pumpkin. We will present a correct proof of this result without this assumption.

Lemma 4.3 (Lemma 5.6 of [8]). *Suppose G is a pumpkin chain. There exists an eigenfunction ψ_1 associated with $\lambda_1(G)$ and a function $\varphi : [0, D] \rightarrow \mathbb{R}$ such that $\psi_1(z) = \varphi(S(z))$ for all $z \in G$.*

Proof. If there exists an eigenfunction ψ associated with $\lambda_1(G)$ which does not vanish on at least one vertex of G , for example, $\psi(v) \neq 0$, then we can construct a new function ψ_1 on G by averaging the value of ψ at each fixed level. Since $\psi(v) \neq 0$, and taking average on a single point will not change the value at that point, we have $\psi_1(v) \neq 0$. Together with continuity, we see that $\psi_1 \not\equiv 0$. We further observe that ψ_1 is also an eigenfunction for $\lambda_1(G)$, since it is constructed as a linear combination of eigenfunctions on each edge. Finally, ψ_1 depends only on the level, since we set ψ_1 's value at the same level to be the average value of the ψ 's values on that level. Therefore, ψ_1 is the desired eigenfunction.

Now we only need to ensure the existence of such an eigenfunction ψ which does not vanish on at least one vertex of G . Suppose there exists an eigenfunction ψ associated with $\lambda_1(G)$ which vanishes at all vertices of G . Consider its longest pumpkin and denote its length by ℓ_{max} . Since ψ is an eigenfunction of G , its restriction to the edges of this longest pumpkin is also an eigenfunction associated with $\lambda_1(G)$. Note that $\lambda_1(G)$ may not be the first eigenvalue on these edges. Since ψ vanishes on all vertices, it vanishes on the endpoints of this pumpkin. By Dirichlet's condition, $\lambda_1(G) \geq \frac{\pi^2}{\ell_{max}^2}$. On the other hand, by Theorem

6.1 of [8], $\lambda_1(G) \leq \frac{\pi^2}{\ell_{max}^2}$. Therefore, $\lambda_1(G) = \frac{\pi^2}{\ell_{max}^2}$. Since $\ell_{max} \geq \ell_e$ for all edges $e \in G$, we have $\frac{\pi^2}{\ell_{max}^2} \leq \frac{\pi^2}{\ell_e^2}$, but Dirichlet's condition gives $\frac{\pi^2}{\ell_{max}^2} \geq \frac{\pi^2}{\ell(e)^2}$. We have $\frac{\pi^2}{\ell_{max}^2} = \frac{\pi^2}{\ell_e^2}$ and hence G is equilateral.

We claim that G has only one pumpkin. If G has $k > 1$ pumpkins with $D(G) = D$, every edge in G has the same length $\frac{D}{k}$. Then $\lambda_1(G) = \frac{\pi^2}{\ell_{max}^2} = \frac{k^2\pi^2}{D^2}$ with an eigenfunction $\psi(z) = \sin\left(\frac{k\pi S(z)}{D}\right)$ for $z \in G$ which vanishes at all vertices of G . However, we can find another eigenvalue $\tilde{\lambda}_1(G) = \frac{\pi^2}{D^2} < \frac{k^2\pi^2}{D^2} = \lambda_1(G)$ with the eigenfunction $\tilde{\psi}(z) = \sin\left(\frac{\pi S(z)}{D}\right)$. Therefore, $\lambda_1(G)$ is not the smallest non-trivial eigenvalue and this is a contradiction. Hence, G has only one pumpkin. (Figure 10)

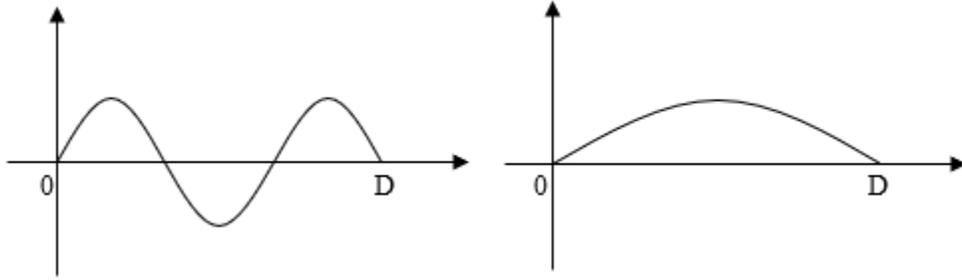


Figure 10: Left: eigenfunction which vanishes at all vertices on a pumpkin chain consisting of 3 equilateral pumpkins. Right: eigenfunction corresponding to λ_1 of the same pumpkin chain.

Since G has only one pumpkin, $\lambda_1(G) = \frac{\pi^2}{D^2}$ with an eigenfunction $\psi(z) = \sin\left(\frac{\pi S(z)}{D}\right)$ for $z \in G$, and ψ vanishes at all vertices of G (here the only vertices of G are the two endpoints of the pumpkin). Define another function $\tilde{\psi}$ on G by $\tilde{\psi}(z) := \cos\left(\frac{\pi S(z)}{D}\right)$. Clearly, $\tilde{\psi}$ is also an eigenfunction of $\lambda_1(G)$, but $\tilde{\psi}(v_0) = 1$ and $\tilde{\psi}(v_D) = -1$. (Figure 11)

In conclusion, for any eigenfunction ψ associated with $\lambda_1(G)$ which vanishes at all vertices of G , we can find another eigenfunction $\tilde{\psi}$ associated with $\lambda_1(G)$ which does not vanish on at least one vertex of G . Hence, we can always perform the averaging strategy to generate the eigenfunction ψ_1 which only depends on the level of points in G . \square

This implies that we only need to consider one-dimensional functions in the Rayleigh

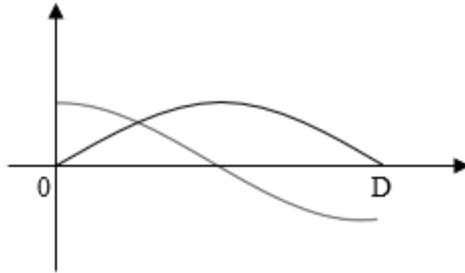


Figure 11: Eigenfunction corresponding to λ_1 on a single pumpkin. There exists a sine eigenfunction which vanishes at endpoints, but also another cosine eigenfunction which does not vanish at endpoints.

quotient with the weight function

$$\rho(x) := \#S^{-1}(x)$$

for $x \in [0, D]$. The weight function counts the number of edges at the given level. Therefore, the formula from Theorem 2.1 reduces to the following:

$$\lambda_1(G) = \inf \left\{ \frac{\int_0^D |u'(x)|^2 \rho(x) dx}{\int_0^D |u(x)|^2 \rho(x) dx} : u \in H^1([0, D]), \int_0^D u(x) \rho(x) dx = 0 \right\}.$$

5 Application: An Estimate in terms of Diameter and Total Length

By Lemma 4.2 and Lemma 4.3, to estimate the spectral gap of quantum graphs in terms of diameter and total length, it suffices to consider the one-dimensional Sturm-Liouville problem on pumpkin chains. Kennedy et al. [8] give the following upper estimate.

Theorem 5.1 (Theorem 7.1 of [8]). *Any quantum graph G satisfying the assumptions in the introduction and having diameter $D > 0$ and total length $L \geq D$ satisfies*

$$\lambda_1(G) \leq \frac{\pi^2}{D^2} \frac{4L - 3D}{D}.$$

In the original proof provided in [8], the test function serving as the upper estimate is defined by

$$\varphi(z) := \begin{cases} A \cos\left(\frac{\pi S(z)}{D}\right) & \text{if } S(z) \leq \frac{D}{2} \\ B \cos\left(\frac{\pi S(z)}{D}\right) & \text{if } S(z) > \frac{D}{2} \end{cases}$$

where A, B are chosen to satisfy the orthogonality condition $\int_G \varphi = 0$. Kennedy et al. [8] claimed that this estimate is far from optimal and is only sharp in the trivial case, meaning when the pumpkin chain consists of a single interval and hence $L = D$. In this section, we will investigate the sharpness of this estimate through an example. To be specific, we will numerically compute the first positive eigenvalue of a specific type of graph by fixing the diameter while altering the total length.

Example 5.2. Consider the pumpkin chain G with diameter D where extra edges are centered around the midpoint of the main diameter. Therefore, G consists of three pumpkins with two single-edge pumpkins on the sides and a thin but tall pumpkin in the middle as shown in Figure 12. Note that all extra edges in the center are equilateral since they belong to the same pumpkin. Denote the length of one extra edge by e , and the number of extra edges by k . Then the total length $L = D + ke$. Let $x \in [0, D]$ be the longitudinal coordinate. Then

$L_1 = \frac{D}{2} - \frac{\epsilon}{2}$ is the coordinate of the left vertex of the extra edges, and $L_2 = \frac{D}{2} + \frac{\epsilon}{2}$ is the coordinate of the right vertex of the extra edges.

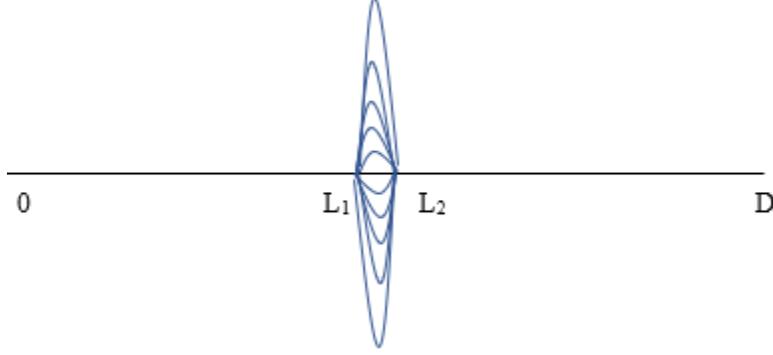


Figure 12: The graph G with $k = 10$.

Recall from the end of section 4 that

$$\lambda_1(G) = \inf \left\{ \frac{\int_0^D |u'(x)|^2 \rho(x) dx}{\int_0^D |u(x)|^2 \rho(x) dx} : u \in H^1([0, D]), \int_0^D u(x) \rho(x) dx = 0 \right\}.$$

Since ρ is piecewise constant, the eigenfunction ψ_1 corresponding to $\lambda_1(G)$ will take the form of sine and cosine of the same frequency σ on each pumpkin, where $\sigma^2 = \lambda_1(G)$. The vertex condition on the end points degrades to Neumann condition, and ψ_1 will only be cosine on the side pumpkins and a linear combination of sine and cosine in the middle pumpkin:

$$\psi_1(x) = \begin{cases} \cos(\sigma x) & x \in [0, L_1] \\ a_1 \cos(\sigma x) + a_2 \sin(\sigma x) & x \in [L_1, L_2] \\ b \cos(\sigma(D - x)) & x \in [L_2, D]. \end{cases}$$

We can assume the coefficient in the first pumpkin to be 1 by rescaling ψ_1 . The coefficients

a_1, a_2, b are chosen to satisfy the vertex condition at L_1, L_2 :

$$\begin{aligned}
\cos(\sigma L_1) - a_1 \cos(\sigma L_1) - a_2 \sin(\sigma L_1) &= 0 \\
\sigma \sin(\sigma L_1) - a_1(k+1)\sigma \sin(\sigma L_1) + a_2(k+1)\sigma \cos(\sigma L_1) &= 0 \\
a_1 \cos(\sigma L_2) - a_2 \sin(\sigma L_2) + b \cos(\sigma(D - L_2)) &= 0 \\
a_1(k+1)\sigma \sin(\sigma L_2) - a_2(k+1)\sigma \cos(\sigma L_2) + b \sigma \sin(\sigma(D - L_2)) &= 0.
\end{aligned}$$

We can rewrite the system of equations in the matrix form. Let

$$A = \begin{pmatrix} \cos(\sigma L_1) & -\cos(\sigma L_1) & -\sin(\sigma L_1) & 0 \\ \sigma \sin(\sigma L_1) & -(k+1)\sigma \sin(\sigma L_1) & (k+1)\sigma \cos(\sigma L_1) & 0 \\ 0 & \cos(\sigma L_2) & -\sin(\sigma L_2) & \cos(\sigma(D - L_2)) \\ 0 & (k+1)\sigma \sin(\sigma L_1) & -(k+1)\sigma \cos(\sigma L_1) & \sigma \sin(\sigma(D - L_2)) \end{pmatrix},$$

and

$$x = \begin{pmatrix} 1 \\ a_1 \\ a_2 \\ b \end{pmatrix}.$$

The homogeneous linear system $Ax = 0$ admits nontrivial solution of the coefficient vector x if and only if $\det(A) = 0$, where it is a function of σ and the spectral gap λ_1 can be computed from its smallest positive root σ_1 . The eigenfunction ψ_1 can be recovered from the nontrivial solution of the coefficient vector x once σ_1 is obtained. Note that ψ_1 will automatically satisfy the orthogonality condition since eigenspaces corresponding to different eigenvalues are orthogonal complements of each other.

In Figure 13, $\psi_1(x)$ takes the form of cosine function on the side pumpkins while tending to a flat line in the middle pumpkin. By Sturm-Liouville theory, $\psi_1(x)$ should have a single

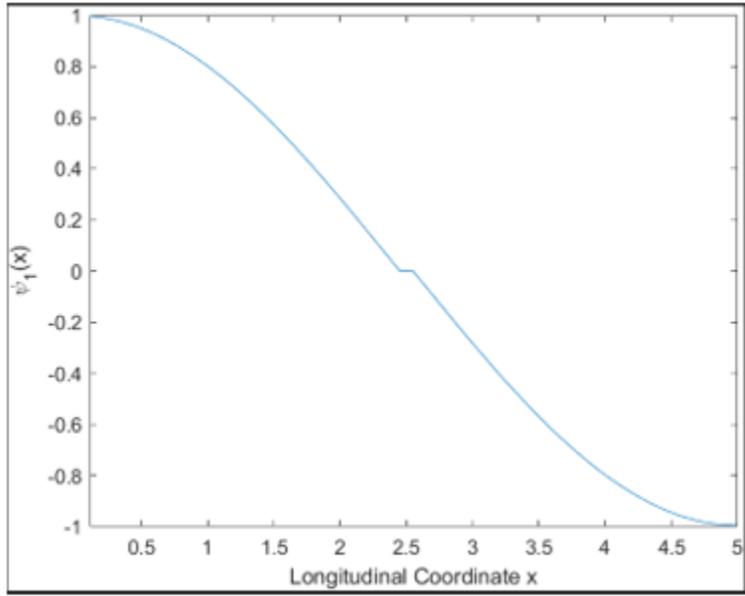


Figure 13: The eigenfunction $\psi_1(x)$. The graph G has $D = 5, e = 0.1, k = 100$.

zero, and we can check that, from Figure 13, $\psi_1(x)$ is decreasing and passes through zero only once.

We can alter the number of extra edges k and thus changing the total length while fixing the diameter. Then observe how λ_1 behaves under this change and compare it with the upper estimate in Theorem 5.1.

In Figure 14, λ_1 lies below the upper bound in Theorem 5.1 for all k values, and this suggests that the upper bound is valid in our example. We can further observe that, when k is small and the total length is not much larger than the diameter, λ_1 is very close to the upper bound. However, as k and L increase, λ_1 nearly remains constant while the upper estimate increases drastically compared to λ_1 . Therefore, in our example, the upper bound in Theorem 5.1 serves as a good estimator of λ_1 when k and L are small but fails to capture its trend as k and L grow larger.

Example 5.2 justifies the comment in [8] which says that the upper bound in Theorem 5.1 is far from optimal. It also suggests that the upper bound may overestimate the contribution from the extra edges to λ_1 . Since the test function adopted in the original proof of Theorem 5.1 assumes no information about the configuration of the extra edges on

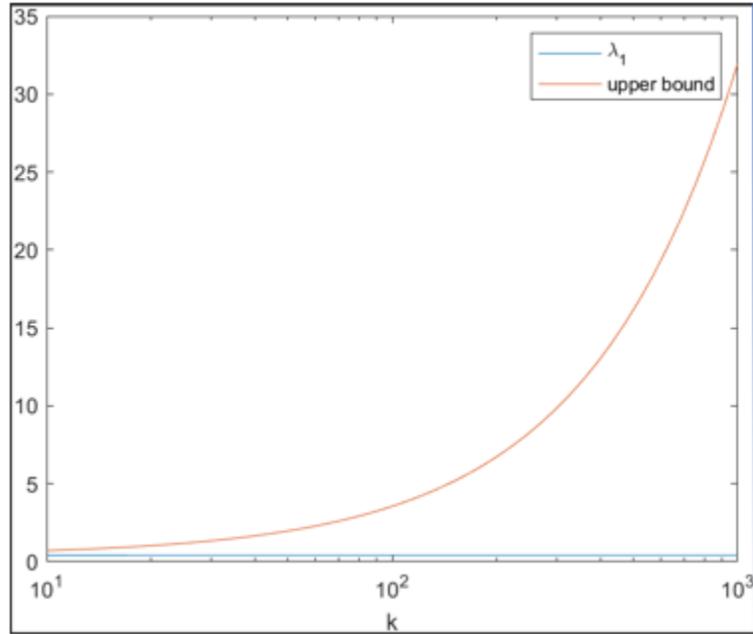


Figure 14: Comparison between the upper bound in Theorem 5.1 and λ_1 with different numbers of extra edges k . The graph G has $D = 5, e = 0.1$.

the pumpkin chain and it fails to approximate the actual first eigenfunction, an improvement on this upper bound may need a test function which suggests more information on the configuration of the maximizer graph.

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