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Article

SPECTRAL BOUNDS FOR LAPLACIAN ENERGY VIA WEIGHTED EIGENVALUE DEVIATIONS

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Abstract: In this paper, we study Laplacian energy using a parameterized spectral framework based on deviations of Laplacian eigenvalues from the average degree. The approach introduces a weighting parameter that allows the contributions of individual eigenvalues to be examined more directly.

Using this formulation, we derive a partitioned lower bound and a quadratic spectral upper bound, both expressed in terms of Laplacian eigenvalues. The bounds depend on a continuous parameter and a discrete partition index, which are optimized according to the structure of the spectrum.

An asymptotic analysis is carried out for representative graph families, showing that the behaviour of the bounds depends on the distribution of the Laplacian eigenvalues. Graphs with concentrated or highly skewed spectra lead to limiting parameter values, while more balanced spectra lead to intermediate values.

Numerical results support these observations and show that the parameters reflect how the Laplacian energy is distributed across the spectrum. In this way, the framework also provides information about the underlying spectral structure of the graph, in addition to bounding the energy.

Keywords: Laplacian energy; spectral graph theory; Laplacian eigenvalues; spectral bounds; weighted spectral deviation; graph spectra..

1. INTRODUCTION

The energy of a graph was introduced by Gutman as a spectral quantity associated with the adjacency matrix of a graph [6]. Since then, the concept of graph energy and its variants have been studied extensively in both mathematics and mathematical chemistry. A comprehensive account of graph energy and its applications can be found in the book by Li, Shi and Gutman [10].

One of the most important matrices associated with a graph is the Laplacian matrix. Its eigenvalues reflect important structural properties of the graph such as connectivity and expansion. Motivated by these considerations, Gutman and Zhou introduced the notion of Laplacian energy [8]. If G is a graph with Laplacian eigenvalues μ_1, μ_2, ..., μ_n and average degree $\underline{d} = 2m/n$, then the Laplacian energy is defined as$LE(G) = \sum_{i=1}^{n} \left|\mu_i - \underline{d}\right|$

This quantity measures the deviation of the Laplacian spectrum from its average value.

After its introduction, Laplacian energy became the subject of considerable study. Various bounds and properties of this invariant have been obtained using both combinatorial and spectral methods. Das [3] derived general

bounds for Laplacian energy in terms of graph parameters such as the number of vertices, the number of edges and the maximum degree. Related spectral estimates were also considered for Laplacian-type energy quantities [7].

However, many of the commonly used bounds are expressed in terms of aggregate graph parameters such as the number of edges or degree variance. While these are convenient and easy to compute, they do not directly reflect how the Laplacian eigenvalues are distributed. Because of this, finer spectral features that influence Laplacian energy may not be fully captured.

The behaviour of Laplacian energy for random graphs has also been studied. In particular, Du, Li and Li derived lower and upper bounds for the Laplacian energy of random graphs using results from random matrix theory. They also showed that these bounds describe the behaviour of Laplacian energy for almost all graphs [4]. These results indicate that the structure of the Laplacian spectrum plays an important role in determining the value of the energy.

More recently, Laplacian energy has been studied for several specific graph classes and graph constructions. For example, Mei [12] investigated the energy and Laplacian energy of chain graphs. D'Souza, Nayak and Bhat [2] studied the Laplacian energy of partial complements of graphs. Preetha, Suresh and Bonyah [13] examined spectral properties and Laplacian energy for graphs with self-loops, while Jusni and Sarmin [9] considered Laplacian energy for conjugacy class graphs associated with generalized quaternion groups.

Extensions of the concept have also been considered in related settings. Anchan, D'Souza, Gowtham and Bhat [1] studied the Laplacian energy of graphs with self-loops and obtained explicit formulas for this generalized case. Another related direction is the study of distance Laplacian energy, where the deviations of distance Laplacian eigenvalues from their average value are analyzed [5]. In addition, Liu et al. [11] recently obtained new bounds for the energy of graphs with self-loops using spectral techniques.

These developments show that spectral methods provide useful tools for studying energy-type graph invariants.

In particular, the distribution of Laplacian eigenvalues plays a central role in the analysis of Laplacian energy.

In this paper we introduce a parameterized weighted spectral deviation framework for the study of Laplacian energy. The idea is to examine the deviations $\left|\mu_i - \underline{d}\right|$ through weights depending on a positive parameter α This formulation provides a flexible spectral setting in which the contributions of individual eigenvalues can be analyzed more directly.

Using this framework, we derive two bounds for Laplacian energy. The first is a partitioned lower bound obtained by isolating the eigenvalues with the largest spectral deviations. The second is a quadratic spectral upper bound derived from a weighted spectral inequality. Both bounds are expressed directly in terms of Laplacian eigenvalues and depend on parameters that can be optimized. These results provide a unified spectral approach for obtaining tighter enclosures of Laplacian energy.

Preliminaries

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $|V(G)| = n$ and $|E(G)| = m$. The degree of a vertex v is denoted by $d(v)$. The average degree of G is

$$\underline{d} = 2m/n$$

The Laplacian matrix of G is defined as

$L(G) = D(G) - A(G)$,

where $A(G)$ is the adjacency matrix of G and $D(G)$ is the diagonal matrix of vertex degrees. The Laplacian matrix is real and symmetric, and hence all its eigenvalues are real. We denote the Laplacian eigenvalues of G by

$\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$.

The Laplacian energy of G is defined by

$$LE(G) = \sum_{i=1}^{n} \left|\mu_i - \underline{d}\right|$$

Since $\mu_n = 0$, this can be written as

$$LE(G) = \sum_{i=1}^{n-1} \left|\mu_i - \underline{d}\right| + \underline{d}$$

Throughout the paper, we use the identities

$$\sum_{i=1}^{n-1} \mu_i = 2m \quad and \quad \mu_i \geq 0 \; \forall \; i$$

which follow from basic properties of the Laplacian matrix.

Parametric Weighted Spectral Deviation Framework

In this section, we introduce a parametric weighted formulation of Laplacian energy. The purpose of this formulation is to rewrite each deviation term $\left|\mu_i - \underline{d}\right|$ in a form that allows the use of spectral inequalities and parameter optimization.

3.1 Definition of the parametric weight

Let $\alpha > 0$ be a fixed real parameter. For $\mu > 0$, we define

$w_\alpha(\mu) = \frac{|\mu - \underline{d}|}{\mu + \alpha \underline{d}}$.

At $\mu = 0$, we define

$$w_\alpha(0) = \frac{\underline{d} - \mu}{\mu + \alpha \underline{d}} = \frac{1}{\alpha}$$

This definition gives a continuous extension of w_α to $\mu = 0$. The denominator $\mu + \alpha \underline{d}$ is strictly positive for all $\mu \geq 0$, so the weight function is well defined.

3.2 Basic properties of the weight function

We now record some elementary properties of w_α which will be used later.

Lemma 3.1. *Let $\alpha > 0$ and $\mu > 0$. Then the following statements hold:*

$w_\alpha(\mu) \geq 0$.

$w_\alpha(\underline{d}) = 0$.

The function w_α is strictly decreasing on $(0, \underline{d})$ and strictly increasing on $(\underline{d}, \infty)$.

Proof. For $\mu > 0$, both $\left|\mu - \underline{d}\right|$ and $\mu + \alpha \underline{d}$ are nonnegative, and the denominator is strictly positive. Hence $w_\alpha(\mu) \geq 0$.

If $\mu = \underline{d}$, then $\left|\mu - \underline{d}\right| = 0$, and therefore $w_\alpha(\underline{d}) = 0$.

For $\mu \neq \underline{d}$, we can write

$$w_\alpha(\mu) = \{\frac{\underline{d} - \mu}{\mu + \alpha \underline{d}}, \;\; 0 < \mu < \underline{d} \; \frac{\mu - \underline{d}}{\mu + \alpha \underline{d}} \; , \mu > \underline{d}$$

Differentiating with respect to μ, we get

$$w'_\alpha(\mu) = \{\frac{-\left((\alpha+1)\underline{d}\right)}{\left(\mu + \alpha \underline{d}\right)^2}, 0 < \mu < \underline{d} \; \frac{\left((\alpha+1)\underline{d}\right)}{\left(\mu + \alpha \underline{d}\right)^2}, \qquad \mu > \underline{d}$$

Since $\alpha > 0$ *and* $\underline{d} > 0$, this shows that w_α is strictly decreasing on $(0, \underline{d})$ and strictly increasing on $(\underline{d}, \infty)$.

Remark 3.2. *The monotonicity of w_α implies that, among the nonzero Laplacian eigenvalues, the maximum value of $w_\alpha(\mu_i)$ is always attained at one of the spectral endpoints μ_1 or μ_{n-1}.*

3.3 Exact parametric decomposition of Laplacian energy

We now give the parametric decomposition of Laplacian energy.

Theorem 3.3. *Let G be a connected graph with Laplacian eigenvalues $\mu_1, \mu_2, \ldots, \mu_n$ and let $\alpha > 0$. Then*

$$LE(G) = \sum_{i=1}^{n-1} (\mu_i + \alpha\underline{d})\, w_\alpha(\mu_i) + \underline{d}$$

Proof. By definition of Laplacian energy, we have

$$LE(G) = \sum_{i=1}^{n} |\mu_i - \underline{d}|$$

Since $\mu_n = 0$, this can be written as

$$LE(G) = \sum_{i=1}^{n-1} |\mu_i - \underline{d}| + |\mu_n - \underline{d}| = \sum_{i=1}^{n-1} |\mu_i - \underline{d}| + \underline{d} \qquad (1)$$

For each $i = 1, 2, \ldots, n-1$, we have $\mu_i > 0$. By the definition of the parametric weight function,

$$w_\alpha(\mu) = \frac{|\mu - \underline{d}|}{\mu + \alpha\underline{d}}$$

and therefore

$$|\mu_i - \underline{d}| = (\mu_i + \alpha\underline{d})\, w_\alpha(\mu_i)$$

Put in eqn (1), we get

$$LE(G) = \sum_{i=1}^{n-1} (\mu_i + \alpha\underline{d})\, w_\alpha(\mu_i) + \underline{d}$$

which proves the result.

Lower bound

In this section, we derive a lower bound for Laplacian energy by isolating the contribution of those Laplacian eigenvalues that deviate most from the average degree.

Let $1 \le k \le n-1$ be an integer. Among the nonzero Laplacian eigenvalues $\mu_1, \mu_2, \ldots, \mu_{n-1}$, consider the k eigenvalues for which the quantities $|\mu_i - \underline{d}|$ are the largest. Let S_k denote the corresponding index set. The remaining indices form the set

$$S_k^c = \{1, 2, \ldots, n-1\} \setminus S_k$$

Define

$$w_{\alpha,min}^{(k)} = w_\alpha(\mu_i)$$

Theorem 4.1 (Partitioned Lower Bound)**.** *Let G be a connected graph with Laplacian eigenvalues $\mu_1, \mu_2, \ldots, \mu_n$ and let $\alpha > 0$. Then, for every $1 \le k \le n-1$,*

$$LE(G) \geq w_{\alpha,min}^{(k)} \left(\sum_{i \in S_k} \mu_i + k\, \alpha \underline{d} \right) + \underline{d}$$

Proof. From the exact parametric decomposition **Theorem 3.3**, we have

$$LE(G) = \sum_{i=1}^{n-1} \left(\mu_i + \alpha \underline{d}\right) w_\alpha(\mu_i) + \underline{d}$$

We split the sum over the index sets S_k and S_k^c:

$$\sum_{i=1}^{n-1} \left(\mu_i + \alpha \underline{d}\right) w_\alpha(\mu_i) = \sum_{i \in S_k} \left(\mu_i + \alpha \underline{d}\right) w_\alpha(\mu_i) + \sum_{i \in S_k^c} \left(\mu_i + \alpha \underline{d}\right) w_\alpha(\mu_i)$$

Since $\mu_i \geq 0$ and $w_\alpha(\mu_i) \geq 0$ for all i, every term in the second sum is nonnegative.

Hence,

$$LE(G) \geq \sum_{i \in S_k} \left(\mu_i + \alpha \underline{d}\right) w_\alpha(\mu_i) + \underline{d} \qquad (2)$$

By definition of $w_{\alpha,min}^{(k)}$ we have

$$w_\alpha(\mu_i) \geq w_{\alpha,min}^{(k)} \quad \forall\, i \in S_k$$

Therefore,

$$\sum_{i \in S_k} \left(\mu_i + \alpha \underline{d}\right) w_\alpha(\mu_i) \geq w_{\alpha,min}^{(k)} \sum_{i \in S_k} \left(\mu_i + \alpha \underline{d}\right) \qquad (3)$$

from (2) and (3) we get

$$LE(G) \geq w_{\alpha,min}^{(k)} \sum_{i \in S_k} \left(\mu_i + \alpha \underline{d}\right) + \underline{d} = w_{\alpha,min}^{(k)} \left(\sum_{i \in S_k} \mu_i + k\, \alpha \underline{d} \right) + \underline{d}$$

Which proves the result.

Remark 4.2. *The strength of the bound depends on the choice of k. For k = 1, the bound isolates the contribution of a single extremal eigenvalue. Larger values of k are more effective when the Laplacian energy is driven by several eigenvalues rather than by a single spectral endpoint.*

4.1 Optimization of lower bound with respect to the parameter α

We now discuss the choice of the parameter α that maximizes the partitioned lower bound given in Theorem 4.1.

Fix an integer k and the corresponding index set S_k. Assume that, for the values of α under consideration, the minimum defining $w_{\alpha,min}^{(k)}$ attained at a fixed eigenvalue $\mu^* \in S_k$.

Let

$$A = \sum_{i \in S_k} \mu_i$$

Then the lower bound can be written in the form

$$LB_{k,\alpha}(G) = \frac{|\mu^* - \underline{d}|}{\mu^* + \alpha\underline{d}}\left(A + k\alpha\underline{d}\right) + \underline{d}$$

Since $\underline{d}$ and $|\mu^* - \underline{d}|$ are constants, the behavior of the bound with respect to α is determined by the function

$$f(\alpha) = \frac{A + k\alpha\underline{d}}{\mu^* + \alpha\underline{d}}$$

Differentiating with respect to α, we get

$$f'(\alpha) = \frac{\underline{d}\,(k\mu^* - A)}{\left(\mu^* + \alpha\underline{d}\right)^2}$$

Hence, the sign of the derivative is determined by the sign of $k\mu^* - A$.

If $k\mu^* > A$, then $f'(\alpha) > 0\ \forall \alpha > 0$, and the lower bound is strictly increasing in α.

In this case, the optimal value of the bound is obtained in the limit $\alpha \to \infty$.

If $k\mu^* < A$, then $f'(\alpha) < 0\ \forall\ \alpha > 0$, and the lower bound is strictly decreasing in α. In this case, the optimal value of the bound is obtained in the limit $\alpha \to 0^+$.

If $k\mu^* = A$, then $f'(\alpha) = 0\ \forall\ \alpha > 0$, and the bound is independent of α.

Consequently, for fixed k, the optimal lower bound is always attained at the boundary of the parameter range, either as $\alpha \to 0^+$ or as $\alpha \to \infty$.

4.2 Numerical evaluation of the lower bound

The partitioned lower bound depends on the integer k and the parameter α. While the bound is valid for every fixed k and $\alpha > 0$, the choice of these parameters influences its sharpness. For numerical purposes, it is therefore convenient to make the optimization explicit.

Fix k and let S_k denote the set of indices corresponding to the k largest values of $|\mu_i - \underline{d}|$. Assume that the minimum defining $w_{\alpha,min}^{(k)}$ attained at an eigenvalue $\mu^* \in S_k$. As shown in the previous section, the lower bound is a monotone function of α, and its optimal value is attained at the boundary of the parameter range. More precisely, the two limiting cases are given by

$$LB_0(G) = L\,B_{k,\alpha}(G) = \frac{|\mu^* - \underline{d}|}{\mu^*} \sum_{i \in S_k} \mu_i + \underline{d}$$

and

$$LB_\infty(G) = L\,B_{k,\alpha}(G) = k\,|\mu^* - \underline{d}| + \underline{d}$$

For fixed k, the optimized lower bound is therefore

$$LB_k^*(G) = \{\, LB_0(G),\, LB_\infty(G)\}$$

Finally, the numerical lower bound is obtained by maximizing over all admissible values of k, that is,

$$LB(G) = L\,B_k^*(G) = \left\{ \frac{|\mu^* - \underline{d}|}{\mu^*} \sum_{i \in S_k} \mu_i + \underline{d},\ k\,|\mu^* - \underline{d}| + \underline{d} \right\}$$

This procedure provides a computable lower bound for the Laplacian energy based solely on the Laplacian spectrum.

Upper bound

In this section, we derive an upper bound for the Laplacian energy using a quadratic inequality. The bound is obtained directly from the exact parametric decomposition and does not depend on any partition of the spectrum.

Theorem 5.1 (Quadratic Spectral Upper Bound)**.** *Let G be a connected graph with Laplacian eigenvalues* $\mu_1, \mu_2, \ldots, \mu_n$ *and let* $\alpha > 0$*. Then*

$$LE(G) \leq \sqrt{\left(2m + (n-1)\alpha\underline{d}\right)\left(\sum_{i=1}^{n-1} \frac{\left(\mu_i - \underline{d}\right)^2}{\mu_i + \alpha\underline{d}}\right)} + \underline{d}$$

Proof. From **Theorem 3.3**, we can have

$$LE(G) - \underline{d} = \sum_{i=1}^{n-1} \left(\mu_i + \alpha\underline{d}\right) w_\alpha(\mu_i) \qquad (4)$$

Using the definition of w_α, in eqn (4), we get

$$LE(G) - \underline{d} = \sum_{i=1}^{n-1} \sqrt{\mu_i + \alpha\underline{d}} \cdot \frac{\left|\mu_i - \underline{d}\right|}{\sqrt{\mu_i + \alpha\underline{d}}}$$

Applying the Cauchy–Schwarz inequality, we get

$$LE(G) - \underline{d} \leq \sqrt{\sum_{i=1}^{n-1} \left(\mu_i + \alpha\underline{d}\right)} \sqrt{\sum_{i=1}^{n-1} \frac{\left(\mu_i - \underline{d}\right)^2}{\mu_i + \alpha\underline{d}}} \qquad (5)$$

Since $\sum_{i=1}^{n-1} \mu_i = 2m$, we get

$$\sum_{i=1}^{n-1} \left(\mu_i + \alpha\underline{d}\right) = 2m + (n-1)\alpha\underline{d}$$

Substituting this in inequality (5), we get the stated result.

5.1 Optimization of upper bound with respect to the parameter α

To study the optimization of the upper bound, we introduce the function

$$F(\alpha) = \left(2m + (n-1)\alpha\underline{d}\right) \sum_{i=1}^{n-1} \frac{\left(\mu_i - \underline{d}\right)^2}{\mu_i + \alpha\underline{d}}$$

which is the expression inside the square root in the quadratic spectral upper bound.

Proposition 5.3 [Existence of a Global Minimizer in the Extended Domain] The function $F(\alpha)$ admits a continuous extension to the compactified interval $[0, \infty]$. Consequently, F attains its global minimum at some $\alpha^* \in [0, \infty]$.

Proof. The function F is continuous on $(0, \infty)$. As $\alpha \to 0^+$,

$$F(\alpha) \to A(0)B(0),$$

which is finite. As $\alpha \to \infty$,

$F(\alpha) \to (n-1) \sum c_i$ where $c_i = \left(\mu_i - \underline{d}\right)^2 \geq 0$

which is also finite. Hence F extends continuously to the compactified interval $[0,\infty]$. Since a continuous function on a compact set attains its minimum, F achieves a global minimum at some $\alpha^* \in [0,\infty]$.

Proposition 5.4 [Optimization Condition] Let G be a connected graph. If the parametric upper bound attains its minimum at an interior point $\alpha^* > 0$, then α^* satisfies the equation

$$(n-1)\sum_{i=1}^{n-1} \frac{(\mu_i - \underline{d})^2}{\mu_i + \alpha^* \underline{d}} = (2m + (n-1)\alpha^* \underline{d}) \sum_{i=1}^{n-1} \frac{(\mu_i - \underline{d})^2}{(\mu_i + \alpha^* \underline{d})^2}$$

Proof. Since,

$$F(\alpha) = (2m + (n-1)\alpha \underline{d}) \sum_{i=1}^{n-1} \frac{(\mu_i - \underline{d})^2}{\mu_i + \alpha \underline{d}}$$

To minimize the bound, it is sufficient to minimize $F(\alpha)$.

Differentiating $F(\alpha)$ with respect to α, we get

$$F'(\alpha) = (n-1)\underline{d} \sum_{i=1}^{n-1} \frac{(\mu_i - \underline{d})^2}{\mu_i + \alpha \underline{d}} + (2m + (n-1)\alpha \underline{d}) \sum_{i=1}^{n-1} \frac{-(\mu_i - \underline{d})^2 \cdot \underline{d}}{(\mu_i + \alpha \underline{d})^2}$$

A critical point α^* satisfies $F'(\alpha^*) = 0$. Since $\underline{d} \neq 0$, so divide with $\underline{d}$ throughout, we get

$$(n-1)\sum_{i=1}^{n-1} \frac{(\mu_i - \underline{d})^2}{\mu_i + \alpha^* \underline{d}} - (2m + (n-1)\alpha^* \underline{d}) \sum_{i=1}^{n-1} \frac{(\mu_i - \underline{d})^2}{(\mu_i + \alpha^* \underline{d})^2} = 0$$

$$\therefore (n-1)\sum_{i=1}^{n-1} \frac{(\mu_i - \underline{d})^2}{\mu_i + \alpha^* \underline{d}} = (2m + (n-1)\alpha^* \underline{d}) \sum_{i=1}^{n-1} \frac{(\mu_i - \underline{d})^2}{(\mu_i + \alpha^* \underline{d})^2}$$

which is required result

Proposition 5.5 [Strict Local Minimum] Let $\alpha^* > 0$ be a solution to the stationarity equation $F'(\alpha) = 0$. Then α^* is a non-degenerate critical point with positive second derivative. Consequently, α^* corresponds to a strict local minimum of the parametric upper bound.

Proof. Let $x = \alpha \underline{d}$. Minimizing the parametric upper bound is equivalent to minimizing the expression inside the square root in **Theorem 5.1**. The stationarity condition for this expression is equivalent to finding the roots of

$$f(x) = \sum_{i=1}^{n-1} c_i \frac{\mu_i - K}{(\mu_i + x)^2} = 0$$

where $c_i = (\mu_i - \underline{d})^2 \geq 0$ and $K = \frac{2m}{n-1}$ is the average of the nonzero eigenvalues. The nature of the critical point is determined by the sign of the second derivative of the objective function, which is proportional to $f(x)$ at the root. Differentiating $f(x)$ with respect to x gives:

$$f'(x) = -2\sum_{i=1}^{n-1} c_i \frac{\mu_i - K}{(\mu_i + x)^3}$$

We partition the summation indices into two sets based on the deviation from the average eigenvalue: $P = \{i : \mu_i > K\}$ and $N = \{j : \mu_j < K\}$. We assume G is not a regular graph, which ensures non-trivial deviations. At the root x^*, the condition $f(x^*) = 0$ implies that the positive and negative contributions balance:

$$\sum_{i\in P} \frac{c_i(\mu_i - K)}{(\mu_i + x^*)^2} = \sum_{j\in N} \frac{c_j(K - \mu_j)}{(\mu_j + x^*)^2} = S$$

where $S > 0$.

For indices in P, we have $\mu_i > K$, which implies $\frac{1}{\mu_i + x^*} < \frac{1}{K + x^*}$. For indices in N, we have $\mu_j < K$, which implies $\frac{1}{\mu_j + x^*} > \frac{1}{K + x^*}$.

Substituting these inequalities into the expansion of $f'(x*)$:

$$f'(x^*) = -2\left(\sum_{i\in P} \frac{1}{\mu_i + x^*}\frac{c_i(\mu_i - K)}{(\mu_i + x^*)^2} - \sum_{j\in N} \frac{1}{\mu_j + x^*}\frac{c_j(K - \mu_j)}{(\mu_j + x^*)^2}\right)$$

The first sum is strictly bounded above by $\frac{S}{K+x^*}$, and the second sum is strictly bounded below by $\frac{S}{K+x^*}$. Thus, the term inside the parentheses is strictly negative i.e.

$$\left(\sum_{i\in P} \frac{1}{\mu_i + x^*}\frac{c_i(\mu_i - K)}{(\mu_i + x^*)^2} - \sum_{j\in N} \frac{1}{\mu_j + x^*}\frac{c_j(K - \mu_j)}{(\mu_j + x^*)^2}\right) < \frac{S}{K + x^*} - \frac{S}{K + x^*} = 0$$

Multiplying by the factor -2, we get $f'(x^*) > 0$.

Since $x = \alpha \underline{d}$ with $\underline{d} > 0$, the sign of the second derivative of the objective function with respect to α coincides with the sign of $f'(x)$. Therefore, $F''(\alpha^*) > 0$. By the Second Derivative Test, α^* is a strict local minimum.

Remark 5.3. *The global minimizer may occur at $\alpha = 0$, at $\alpha = \infty$, or in the interior $(0, \infty)$. If it lies in the interior, Propositions 5.4 and 5.5 apply. Determining whether the minimizer is interior depends on the sign of $F'(0)$ and the asymptotic behavior of $F'(\alpha)$.*

Asymptotic Comparison with the Gutman–Zhou Bound for Star Graphs

We compare the upper bound with the classical Gutman–Zhou Laplacian energy bound for the family of star graphs.

Theorem 6.1 (Asymptotic dominance for star graphs)**.** *Let S_n be the star graph on n vertices. Let $m = n - 1$ denote the number of edges and $\underline{d} = 2m/n = 2(n-1)/n$ the average degree.*

Define the classical Gutman–Zhou quantity

$$M(G) = m + \frac{1}{2}\sum_{i=1}^{n} \left(d_i - \underline{d}\right)^2$$

and the corresponding upper bound $UB_{GZ}(G) = \sqrt{2M(G)n}$

Let $UB_\alpha(G)$ denote the parametric upper bound

$$UB_\alpha(G) = \sqrt{(2m + (n-1)\alpha\underline{d}\left(\sum_{i=1}^{n-1} \frac{(\mu_i - \underline{d})^2}{\mu_i + \alpha\underline{d}}\right)} + \underline{d}$$

for fixed $\alpha > 0$.

Then for every fixed $\alpha > 0$,

$$\frac{UB_{GZ}(S_n)}{UB_{\alpha}(S_n)} \to \infty \quad as\ n \to \infty$$

In particular,

$$UB_{GZ}(S_n) = \Theta\left(n^{3/2}\right), \qquad UB_{\alpha}(S_n) = \Theta(n)$$

Proof. We first describe the degree structure of S_n. In S_n graph,

$$d_1 = n-1, \qquad d_2 = \cdots = d_n = 1, \qquad m = n-1, \qquad \underline{d} = \frac{2(n-1)}{n}$$

We now compute the asymptotic behavior of $M(S_n)$.

Compute the degree deviations. For the central vertex,

$$d_1 - \underline{d} = (n-1) - \frac{2(n-1)}{n} = \frac{(n-1)(n-2)}{n}$$

Thus

$$\left(d_1 - \underline{d}\right)^2 = \frac{(n-1)^2(n-2)^2}{n^2}$$

For each leaf vertex,

$$d_i - \underline{d} = 1 - \frac{2(n-1)}{n} = -1 + \frac{2}{n}$$

$$\therefore \left(d_i - \underline{d}\right)^2 = \left(-1 + \frac{2}{n}\right)^2 = 1 - \frac{4}{n} + O(n^{-2})$$

Summing over all vertices,

$$\sum_{i=1}^{n} \left(d_i - \underline{d}\right)^2 = \frac{(n-1)^2(n-2)^2}{n^2} + (n-1)\left(1 - \frac{4}{n} + O(n^{-2})\right)$$

On expansion we get

$$\sum_{i=1}^{n} \left(d_i - \underline{d}\right)^2 = n^2 + O(n)$$

Therefore,

$$M(S_n) = (n-1) + \frac{1}{2}\left(n^2 + O(n)\right) = \frac{1}{2}n^2 + O(n)$$

Using this, we obtain the asymptotic behavior of $UB_{GZ}(S_n)$

$$UB_{GZ}(S_n) = \sqrt{2M(S_n)n}$$

we get

$$UB_{GZ}(S_n) = n^{3/2}\sqrt{1 + O(n^{-1})} = \Theta\left(n^{3/2}\right)$$

The Laplacian spectrum of S_n is given by

$\mu_1 = n, \quad \mu_2 = \cdots = \mu_{n-1} = 1, \quad \mu_n = 0$

Define $c_i = \left(\mu_i - \underline{d}\right)^2$

For $\mu_1 = n$, $c_1 = \left(n - \frac{2(n-1)}{n}\right)^2 = n^2 + O(n)$

For $\mu_i = 1$, $c_i = \left(1 - \frac{2(n-1)}{n}\right)^2 = 1 + O(n^{-1})$

We now analyze the asymptotic behavior of $UB_\alpha(Sn)$.

First compute

$$A(\alpha) = 2m + (n-1)\alpha\underline{d} = 2(n-1) + (n-1)\alpha\frac{2(n-1)}{n}$$

Hence

$$A(\alpha) \;=\; 2(1 \;+\; \alpha)n \;+\; O(1),$$

so $A(\alpha) \;=\; \Theta(n)$.

Now consider

$$B(\alpha) = \frac{c_1}{n + \alpha\underline{d}} + \sum_{i=2}^{n-1} \quad \frac{c_i}{1 + \alpha\underline{d}}$$

Since $n + \alpha\underline{d} = n + O(1)$ and $1 + \alpha\underline{d} = 1 + O(1)$, we get

$$B(\alpha) = \frac{n^2 + O(n)}{n + O(1)} + \frac{(n-2)\left(1 + O(n^{-1})\right)}{1 + O(1)}$$

Therefore

$$B(\alpha) \;=\; C(\alpha)n \;+\; O(1),$$

for some positive constant $C(\alpha)$. Thus $B(\alpha) \;=\; \Theta(n)$.

Hence

$$A(\alpha)B(\alpha) = \Theta(n^2)$$

and

$$UB_\alpha(S_n) = \sqrt{\Theta(n^2)} + \underline{d} = \Theta(n)$$

Combining the two growth estimates,

$$\frac{UB_{GZ}(S_n)}{UB_\alpha(S_n)} = \frac{\Theta\left(n^{3/2}\right)}{\Theta(n)} = \Theta\left(n^{1/2}\right) \to \infty$$

This completes the proof.

This difference in growth arises from the underlying structure of the two bounds. The Gutman–Zhou bound is driven by degree-based quantities, which become large in graphs with strong degree imbalance such as star graphs. In contrast, the proposed bound depends directly on the Laplacian eigenvalues, and the normalization in the weighted terms controls the contribution of large eigenvalues. As a result, the bound grows only linearly with n.

Numerical Analysis and Discussion

In this section we illustrate the behaviour of the bounds derived in the previous sections by numerical experiments on several graph families.

Both small graphs and large graphs are considered in order to observe how the bounds perform across different structural regimes. In this numerical study, we compare the bounds obtained in this paper with the classical bounds of Gutman and Zhou.

Classical bounds. Let G be a graph with n vertices and m edges. Let $d_1, d_2, \dots, d_n$ be the vertex degrees and let $\underline{d} = \frac{2m}{n}$ be the average degree. Following Gutman and Zhou, these degree-based quantities are defined as

$$M = m + \frac{1}{2}\sum_{i=1}^{n} \left(d_i - \underline{d}\right)^2$$

The classical lower and upper bounds for Laplacian energy are

$$LB_{GZ} = 2\sqrt{M}, \qquad UB_{GZ} = \sqrt{2Mn}$$

These bounds are taken as reference values in the tables. These bounds depend only on degree-based aggregate quantities and do not explicitly involve the Laplacian eigenvalues.

Bounds from this paper. The quantity LB_{part} denotes the partitioned lower bound obtained from Theorem 4.1, while UB_{QS} denotes the quadratic spectral upper bound given in Theorem 5.1. Both bounds are computed directly from the Laplacian spectrum, allowing them to reflect the distribution of eigenvalues rather than relying on coarse structural summaries.

Measure of improvement. To see how much the partitioned lower bound improves upon the classical lower bound, we use the following percentage measure:

$$Improvement(\%) = \frac{LB_{part} - LB_{GZ}}{LE(G) - LB_{GZ}} \times 100$$

This value shows how much of the gap between the classical lower bound and the exact Laplacian energy is covered by the partitioned lower bound.

In the numerical tables, we list the exact Laplacian energy $LE(G)$, the classical Gutman– Zhou bounds, the partitioned lower bound, the quadratic spectral upper bound, and the corresponding percentage improvement. This makes it easy to see the gain obtained by the proposed lower bound and the behaviour of the new upper bound in comparison with the classical one.

Definition of the upper bound gap. For the quadratic spectral upper bound, we define the gap by

Gap = $UB_{\text{QS}} - LE(G)$.

This quantity measures how far the upper bound is from the exact Laplacian energy. A smaller gap indicates that the upper bound is tighter and closer to the true value. A gap equal to zero means that the upper bound coincides with the exact Laplacian energy.

Table 1 presents the behaviour of the classical Gutman–Zhou bounds and the proposed parametric bounds for several small graph families. The results illustrate how the bounds vary across different structural types even at small orders.

For symmetric graphs such as K5 and K3,3, the partitioned lower bound coincides with the exact Laplacian energy. In particular, for K3,3 exactness is achieved with a single eigenvalue partition ($k* = 1$), reflecting the uniform spectral structure of the graph.

For graphs with strong degree heterogeneity, including the star S6 and the wheel W6, the degree-based upper bound takes relatively large values. The quadratic spectral upper bound remains close to the exact Laplacian energy. In these cases, the optimization leads to small positive values of $\alpha*$, which moderates the contribution of large eigenvalues. The lower bound also captures a substantial portion of the Laplacian energy.

For sparse and nearly regular graphs such as the cycle C6 and the path P5, the optimization behaves differently. The parameter $\alpha*$ increases beyond 1, leading to a more balanced contribution across the spectrum. The partitioned lower bound remains stable across these cases.

The discrete partition index k∗ and the continuous parameter α∗ adjust according to the spectral distribution of each graph. Even for small networks, the framework adapts to different structural patterns through these parameters.

Table 1: Laplacian Energy Bounds for Small Graph Families

Graph (*G*)	*n*	*LE*(*G*)	LB_{GZ}	LB_{part} (k^*)	**LB Imp (%)**	UB_{GZ}	UB_{QS} (α^*)	**UB Gap**
Complete K_5	5	8.0000	6.3246	8.0000 (4)	100.00	10.0000	8.0000 (∞)	0.0000
Bipartite $K_{3,3}$	6	6.0000	6.0000	6.0000 (1)	100.00	10.3923	8.1962 (≈ 0)	2.1962
Star S_6	6	8.6667	6.8313	8.3333 (5)	81.84	11.8322	8.6720 (≈ 0)	0.0053
Wheel W_6	6	10.4721	6.8313	8.8972 (5)	56.74	12.6491 (0.03)	10.6266	0.1545
Cycle C_6	6	8.0000	4.8990	7.0000 (5)	67.75	8.4853	8.1579 (1.67)	0.1579
Path P_5	5	6.0721	4.2895	4.6541 (3)	20.45	7.2111	6.5926 (2.45)	0.5204

Note: LB Imp (%) represents the percentage of the gap closed relative to the Gutman-Zhou baseline. UB Gap represents the absolute deviation of the proposed upper bound from the exact Laplacian energy.

Table 2 presents the behaviour of Laplacian energy bounds for several large graph families across different structural regimes. The graphs are grouped according to their structural properties in order to illustrate how the parameters k∗ and α∗ vary with the underlying spectral distribution.

For highly symmetric graphs such as the complete graph K5000 and dense Erdos–Renyi graphs G(n,0.8), the Laplacian spectrum is strongly concentrated around the average degree. In these cases, the optimization produces very large values of α∗. For the complete graph the upper bound coincides with the exact Laplacian energy, reflecting the uniform structure of the spectrum. In this case, $\alpha* \to \infty$ indicates that the bound is independent of α.

A different behaviour is observed in graphs with strong degree heterogeneity, including the star graph S5000, the wheel graph W5000 and Barabasi–Albert scale–free networks. These graphs contain vertices of very large degree, and their Laplacian spectra include dominant eigenvalues associated with these hubs. In these cases, the optimization produces small values of α∗, which moderates the contribution of large eigenvalues in the weighted deviation term. In particular, for star graphs this reflects the presence of a dominant eigenvalue, whose influence is controlled through the weighting mechanism. As a result, the upper bound remains close to the Laplacian energy. This behaviour is consistent with the asymptotic analysis for star graphs, where the growth of the bound is linear in n.

For graphs with more evenly distributed spectra, such as paths, cycles and sparse Erdos–Renyi graphs G(n,0.2), the optimized parameter takes moderate values. In these graphs the Laplacian eigenvalues are distributed more uniformly around the average degree, and the optimization balances the contributions of the spectral deviations.

The behaviour of the partition index k∗ is also consistent across the examples. For random and scale–free graphs the optimal value is typically close to one half of n, indicating that a substantial portion of the spectrum contributes to the lower bound. For highly symmetric graphs such as K5000 and S5000 the optimal value becomes $k* = n - 1$, corresponding to the full spectrum.

These observations show that the parameters α∗ and k∗ reflect different aspects of the spectral structure. The parameter α∗ adjusts the relative influence of large and small eigenvalues, while k∗ determines how many of the

dominant spectral deviations are captured. In this way, the framework provides information about how the Laplacian energy is distributed across the spectrum, rather than summarizing it through aggregate graph quantities.

Table 2: Laplacian Energy Bounds for Large Graph Families Across Different Structural Regimes

Regime	**Graph (G)**	n	$LE(G)$	LB_{GZ}	LB_{part} (k^*)	UB_{GZ}	UB_{QS} (α^*)	**UB Gap**
Sparse Structured	Path P_{5000}	5000	6366.20	141.42	3573.84 (2739)	7071.07	7070.95 (3749)	704.75
	Cycle C_{5000}	5000	6366.20	141.42	3575.35 (2741)	7071.07	7070.95 (7493)	704.75
	Wheel W_{5000}	5000	12174.19	7067.53	7241.45 (1667)	353376.71	16584.79 (0.35)	4410.60
Dense / Regular	Complete K_{5000}	5000	9998.00	7070.36	9998.00 (4999)	353518.03	9998.00 ($\to\infty$)	0.00
	Bipartite $K1000,1000$	2000	2000.00	2000.00	2000.00 (1)	63245.55	32622.82 ($\to$ 0)	30622.82
	Erdos–Renyi $G(n,0.8)$	800	11381.37	1109.93	5626.76 (377)	22198.52	13506.36 (10^4)	2124.99
Random Sparse	Erdos–Renyi $G(n,0.2)$	800	10729.51	672.39	5063.52 (381)	13447.79	12809.52 (4.67)	2080.01
Hub-Dominated	Star S_{5000}	5000	9996.00	7068.95	9996.00 (4999)	353553.39	9996.00 ($\to$ 0)	0.00
	BA(n,50)	1000	41182.14	2591.36	17733.58 (563)	57944.62	47399.51 (0.21)	6217.37

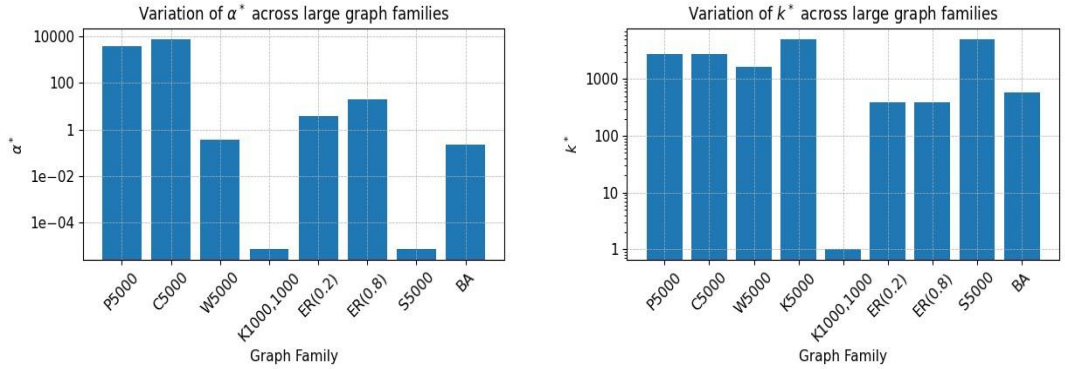

Figure 1: Variation of the optimal parameters α^* and k^* across large graph families (logarithmic scale).

Figures 1a and 1b show how the optimal parameters vary across different graph families.

From Figure 1(a), we see that the value of $\alpha*$ changes a lot depending on the graph structure. For graphs with a more uniform spectrum, such as dense graphs, $\alpha*$ becomes large. For graphs like star and bipartite graphs, where a few eigenvalues dominate, $\alpha*$ becomes very small. For paths, cycles, and random graphs, the values lie somewhere in between.

Figure 1(b) shows how the partition index $k*$ behaves. In graphs where many eigenvalues

contribute to the energy, $k*$ is close to n. On the other hand, in graphs like complete bipartite graphs, $k*$ is very small, which means only a few eigenvalues play a major role. For random and scale-free graphs, $k*$ takes moderate values.

Together, these plots show that the parameters α∗ and k∗ adjust according to how the Laplacian eigenvalues are distributed. The parameter α∗ controls how strongly different eigenvalues are weighted, while k∗ shows how many of them contribute significantly to the energy.

2. CONCLUSION

In this paper, we studied Laplacian energy using a parameterized spectral framework based on the deviations of

Laplacian eigenvalues from the average degree. We obtained a partitioned lower bound and a quadratic spectral upper bound,

both written directly in terms of the Laplacian eigenvalues. The parameters α and k are used to adjust the bounds, and their optimized values depend on how the eigenvalues are distributed.

The asymptotic analysis shows that the behaviour of the bounds is linked to the distribution of the Laplacian spectrum. When the spectrum is highly concentrated or uneven, the parameters move towards limiting values. When the spectrum is more balanced, the parameters take moderate values.

The numerical results show the same pattern. The values of α^* and k^* change across different graph families and reflect how the Laplacian energy is spread among the eigenvalues. Small values of α^* shows the presence of dominant eigenvalues, while larger values indicate a more uniform distribution. The parameter k^* shows how many eigenvalues contribute significantly to the energy.

These observations indicate that the parameters α^* and k^* carry information about the spectral structure of the graph, in addition to defining the bounds. In this way, the framework provides a spectral view of how Laplacian energy is distributed across the eigenvalues. The same approach can be explored for other spectral quantities in future work..

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