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On Radenković and Gutman Conjecture for certain Classes of Trees

Afeefa Maryam[1], M. Tariq Rahim[1,✉], Fawad Hussain[1]

[1] *Department of Mathematics, Abbattabad University of Science and Technology, Pakistan*

ABSTRACT

The Radenković and Gutman conjecture establishes a relationship between the Laplacian eigenvalues of any tree T_n, the star graph S_n and the path graph P_n, i.e., $\mathbb{LE}(P_n) \leq \mathbb{LE}(T_n) \leq \mathbb{LE}(S_n)$. In this paper, we prove this conjecture for a class of trees with n vertices and having diameter 16 to 30.

Keywords: Laplacian energy, Laplacian characteristics polynomial, Tree, Laplacian eigenvalues

1. Introduction

The "energy" of a graph is a concept that comes from spectral graph theory, a branch of graph theory that emphasizes the connections between the eigenvalues and eigenvectors of certain matrices associated with a graph. Graph energy have wide range of applications in the field of chemistry particularly in the study of molecular graphs and their properties. The energy of graph has been served as a structure descriptor in case of σ-electron systems. The graph energy gives better results than the traditional structure-descriptors. In this context, Liu et al. [8, 7] introduced Hosoya index of graphs formed by a fractal graph and minimize Kirchhoff index among graphs with a given vertex bipartiteness. Understanding the structure, stability, and reactivity of molecules in many chemical situations is made possible by the useful tools provided by graph energy and Laplacian energy analyses, which further advances synthetic chemistry.

Energy of graph is defined as the total of the absolute eigenvalues values of the adjacency matrix $\mathbf{A}(\mathbb{G})$ denoted by

$$\mathbb{E}(\mathbb{G}) = \sum_{r=1}^{n} |\lambda_r|,$$

✉ Corresponding author.

E-mail addresses: afifamalik0640@gmail.com (A. Maryam), tariqsms@gmail.com (M. T. Rahim), fawadhussain998@hotmail.com (F. Hussain).

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of $\mathbf{A}(\mathbb{G})$.

The Laplacian energy of a directed graph is denoted by

$$\mathbb{LE}(\mathbb{G}) = \sum_{r=1}^{n} |\mu_r - \frac{2m}{n}|,$$

where m is total number of edges and n is total number of vertices and $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of $L(\mathbb{G})$. The Laplacian matrix is defined as $L(\mathbb{G}) = D(\mathbb{G}) - \mathbf{A}(\mathbb{G})$, where $D(\mathbb{G})$ is the degree matrix.

Fiedler's theorem [3] established that if the second smallest eigenvalue of the Laplacian matrix $L(\mathbb{G})$ of a graph is equal to zero i.e $\mu_2 = 0$, then the graph is disconnected. Consequently, this eigenvalue, denoted as $a(\mathbb{G})$, is defined as the algebraic connectivity of the graph $\mathbb{G}$. The corresponding eigenvectors are referred as Fiedler vectors of $\mathbb{G}$. The relationship among energy and Laplacian energy of trees was investigated by Radenkovic and Gutman in [9].

Conjecture 1.1. *Let T_n be the set of trees with n vertices. Then,*

$$\mathbb{LE}(P_n) \leq \mathbb{LE}(T_n) \leq \mathbb{LE}(S_n).$$

If this hypothesis is correct, it suggests that the Laplacian energy's extremal energy trees show an unusual inversion when compared to the extremal energy trees. This surprising result implies that the structural features that raise a tree's energy actually decrease its Laplacian energy, and conversely, the structural features that decrease a tree's energy increase its Laplacian energy. This finding highlights a striking and illogical link between these two energy measurements.

Ganie et al. [4] showed the truth of conjecture for all trees with number of non-pendent vertices at most $\frac{9n}{25} - 2$. It is possible to repeat Radenković and Gutman's experiment and validate that the star has the highest Laplacian energy and the path structure has the lowest Laplacian energy for all the trees in the database. The conjecture was confirmed by Trevisan et al. [11] for all trees with a diameter of 3 and trees with a maximum of 18 vertices also Rahman et al. [10] investigate this conjecture's validity for all the trees of diameter 4.

In this work, we established the validity of Conjecture 1.1 for trees with diameter 16 to 30. Two stars with diameter 16 can be observed in a tree having 14 edges connecting the cores of them as shown in Figure 1, diameter 17 can be seen as two stars with 15 edges connecting the cores of them and so on till diameter 30. In this note, a class of trees of diameter 16 to 30 with n vertices will be represented by $T_{n_i}(v, w)$ for $1 \leq i \leq 15$, respectively. Where $n_i = v + w + (13 + i)$ is the total number of vertices and $v \geq w \geq 1$ are the leaves at each end of $T_{n_i}(v, w)$. We demonstrate that,

$$\mathbb{LE}(P_n) \leq \mathbb{LE}(T_{n_i}(v, w)) \leq \mathbb{LE}(S_n), \text{ where } 1 \leq i \leq 15.$$

In the class of trees of diameter 16 to 30, we also provide a total order by indicating that the Laplacian energies within $T_{n_i}(v, w)$ for $1 \leq i \leq 15$, are strictly reducing as a function of v. Furthermore, we observe that in this class of trees, the order by Laplacian energy depends only on their algebraic connectivity, or more specifically, the Laplacian energy of $T_{n_i}(v, w)$ for $1 \leq i \leq 15$, increases as their algebraic connectivity decreases.
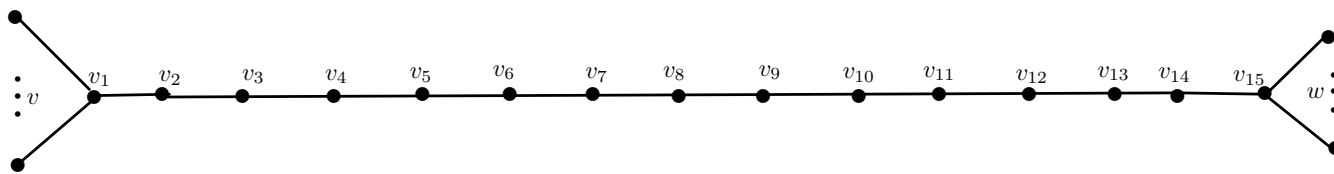
Fig. 1. $T_{n_1}(v, w)$ Tree with diameter 16

Theorem 1.2. *Let T_n be a trees with n vertices such that $T_n \neq S_n$. Then,*

$$\mathbb{LE}(T_n) \leq \mathbb{LE}(S_n).$$

The theorem mentioned above suggests that Conjecture 1.1's upper bound holds true for each tree T_n with n vertices. It is still unclear what the lower border suggested by Conjecture 1.1. While it is often easy to show that $\mathbb{LE}(P_n) \leq \mathbb{LE}(T_n)$, for some specific circumstances, the difficulty occurs when dealing with trees of higher diameters like trees diameter 16 to 30. Due to the set T_n's unlimited number of trees, the problem still exists in these situations.

Consider the following trees $T_{n_i}(v, w)$ for $1 \leq i \leq 15$, of diameter 16 to 30, respectively. Note that the integers $v, w \geq 1$ are the number of pendent vertices of tree. The order of $T_{n_i}(v, w)$ is $n_i = v + w + (13 + i)$, where $1 \leq i \leq 15$.

Theorem 1.3. *Let P_n be a path on n vertices. Then,*

$$\mathbb{LE}(P_n) \leq \mathbb{LE}(T_n).$$

This paper follows the following structure. In section 2 some history and important definitions are reviewed. Section 3 is dedicated to explore the Laplacian characteristic polynomials of $T_{n_i}(v, w)$, where $1 \leq i \leq 15$ having diameter 16 to 30, respectively. Additionally, in the same part, count of Laplacian eigenvalues that exceed the average degree of $T_{n_i}(v, w)$, where $1 \leq i \leq 15$ will be examined and the Conjecture 1.1 is proved with the help of related results. Finally, in the concluding section 4, we summarize our findings and draw conclusions.

2. Meterials and Methods

For a simple graph $\mathbb{G} = (V, E)$ with vertex set $V = \{v_1, \ldots, v_n\}$, the adjacency matrix is basically a square matrix $\mathbf{A}$ such that its element A_{ij} is 1 when there is an edge between vertex v_i and vertex v_j, and 0 when there is no edge. The degree matrix $D(\mathbb{G})$ is a diagonal matrix that tells the degree of each vertex (number of edges connecting to it) of the graph.

For a simple and undirected graph $\mathbb{G} = (V, E)$ of order n, with adjacency matrix $\mathbf{A}(\mathbb{G})$and the degree matrix $D(\mathbb{G})$, we will denote the eigenvalues of $\mathbf{A}(\mathbb{G})$ by $\lambda_1, \lambda_2, \ldots, \lambda_n$, which follow to the preceding relations:

$$\sum_{r=1}^{n} \lambda_r = 0; \quad \sum_{r=1}^{n} \lambda_r^2 = 2m. \tag{1}$$

The energy of a graph can be expressed as the total of the absolute values of the of adjacency matrix's eigenvalues denoted by

$$\mathbb{E}(\mathbb{G}) = \sum_{r=1}^{n} |\lambda_r|. \tag{2}$$

The Laplacian matrix, denoted by $L(\mathbb{G})$, is defined as $L(\mathbb{G}) = D(\mathbb{G}) - \mathbf{A}(\mathbb{G})$ and the eigenvalues of $L(\mathbb{G})$ denoted by $\mu_1, \mu_2, \ldots, \mu_n$. A well known fact about $L(\mathbb{G})$ is that it is positive semi-definite with smallest eigenvalue $\mu_n = 0$. Algebraic concreteness, or the eigenvalue μ_{n-1}, is always smaller than 1. The eigenvalues of $L(\mathbb{G})$ correspond to the subsequent relations:

$$\sum_{r=1}^{n} \mu_r = 2m; \quad \sum_{r=1}^{n} \lambda_r{}^2 = 2m + \sum_{r=1}^{n} d_r{}^2. \tag{3}$$

The Laplacian energy of an undirected graph is denoted by

$$\mathbb{LE}(\mathbb{G}) = \sum_{r=1}^{n} |\mu_r - \hat{d}|, \tag{4}$$

where $\hat{d}$ is the average degree of $\mathbb{G}$. It's important to note that there is a discussion available regarding the graph's signless Laplacian matrix $\mathbb{G}$ in [1]. Let x_i denote the number of vertices of degree $i, 0 \leq i \leq n-1$. We represent by $(x_1, x_2, \cdots, x_{n-1})$, the degree vector of any graph $\mathbb{G}$. a tree with degree vector isomorphic to $(2, n-1, 0, \cdots, 0)$ is called a path graph, denoted by P_n, and a graph with degree vector isomorphic to $(n-1, 0, 0, \cdots, 0, 1)$ is called a star graph and is denoted by S_n. It is a well-known fact that the size of any tree T_n of order n is $n-1$. The average degree d of trees was determined by Trevisan et al. [11].

Lemma 2.1. *Let T_n be the set of trees with n vertices. Then, its average degree $\hat{d} = \frac{2(n-1)}{n} = 2 - \frac{2}{n}$.*

Trevisan et al. [11] have established a lemma regarding the Laplacian energy of path P_n.

Lemma 2.2. *Let P_n be the set of trees with n vertices. Then, $\mathbb{LE}(P_n) \leq 2 + \frac{4n}{\pi}$.*

We can now delve into a discussion regarding Laplacian eigenvalues and the Laplacian characteristic polynomial, specifically focusing on trees. There exists a notable lemma in this context, credited to Brouwer and Haemers [2].

Lemma 2.3. *Consider a connected graph G with Laplacian eigenvalues as $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n$. Then,*

$$\mu_r \geq d_r - r + 2, \ r = 1, 3, \ldots, n,$$

where $d_1 \geq d_2 \geq \ldots \geq d_n$ is the degree sequence of the vertices of G.

We use the technique described in references [6] and [5] to determine the characteristic polynomial of a tree T_n with n vertices. This approach may be simply modified to determine the characteristic polynomial of the Laplacian matrix because it is made to operate directly on the tree structure. Let's give a brief summary of this process in order to assure a thorough knowledge.

The algorithm functions by assigning a rational function $a(v) = \frac{t}{c}$ to each vertex v in the tree, where both t and c are polynomials within the polynomial ring $\mathbf{Q}[\lambda]$. Beginning with the tree's leaves, which are originally given the value $\lambda - 1$ (assuming the tree is rooted arbitrarily), the process follows a bottom-up methodology. After all of v's children have undergone this computation, vertex v is then assigned the resulting rational function.

$$a(v) = \lambda - d_v - \sum_{c \in C} \frac{1}{a(c)}, \tag{5}$$

where d_v is the degree of vertex v and C is the collection of its offspring. Following this procedure for each vertex, the characteristic polynomial is calculated by multiplying each function $a(v)$ by the total number of vertices.

$$\chi(\lambda) = \prod_{v \in V} a(v). \tag{6}$$

3. Results and Discussions

3.1. Construction of Laplacian characteristic polynomial and Laplacian eigenvalues

In this section, we will explore characteristic polynomials of trees $T_{n_i}(v, w)$, where $1 \le i \le 15$, having diameters 16 to 30 respectively, using the above mentioned algorithm. The number of Laplacian eigenvalues greater than the average degree value will also be investigated. Further, the relationship between Laplacian energies of path graphs, trees of diameters 16 to 30 and star graphs will be discussed by proving the Radenković and Gutman conjecture, that is

$$\mathbb{LE}(P_n) \le \mathbb{LE}(T_n) \le \mathbb{LE}(S_n).$$

Proposition 3.1. *Let $T_{n_i}(v, w)$ for $1 \le i \le 15$, be the class of trees with n vertices having diameter 16 to 30, respectively. The Laplacian characteristic polynomial of $T_{n_i}(v, w)$ for $i = 1$, of diameter 16 is as follows:*

(i) $\chi(T_{n_1}(v, w)) = (-1 + \mu)^{(n-17)}\mu(15 - 590\mu + 7323\mu^2 - 44760\mu^3 + 162214\mu^4 - 384540\mu^5 + 631788\mu^6 - 745484\mu^7 + 645525\mu^8 - 414942\mu^9 + 198605\mu^{10} - 70404\mu^{11} + 18201\mu^{12} - 3330\mu^{13} + 408\mu^{14} - 30\mu^{15} + \mu^{16} + v - 106\mu v + 1925\mu^2 v - 14196\mu^3 v + 56134\mu^4 v - 136136\mu^5 v + 218348\mu^6 v - 242250\mu^7 v + 190893\mu^8 v - 108262\mu^9 v + 44275\mu^{10} v - 12926\mu^{11} v + 2625\mu^{12} v - 352\mu^{13} v + 28\mu^{14} v - \mu^{15} v + w - 106\mu w + 1925\mu^2 w - 14196\mu^3 w + 56134\mu^4 w - 136136\mu^5 w + 218348\mu^6 w - 242250\mu^7 w + 190893\mu^8 w - 108262\mu^9 w + 44275\mu^{10} w - 12926\mu^{11} w + 2625\mu^{12} w - 352\mu^{13} w + 28\mu^{14} w - \mu^{15} w - 14\mu v w + 455\mu^2 v w - 4368\mu^3 v w + 19448\mu^4 v w - 48620\mu^5 v w + 75582\mu^6 v w - 77520\mu^7 v w + 54264\mu^8 v w - 26334\mu^9 v w + 8855\mu^{10} v w - 2024\mu^{11} v w + 300\mu^{12} v w - 26\mu^{13} v w + \mu^{14} v w);$

Proof. *The algorithm depicted in the previously mentioned section 2 is applied here.* □

In the forthcoming lemma, we will examine the number of Laplacian eigenvalues that exceed the average degree of $T_{n_i}(v, w)$ for $1 \le i \le 15$, respectively.

Lemma 3.2. *Consider the class of trees $T_{n_i(v,w)}$ for $1 \le i \le 15$, with n vertices. Then $T_{n_i}(v, w)$ has exactly 2 Laplacian eigenvalues greater than $\hat{d} = 2 - \frac{2}{n}$, where $1 \le i \le 15$.*
Proof. *We prove the result by considering $T_{n_1}(v, w)$ for $i = 1$. By Proposition 3.1, it is evident that the multiplicity of Laplacian eigenvalue 1 is $n\check{}17$. The Laplacian eigenvalues $\mu_n = 0$ and $\mu_{n-1} \le 1$ are also known. This indicates that there are at least $n\check{}15$, Laplacian eigenvalues less than $\hat{d}$, since $1 < \hat{d} < 2$. By Lemma 2.3, we have*

$$\mu_1 \ge d_1 + 1 = v + 2 \ge 3, \text{ for } v \ge 1,$$

$$\mu_2 \ge d_2 = w + 1 \ge 2, \text{ for } w \ge 1.$$

As a result, precisely two Laplacian eigenvalues exceed the value of $\hat{d}$. Using a similar approach, we can establish the same conclusion for the remaining cases. □

3.2.   Proof of Conjecture

Now we will prove that left side of the Conjecture 1.1 is true for class of trees $T_{n_i}(v, w)$ for $1 \leq i \leq 15$, having diameters 16 to 30, respectively.

Theorem 3.3. *Let P_n be a path on n vertices. Then,*

$$\mathbb{LE}(P_n) \leq \mathbb{LE}(T_{n_i}(v, w)) \ for \ 1 \leq i \leq 15.$$

Proof. Initially, it is important to acknowledge that Trevisan et al. [11], asserted the validity of the inequality $\mathbb{LE}(P_n) \leq \mathbb{LE}(T_n)$ for n vertices in the context of any tree T_n, specifically for cases where $n \leq 18$. In the course of our proof, we can safely suppose that $n \geq 19$. Consider the case $T_{n_i}(v, w)$, for $i = 1$.

From Eq. (5), by Proposition 3.1 and by Lemma 3.2, we see that

$$\mathbb{LE}(T_{n_1}(v, w)) = |\mu_1 - \hat{d}| + |\mu_2 - \hat{d}| + |\mu_3 - \hat{d}| + \ldots + |\mu_{15} - \hat{d}| + (n - 17)|1 - \hat{d}| + |\mu_{n-1} - \hat{d}| + |\mu_n - \hat{d}|$$
$$= \hat{d} + (n - 17)(\hat{d} - 1) + (\mu_1 - \hat{d}) + (\mu_2 - \hat{d}) + (\hat{d} - \mu_3) + \ldots + (\hat{d} - \mu_{15}) + (\hat{d} - \mu_{n-1})$$
$$= 13\hat{d} + (n - 17)(\hat{d} - 1) + (\mu_1 + \mu_2) - (\mu_3 + \ldots + \mu_{15} + \mu_{n-1}). \tag{7}$$

through the use of Proposition 3.1 and Eq. (6), we observe that $\mu_1 + \ldots + \mu_{15} + \mu_{n-1} = v + w + 29 = n + 15$ and substituting $\hat{d} = 2 - \frac{2}{n}$, Eq. (7) implies that:

$$\mathbb{LE}(T_{n_1}(v, w)) = 2n + 24 + \frac{8}{n} - 2(\mu_3 + \ldots + \mu_{15} + \mu_{n-1}). \tag{8}$$

through the use of Lemma 2.2 and Eq. (8), the above equation becomes:

$$\mathbb{LE}(P_n) - \mathbb{LE}(T_{n_1}(v, w)) \leq n\left(\frac{4}{\pi} - 2\right) - \frac{8}{n} - 22 + 2(\mu_3 + \ldots + \mu_{15} + \mu_{n-1}).$$

Since $\mu_3 + \ldots + \mu_{15} < 2$, $\quad \mu_{n-1} < 1$ and $\frac{8}{n} > 0$, so it follows;

$$\mathbb{LE}(P_n) - \mathbb{LE}(T_{n_1}(v, w)) \leq n\left(\frac{4}{\pi} - 2\right) - \frac{8}{n} + 6,$$

which is negative for $n > 18$. □

Corollary 3.4. *Let P_n be a path and S_n be a star with n vertices. Then,*

$$\mathbb{LE}(P_n) \leq \mathbb{LE}(T_{n_i}(v, w)) \leq \mathbb{LE}(S_n), \ where \ 1 \leq i \leq 15.$$

Remark 3.5. Using a similar approach, results concerning the remaining classes of trees of diameter between 17 to 30 with Laplacian characteristic polynomials determined in Proposition 3.1, and thus establishing the Conjecture 1.1, for all these classes of trees.

4.   Conclusion

In this research study, Conjecture 1.1 was examined for some special classes of trees $T_{n_i}(v, w)$, where $1 \leq i \leq 15$, having diameters 16 to 30, respectively.

References

[1] A. Z. Abdian, S. Pouyandeh, and B. Askari. Which multicone graphs are determined by their signless laplacian spectrum?(the proof of a conjecture). *Journal of Discrete Mathematical Sciences and Cryptography*, 22(1):91–99, 2019. https://doi.org/10.1080/09720529.2019.1578082.

[2] A. E. Brouwer and W. H. Haemers. A lower bound for the laplacian eigenvalues of a graph—proof of a conjecture by guo. *Linear Algebra and its Applications*, 429(8-9):2131–2135, 2008. https://doi.org/10.1016/j.laa.2008.06.008.

[3] M. Fiedler. Laplacian of graphs and algebraic connectivity. *Banach Center Publications*, 1(25):57–70, 1989.

[4] H. A. Ganie, B. A. Rather, and S. Pirzada. On a conjecture of laplacian energy of trees. *Discrete Mathematics, Algorithms and Applications*, 14(06):2250009, 2022. https://doi.org/10.1142/S1793830922500094.

[5] D. Jacobs, V. Trevisan, and F. Tura. Computing the characteristic polynomial of threshold graphs. *Journal of Graph Algorithms and Applications*, 18(5):709–719, 2014. https://doi.org/10.7155/jgaa.00342.

[6] D. P. Jacobs and V. Trevisan. How to construct the characteristic polynomial of a tree's adjacency matrix, 1996.

[7] J.-B. Liu and X.-F. Pan. Minimizing kirchhoff index among graphs with a given vertex bipartiteness. *Applied mathematics and computation*, 291:84–88, 2016. https://doi.org/10.1016/j.amc.2016.06.017.

[8] J.-B. Liu, J. Zhao, J. Min, and J. Cao. The hosoya index of graphs formed by a fractal graph. *Fractals*, 27(08):1950135, 2019. https://doi.org/10.1142/S0218348X19501354.

[9] S. Radenković and I. Gutman. Total π-electron energy and laplacian energy: how far the analogy goes? *Journal of the Serbian Chemical Society*, 72(12):1343–1350, 2007. https://doi.org/10.2298/JSC0712343R.

[10] J. U. Rahman, U. Ali, and M. U. Rehman. The laplacian energy of diameter 4 trees. *Journal of Discrete Mathematical Sciences and Cryptography*, 24(1):119–128, 2021. https://doi.org/10.1080/09720529.2019.1670943.

[11] V. Trevisan, J. B. Carvalho, R. R. Del Vecchio, and C. T. Vinagre. Laplacian energy of diameter 3 trees. *Applied mathematics letters*, 24(6):918–923, 2011. https://doi.org/10.1016/j.aml.2010.12.050.