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On the ABS Spectral Radius of Trees and Unicyclic Graphs

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ABSTRACT: Characterization of extremal graphs with respect to the spectral radius of the adjacency matrix weighted by topological indices is one of the interesting problems in the study of graph matrices. Recently, attempts have been made to unify the study of the spectral radius of the adjacency matrix weighted by topological indices. As a result, extremal trees and unicyclic graphs for the spectral radius of several topological matrices have been characterized. One of the topological matrices that do not come under the unified approaches studied so far is the atom-bound sum connectivity matrix $\mathcal{ABS}(G)$ of a graph G. Until now, it is known that among all trees with n vertices, the star graph has maximum spectral radius with respect to the matrix $\mathcal{ABS}(G)$ (called ABS spectral radius), whereas the path graph has minimum ABS spectral radius. Motivated by these works, in this paper, we determine trees with second-largest, third-largest, fourth-largest, and fifth-largest ABS spectral radius. We show that among all unicyclic graphs on n vertices, the graph S_n+e has maximum ABS spectral radius. Also, we obtain an upper bound for the ABS spectral radius of unicyclic graphs with girth at least 5.

Keywords: ABS matrix, ABS spectral radius, trees, unicyclic graphs.

Contents

1. Introduction

Throughout the paper, G is a simple graph with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$. We denote the degree of v_i as $d_G(v_i)$ or d_i. If v_i is adjacent to v_j, we write $v_i\sim v_j$ or $i\sim j$. The adjacency matrix $\mathcal{A}(G)$ of G is a square matrix whose rows and columns are indexed by the vertices of G, and the $(i,\ j)$-th entry is 1 if $v_i\sim v_j$ and 0, otherwise. Since $\mathcal{A}(G)$ is a symmetric $(0,1)$ matrix, all its eigenvalues are real, and we denote the i-th largest eigenvalue of $\mathcal{A}(G)$ by $\lambda_i(G)$ or λ_i. Further, by Perron–Frobenius theory of non-negative matrices, λ_1 is the spectral radius of $\mathcal{A}(G)$.

Topological indices are well-known graph parameters that play a major role in chemical graph theory. There are various types of topological indices based on concepts such as degree, distance, and eccentricity. Most of the topological indices can generally be expressed as $\sum\limits_{i\sim j} f(d_i,d_j)$, where f is a symmetric bi-variant function. The atom-bond sum-connectivity index (ABS) is a new topological index introduced in [2] and is defined as $ABS(G)=\sum\limits_{i\sim j}\sqrt{\dfrac{d_i+d_j-2}{d_i+d_j}}$. It was presented as a combination of the atom-bond connectivity index [10] and the sum-connectivity index [31]. The mathematical properties of the ABS index, including its extremal results and bounds, are discussed in [12,1]. For more details, we refer to a recent survey article [3]. For each topological index of the form $\sum\limits_{i\sim j} f(d_i,d_j)$, where f is a symmetric bi-variate function, one can associate a general extended adjacency matrix/topological matrix $A_f(G)$ [8]. The (i,j)-th entry of this matrix is given by $f(d_i,d_j)$ if $i\sim j$, and it is 0 otherwise. In recent years, the concept of the general extended matrix, also known as the adjacency matrix weighted by topological indices [8,26,27,7], has gained attention among researchers, leading to the publication of several papers

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on this topic. However, most of these studies focus on specific topological indices and lack a unified approach. See [17,25,15,9] for more details.

The ABS matrix of G, denoted by $\mathcal{ABS}(G)$, is the adjacency matrix weighted by the ABS index. Therefore, the (i,j)-th entry of this matrix is $\sqrt{\dfrac{d_i+d_j-2}{d_i+d_j}}$ if $v_i \sim v_j$ and 0, otherwise. We denote the eigenvalues of $\mathcal{ABS}(G)$ as $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$. Thus, η_1 represents the spectral radius of $\mathcal{ABS}(G)$, which is referred to as the ABS spectral radius. In [22] Lin et al. studied ABS Estrada index ($\sum_{i=1}^{n} e^{\eta_i}$) of trees and proved that it is maximum for the star graph and minimum for the path graph. In [23], the authors showed that ABS spectral radius of trees with order n is maximum for the star graph and minimum for the path graph. In [22,23], the chemical significance of the ABS Estrada index and the ABS spectral radius are examined separately. This indicates that both the ABS Estrada index and the ABS spectral radius can aid in predicting specific molecular properties. Some bounds on ABS spectral radius and ABS energy were obtained in [29]. The authors also investigated the chemical importance of ABS energy.

Recently, attempts have been made to unify the study of the spectral radius of the adjacency matrix $A_f(G)$ weighted by topological indices. In [20], it has been proven that the tree with the largest spectral radius of $A_f(G)$ is either a star or a double star, given that $f(x,y)$ is increasing and convex in the variable x. The function f is said to satisfy the property P^* [30] if $f(x,y) > 0$ is increasing and convex in variable x, and for any $x_1 + y_1 = x_2 + y_2$ and $|x_1 - y_1| > |x_2 - y_2|$, $f(x_1, y_1) \geq f(x_2, y_2)$. In [30], the authors identified the extremal trees with both the smallest and largest spectral radii, as well as the extremal unicyclic graphs with the smallest spectral radius and the three largest spectral radii of $A_f(G)$ when f satisfies the property P^*. These works encompass nearly all of the main topological indices. It is important to note that $f(x,y) = \sqrt{1 - \dfrac{2}{x+y}}$ is concave in x, and therefore does not fall under the aforementioned unified approaches.

Motivated by these works, in this article, we identify the trees with first five largest values of the ABS spectral radius. We show that among all unicyclic graphs on n vertices, the graph $S_n + e$ (see Fig. 4) has maximum ABS spectral radius. Also, we obtain an upper bound for the ABS spectral radius of unicyclic graphs with girth at least 5. We note that similar findings have recently appeared in [18,19], although the methods employed there differ from those used in this paper. The present work predates [18,19] and was already under review at another journal when those manuscripts were published.

2. *ABS* spectral radius of trees

In this section, we classify trees that have the second-largest, third-largest, fourth-largest and fifth-largest ABS spectral radius. We denote by $\mathscr{T}_n$, the class of tress on n vertices. Let $S_n^2, S_n^3, S_n^4, S_n^5$, and S_n^6 denote the trees on n vertices as depicted in Fig. 1. The following lemmas are essential to obtain our main results.

Lemma 2.1 [13] Let T be a tree in $\mathscr{T}_n n \left\{S_n, S_n^2\right\}$. Then $\lambda_1(T) \leq \sqrt{\frac{1}{2}(n-1+\sqrt{n^2-10n+33})}$ for $n \geq 4$, and the equality holds if and only if $T \cong S_n^3$.

Lemma 2.2 [6] Let T be a tree in $\mathscr{T}_n n \left\{S_n, S_n^2, S_n^3, S_n^4, S_n^5\right\}$. Then for $n \geq 11$, $\lambda_1(T) \leq \sqrt{\frac{1}{2}(n-1+\sqrt{n^2-14n+61})}$ and the equality holds if and only if $T \cong S_n^6$.

Let B_1 and B_2 be two real matrices of same order, we write $B_1 \preceq B_2$ if every entry in B_1 does not exceeds the counterpart in B_2.

Lemma 2.3 [14] *Let B_1, B_2 be non-negative matrices of order n with spectral radius $\rho(B_1)$ and $\rho(B_2)$, respectively. If $B_1 \preceq B_2$, then $\rho(B_1) \leq \rho(B_2)$. Further, if B_1 is irreducible and $B_1 \neq B_2$, then $\rho(B_1) < \rho(B_2)$.*

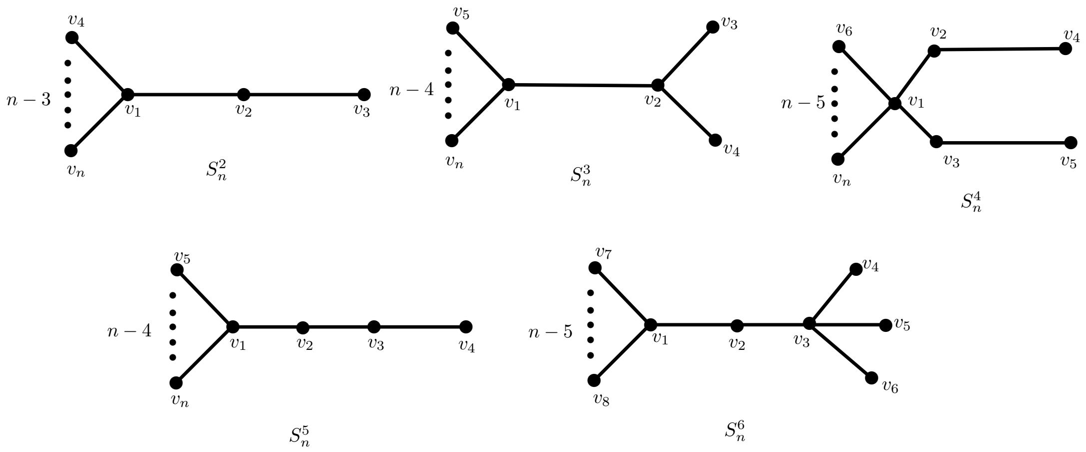


Figure 1: Trees S_n^2, S_n^3, S_n^4, S_n^5 and S_n^6.

Remark 2.1 *For any tree $T \in \mathscr{T}_n$, the matrices $\mathcal{ABS}(T)$ and $\mathcal{A}(T)$ are irreducible with $\mathcal{ABS}(T) \preceq \sqrt{\frac{n-2}{n}}\mathcal{A}(T)$ and $\mathcal{ABS}(T) \neq \sqrt{\frac{n-2}{n}}\mathcal{A}(T)$. Thus, by Lemma 2.3, $\eta_1(T) < \sqrt{\frac{n-2}{n}}\lambda_1(T)$.*

In the following theorem, we prove that the ABS spectral radius of the tree S_n^2 is the second-largest among all trees in $\mathscr{T}_n$.

Theorem 2.1 *Let T be a tree on $n \geq 7$ vertices. If $T \ncong S_n$, then*

$$\eta_1^2(T) \leq \frac{3n^3 - 14n^2 + 17n + 6 + \sqrt{9n^6 - 96n^5 + 382n^4 - 620n^3 + 229n^2 + 204n + 36}}{6n(n-1)}$$

and the equality holds if and only if $T \cong S_n^2$.

Proof: The ABS matrix of S_n^2, with the vertex labels as shown in the Fig. 1 is given by

$$\mathcal{ABS}(S_n^2) = \begin{bmatrix} 0 & \sqrt{\frac{n-2}{n}} & 0 & \sqrt{\frac{n-3}{n-1}} & \cdots & \sqrt{\frac{n-3}{n-1}} \\ \sqrt{\frac{n-2}{n}} & 0 & \sqrt{\frac{1}{3}} & 0 & \cdots & 0 \\ 0 & \sqrt{\frac{1}{3}} & 0 & 0 & \cdots & 0 \\ \sqrt{\frac{n-3}{n-1}} & 0 & 0 & 0 & \cdots & 0 \\ \vdots & & \vdots & & & \vdots \\ \sqrt{\frac{n-3}{n-1}} & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

Upon applying the elementary row operations, $R_i' \leftarrow R_i - R_4$ for $5 \leq i \leq n$, and then performing the column operations, $C_4' \leftarrow C_4 + C_j$ for $5 \leq j \leq n$, the matrix $xI_n - \mathcal{ABS}(S_n^2)$ gets transformed into the following block upper triangular matrix.

$$\left[\begin{array}{cccc|cccc}
x & -\sqrt{\dfrac{n-2}{n}} & 0 & -(n-3)\sqrt{\dfrac{n-3}{n-1}} & -\sqrt{\dfrac{n-3}{n-1}} & . & . & . & -\sqrt{\dfrac{n-3}{n-1}} \\
-\sqrt{\dfrac{n-2}{n}} & x & -\sqrt{\dfrac{1}{3}} & 0 & 0 & . & . & . & 0 \\
0 & -\sqrt{\dfrac{1}{3}} & x & 0 & 0 & . & . & . & 0 \\
-\sqrt{\dfrac{n-3}{n-1}} & 0 & 0 & x & 0 & . & . & . & 0 \\
\hline
0 & 0 & 0 & 0 & x & . & . & . & 0 \\
. & & . & & & & & & . \\
. & & . & & & & \ddots & & . \\
. & & . & & & & & & . \\
0 & 0 & 0 & 0 & 0 & . & . & . & x
\end{array}\right].$$

Thus, $det\left(xI_n - \mathcal{ABS}(S_n^2)\right) = x^{n-4}\left(x^4 + \dfrac{14n^2-3n^3-17n-6}{3n(n-1)}x^2 + \dfrac{(n-3)^2}{3(n-1)}\right)$.
So,

$$\eta_1^2(S_n^2) = \frac{3n^3-14n^2+17n+6+\sqrt{9n^6-96n^5+382n^4-620n^3+229n^2+204n+36}}{6n(n-1)}. \tag{2.1}$$

Suppose $T \notin \left\{S_n, S_n^2\right\}$. Then by Lemma 2.1 and Remark 2.1,

$$\eta_1^2(T) < \frac{n-2}{2n}(n-1+\sqrt{n^2-10n+33}). \tag{2.2}$$

Claim: $3(n-1)(n-2)(n-1+\sqrt{n^2-10n+33}) < 3n^3-14n^2+17n+6+\sqrt{A}$, where $A = 9n^6-96n^5+382n^4-620n^3+229n^2+204n+36$.
For $n=7$, the above inequality holds. Let $n \geq 8$. We have $A - 9(n^2-2n+4)^2(n^2-10n+33) = 30n^5-383n^4+1792n^3-4919n^2+6396n-4716$. Since $h(x) := 30x^5-383x^4+1792x^3-4919x^2+6396x-4716$ is an increasing function for $x \geq 8$ and $h(8) > 0$,

$$\begin{aligned}
\sqrt{A} &> 3(n^2-2n+4)\sqrt{n^2-10n+33} \\
&= 3(n-1)(n-2)\sqrt{n^2-10n+33} + 3(n+2)\sqrt{n^2-10n+33} \\
&> 3(n-1)(n-2)\sqrt{n^2-10n+33} + 2(n+2)(n-3).
\end{aligned}$$

Thus,

$$\begin{aligned}
\frac{\sqrt{A}}{6n(n-1)} &> \frac{(n-2)}{2n}\sqrt{n^2-10n+33} + \frac{(n+2)(n-3)}{3n(n-1)} + \frac{(n-2)(n-1)}{2n} - \frac{(n-2)(n-1)}{2n} \\
&= \frac{n-2}{2n}(n-1+\sqrt{n^2-10n+33}) - \frac{3n^3-14n^2+17n+6}{6n(n-1)}.
\end{aligned}$$

Therefore, our claim is valid, and based on equations (2.1) and (2.2), $\eta_1(T) < \eta_1(S_n^2)$. Proving the theorem. $\square$

In the following theorem, we show that the tree S_n^5 has the largest ABS spectral radius among all trees in the class $\mathscr{T}_n n\left\{S_n, S_n^2, S_n^3, S_n^4\right\}$.

Theorem 2.2 *Let $T \in \mathscr{T}_n n\left\{S_n, S_n^2, S_n^3, S_n^4\right\}$. Then for $n \geq 11$,*

$$\eta_1^2(T) \;\leq\; \frac{6n^3-43n^2+99n-50+\sqrt{36n^6-636n^5+4429n^4-15090n^3+25717n^2-20076n+5764}}{12(n-1)(n-2)}$$

and the equality holds if and only if $T = S_n^5$.

Proof: The ABS matrix of S_n^5, with the vertex labels as shown in the Fig. 1 is given by

$$\mathcal{ABS}(S_n^5)=\begin{bmatrix} 0 & \sqrt{\frac{n-3}{n-1}} & 0 & 0 & \sqrt{\frac{n-4}{n-2}} & \cdots & \sqrt{\frac{n-4}{n-2}} \\ \sqrt{\frac{n-3}{n-1}} & 0 & \sqrt{\frac{1}{2}} & 0 & 0 & \cdots & 0 \\ 0 & \sqrt{\frac{1}{2}} & 0 & \sqrt{\frac{1}{3}} & 0 & \cdots & 0 \\ 0 & 0 & \sqrt{\frac{1}{3}} & 0 & 0 & \cdots & 0 \\ \sqrt{\frac{n-4}{n-2}} & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & & & \vdots & & & \vdots \\ \sqrt{\frac{n-4}{n-2}} & 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

The characteristic equation of S_n^5 is given by

$$x^{n-4}\left(x^4+\frac{43n^2-6n^3-99n+50}{6(n-1)(n-2)}x^2+\frac{5n^3-43n^2+110n-68}{6(n-1)(n-2)}\right)=0. \tag{2.3}$$

Solving equation (2.3), we get $\eta_1^2(S_n^5)=\dfrac{6n^3-43n^2+99n-50+\sqrt{B}}{12(n-1)(n-2)}$, where $B=36n^6-636n^5+4429n^4-15090n^3+25717n^2-20076n+5764$.

Suppose $T\notin\{S_n,S_n^2,S_n^3,S_n^4,S_n^5\}$. Then by Lemma 2.2 and Remark 2.1,

$$\eta_1^2(T)<\frac{n-2}{2n}\left(n-1+\sqrt{n^2-14n+61}\right). \tag{2.4}$$

Claim : $\dfrac{n-2}{2n}\left(n-1+\sqrt{n^2-14n+61}\right)<\eta_1^2(S_n^5)$.

Note that,

$n^2B-\left(6(n-2)^2(n-1)(n-\frac{57}{10})+7n^3-21n^2-22n+24\right)^2=\dfrac{3(n-1)(n-2)k(n)}{25}$, where $k(n):=420n^5-8897n^4+67439n^3-213046n^2+266660n-107736$ is an increasing function for $n\geq 11$ and $k(11)>0$.

Thus,

$$\begin{aligned} n\sqrt{B} &> 6(n-2)^2(n-1)(n-\frac{57}{10})+7n^3-21n^2-22n+24 \\ &> 6(n-1)^2(n-1)\sqrt{n^2-14n+61}+7n^3-21n^2-22n+24. \end{aligned}$$

Therefore,

$$\begin{aligned} \frac{\sqrt{B}}{12(n-1)(n-2)} &> \frac{(n-2)\sqrt{n^2-14n+61}}{2n}+\frac{7n^3-21n^2-22n+24}{12n(n-1)(n-2)} \\ &\quad +\frac{(n-1)(n-2)}{2n}-\frac{(n-1)(n-2)}{2n} \\ &= \frac{n-2}{2n}\left(n-1+\sqrt{n^2-14n+61}-\frac{6n^3-43n^2+99n-50}{12(n-1)(n-2)}\right). \end{aligned}$$

Proving our claim. Consequently, by equation (2.4), we have $\eta_1(T)<\eta_1(S_n^5)$. □

In the following lemma, we prove that $\eta_1(S_n^4)>\eta_1(S_n^5)$.

Lemma 2.4 *For $n \geq 6$,*
$\eta_1^2(S_n^4) = \dfrac{3n^3 - 23n^2 + 54n - 22 + \sqrt{9n^6 - 150n^5 + 1009n^4 - 3348n^3 + 5452n^2 - 3792n + 964}}{6(n^2 - 3n + 2)}$ *and*
$\eta_1(S_n^4) > \eta_1(S_n^5)$.

Proof: The ABS matrix of S_n^4, with the vertex labels as shown in the Fig. 1 is given by

$$\mathcal{ABS}(S_n^4)=\begin{bmatrix} 0 & \sqrt{\frac{n-3}{n-1}} & \sqrt{\frac{n-3}{n-1}} & 0 & 0 & \sqrt{\frac{n-4}{n-2}} & . \; . \; . & \sqrt{\frac{n-4}{n-2}} \\ \sqrt{\frac{n-3}{n-1}} & 0 & 0 & \sqrt{\frac{1}{3}} & 0 & 0 & . \; . \; . & 0 \\ \sqrt{\frac{n-3}{n-1}} & 0 & 0 & 0 & \sqrt{\frac{1}{3}} & 0 & . \; . \; . & 0 \\ 0 & \sqrt{\frac{1}{3}} & 0 & 0 & 0 & 0 & . \; . \; . & 0 \\ 0 & 0 & \sqrt{\frac{1}{3}} & 0 & 0 & 0 & . \; . \; . & 0 \\ \sqrt{\frac{n-4}{n-2}} & 0 & 0 & 0 & 0 & 0 & . \; . \; . & 0 \\ \vdots & & & & & \vdots & & \vdots \\ \sqrt{\frac{n-4}{n-2}} & 0 & 0 & 0 & 0 & 0 & . \; . \; . & 0 \end{bmatrix}.$$

The characteristic polynomial of S_n^4 is given by

$$x^{n-6}\left(x^6 + \frac{66n^2 - 9n^3 - 153n + 60}{9(n-1)(n-2)}x^4 + \frac{6n^3 - 53n^2 + 141n - 82}{9(n-1)(n-2)}x^2 + \frac{10n^2 - n^3 - 29n + 20}{9(n-1)(n-2)}\right). \quad (2.5)$$

Solving equation (2.5), we get
$\eta_1^2(S_n^4) = \dfrac{3n^3 - 23n^2 + 54n - 22 + \sqrt{C}}{6(n^2 - 3n + 2)}$, where $C = 9n^6 - 150n^5 + 1009n^4 - 3348n^3 + 5452n^2 - 3792n + 964$.

To prove that $\eta_1(S_n^4) > \eta_1(S_n^5)$, where $\eta_1(S_n^5)$ is given in Theorem 2.2, it suffices to prove, $2\sqrt{C} - \sqrt{B} > 3(n^2 - 3n - 2)$,where $B = 36n^6 - 636n^5 + 4429n^4 - 15090n^3 + 25717n^2 - 20076n + 5764$. Equivalently, it is enough to show that, $4C + B - 9(n^2 - 3n - 2)^2 > 4\sqrt{CB}$.

Now, $(4C + B - 9(n^2 - 3n - 2)^2)^2 - 16CB = 576(n-5)(n-2)(n-1)(3n^6 - 3n^5 - 239n^4 + 1435n^3 - 3032n^2 + 2300n - 512)$. Since $f(x) := 576(x-5)(x-2)(x-1)(3x^6 - 3x^5 - 239x^4 + 1435x^3 - 3032x^2 + 2300x - 512)$ is an increasing function for $x \geq 6$ with $f(6) > 0$, $(4C + B - 9(n^2 - 3n - 2)^2)^2 - 16CB > 0$. Therefore, $\eta_1^2(S_n^4) > \eta_1^2(S_n^5)$. □

In the following lemma, we prove that $\eta_1(S_n^3) > \eta_1(S_n^4)$.

Lemma 2.5 *For $n \geq 6$,*
$\eta_1^2(S_n^3) = \dfrac{n^3 - 6n^2 + 10n + 4 + \sqrt{n^6 - 16n^5 + 96n^4 - 240n^3 + 180n^2 + 80n + 16}}{2n(n-2)}$ *and* $\eta_1(S_n^3) > \eta_1(S_n^4)$.

Proof: The ABS matrix of S_n^3, with the vertex labels as shown in the Fig. 1 is given by

$$\mathcal{ABS}(S_n^3)=\begin{bmatrix} 0 & \sqrt{\dfrac{n-2}{n}} & 0 & 0 & \sqrt{\dfrac{n-4}{n-2}} & \cdots & \sqrt{\dfrac{n-4}{n-2}} \\ \sqrt{\dfrac{n-2}{n}} & 0 & \sqrt{\dfrac{1}{2}} & \sqrt{\dfrac{1}{2}} & 0 & \cdots & 0 \\ 0 & \sqrt{\dfrac{1}{2}} & 0 & 0 & 0 & \cdots & 0 \\ 0 & \sqrt{\dfrac{1}{2}} & 0 & 0 & 0 & \cdots & 0 \\ \sqrt{\dfrac{n-4}{n-2}} & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & & & & \vdots & & \vdots \\ \sqrt{\dfrac{n-4}{n-2}} & 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

The characteristic polynomial of S_n^3 is given by

$$x^{n-4}\left(x^4+\frac{6n^2-n^3-10n-4}{n(n-2)}x^2+\frac{n^3-8n^2+16n}{n(n-2)}\right).$$

So,
$\eta_1^2(S_n^3)=\dfrac{n^3-6n^2+10n+4+\sqrt{D}}{2n(n-2)}$, where $D=n^6-16n^5+96n^4-240n^3+180n^2+80n+16$.

To prove that $\eta_1(S_n^3)>\eta_1(S_n^4)$, where $\eta_1(S_n^4)$ is given in Lemma 2.4. It is enough to show that, $n\sqrt{C}-3(n-1)\sqrt{D}<2(n-3)(n^2+2)$, where $C=9n^6-150n^5+1009n^4-3348n^3+5452n^2-3792n+964$. Equivalently, it suffices to prove, $n^2C+9(n-1)^2D-4(n-3)^2(n^2+2)^2<6n(n-1)\sqrt{CD}$.

Now, $(n^2C+9(n-1)^2D-4(n-3)^2(n^2+2)^2)^2-36n^2(n-1)^2CD=-144n^2(n-2)(n-4)(n-1)^2(2n^7-21n^6+78n^5+15n^4-858n^3+1800n^2-824n+240)$. Since $g(x)=2x^7-21x^6+78x^5+15x^4-858x^3+1800x^2-824x+240$ is an increasing function for $x\geq 6$ with $g(6)>0$, $(n^2C+9(n-1)^2D-4(n-3)^2(n^2+2)^2)^2-36(n-1)^2CD<0$. Therefore, $\eta_1(S_n^3)>\eta_1(S_n^4)$. $\square$

The following two theorems present trees that have third-largest and fourth-largest *ABS* spectral radius. Their proofs directly follow from Theorem 2.2, Lemma 2.5, and Lemma 2.4.

Theorem 2.3 *Let $n\geq 11$ and $T\in\mathscr{T}_n n\left\{S_n,S_n^2\right\}$. Then* $\eta_1^2(T)\leq\dfrac{n^3-6n^2+10n+4+\sqrt{n^6-16n^5+96n^{-}240n^3+180n^2+80n+16}}{2n(n-2)}$ *and equality holds if and only if $T=S_n^3$.*

Theorem 2.4 *Let $n\geq 11$ and $T\in\mathscr{T}_n n\left\{S_n,S_n^2,S_n^3\right\}$. Then* $\eta_1^2(T)\leq\dfrac{3n^3-23n^2+54n-22+\sqrt{9n^6-150n^5+1009n^4-3348n^3+5452n^2-3792n+964}}{6(n^2-3n+2)}$ *and equality holds if and only if $T=S_n^4$.*

3. *ABS* spectral radius of unicyclic graphs

The following lemma proved in [11] gives an upper bound for the spectral radius of a graph with girth at least 5.

Lemma 3.1 *[11] For any graph G of order n with girth at least 5, $\lambda_1\leq\sqrt{n-1}$.*

Theorem 3.1 *Let G be a unicyclic graph of order n and girth at least 5. Then $\eta_1(G)\leq\sqrt{n-3}$. Further, equality holds if and only if $G=C_5$.*

Proof: Let v_i and v_j be two vertices of G. Since G is of girth at least 5, there exist at least 3 vertices v_p, v_q and v_r on the unique cycle of G which are distinct from the vertices v_i and v_j. Therefore, $d_i + d_j = 2n - d_p - d_q - d_r - \sum\limits_{\substack{k=1 \\ k \notin \{i,j,p,q,r\}}}^{n} d_k \leq 2n - 6 - \sum\limits_{k \notin \{i,j,p,q,r\}} d_k \leq n-1$. That is, $d_i + d_j \leq n - 1$. Thus, $\sqrt{1 - \dfrac{2}{d_i + d_j}} \leq \sqrt{\dfrac{n-3}{n-1}}$, and so $\mathcal{ABS}(G) \preceq \sqrt{\dfrac{n-3}{n-1}}\mathcal{A}(G)$.

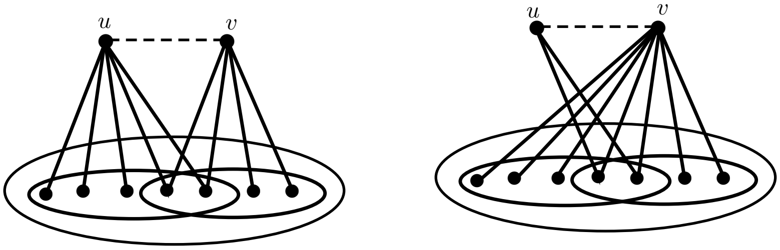
Hence, by Lemma 2.3 and Lemma 3.1, $\eta_1(G) \leq \sqrt{\dfrac{n-3}{n-1}}\lambda_1(G) \leq \sqrt{n-3}$. Proving the upper bound.

Suppose $\eta_1(G) = \sqrt{n-3}$. Then $\mathcal{ABS}(G) = \sqrt{\dfrac{n-3}{n-1}}\mathcal{A}(G)$. This implies that, $d_i + d_j = n - 1$, for all $i \sim j$. Assume that G is not a cycle. In this case, a quasi-pendant vertex of G, say v_k, must be of degree $n-2$. If $d_k \neq n-2$, then $d_k + d_j \neq n-1$ for a pendant vertex v_j of G, which is adjacent to v_k, a contradiction. Since G is connected and $d_k = n-2$, the vertex of G that is not adjacent to v_k must be adjacent to v_j for some j. Consequently, we find that $d_k + d_j > n-1$, which again results in a contradiction. So, G must be a cycle with $d_i + d_j = n-1$, for all $i \sim j$. Hence $G \cong C_5$. The converse part is direct. □

The Kelmans operation [16] described below is essential to proceed further in this section.

Let u, v be two vertices of the graph G and let $\Omega_1 = N(u) - N[v]$, $\Omega_2 = N(v) - N[u]$, $\Omega_3 = N(u) \cap N(v)$. Replace the edge uw of G by a new edge vw for all vertices $w \in \Omega_1$. This graph operation is referred to as Kelmans operation on G, and we denote the resulting graph as G_{uv^+}. See Fig. 2.

Remark 3.1 *The graphs G_{uv^+} and G_{vu^+} are isomorphic.*



Graph G Graph G^+_{uv}

Figure 2: Graph G and resultant graph G_{uv^+}.

The following lemma is the well-known Rayleigh's inequality [5].

Lemma 3.2 *[5] Let A be an $n \times n$ symmetric nonnegative matrix. Then $\rho(A) \geq \boldsymbol{x}^T A \boldsymbol{x}$ for any unit vector $\boldsymbol{x}$, with equlity holds if and only if $A\boldsymbol{x} = \rho(A)\boldsymbol{x}$.*

Lemma 3.3 *Let G be a connected graph of order n. Suppose $uv \in E(G)$ such that $|\Omega_1| \geq 1$, $|\Omega_2| \geq 1$ and $\Omega_3 = \emptyset$. Then $\eta_1(G) < \eta_1(G_{uv^+})$.*

Proof: Let $\mathbf{x}$ be the unit Perron vector of $\mathcal{ABS}(G)$ and let the component of $\mathbf{x}$ corresponding to the vertex w of G be denoted as x_w. By Remark 3.1, without loss of generality, we assume that $x_u \leq x_v$.

Consider,

$$\begin{aligned}\mathbf{x}^T\mathcal{ABS}(G_{uv^+})\mathbf{x}-\mathbf{x}^T\mathcal{ABS}(G)\mathbf{x} &= 2\sum_{w\in\Omega_1}\Bigg[\left(\sqrt{1-\frac{2}{d_v+|\Omega_1|+d_w}}\right)x_vx_w\\ &- \left(\sqrt{1-\frac{2}{d_u+d_w}}\right)x_ux_w\Bigg]+2\sum_{w\in\Omega_2}\Bigg[\left(\sqrt{1-\frac{2}{d_v+|\Omega_1|+d_w}}\right.\\ &- \left.\sqrt{1-\frac{2}{d_v+d_w}}\right)\Bigg]x_vx_w. \end{aligned}\tag{3.1}$$

Since $|\Omega_1| = d_u - 1 \geq 1$, $|\Omega_2| \geq 1$ and $x_v \geq x_u$, it follows from equation (3.1) that $\mathbf{x}^T\mathcal{ABS}(G_{uv^+})\mathbf{x} - \mathbf{x}^T\mathcal{ABS}(G)\mathbf{x} > 0$. Thus, by Lemma 3.2, $\eta_1(G) < \eta_1(G_{uv^+})$. □

The class of unicyclic graphs of order n with girth g, and p pendant vertices is denoted as $\mathcal{U}_{g,p}$, where $n = g + p$.

Corollary 3.1 *Let G be a unicyclic graph of order n with the largest ABS spectral radius. Then $G \in \mathcal{U}_{3,n-3}$.*

Proof: Let G be a unicyclic graph with order n, girth g, and p pendant vertices. Applying Kelmans operation repeatedly on the non-pendant edges of G that are not on the unique cycle of G, the graph G gets transformed into the graph $\mathcal{U}_{g,p}$ (for example, see Fig. 3). Therefore, by Lemma 3.3, $\eta_1(G) < \eta_1(\mathcal{U}_{g,p})$. If g=3, then we are done. Otherwise $g > 3$. In this case, we apply Kelmans operation repeatedly on the edges of the cycle in $\mathcal{U}_{g,p}$ to obtain the graph $\mathcal{U}_{3,p}$ (see Fig. 3). Therefore, by Lemma 3.3, $\eta_1(G) < \eta_1(\mathcal{U}_{g,p}) < \eta_1(\mathcal{U}_{3,p})$. This completes the proof. □

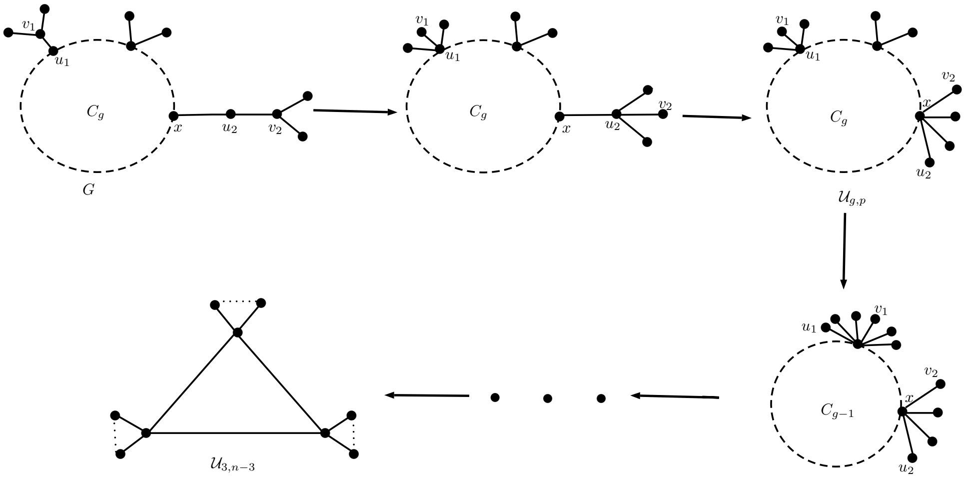


Figure 3: Graph G and its transformation into the graph $\mathcal{U}_{3,p}$ under the Kelmans operation.

We denote the class of unicyclic graphs of diameter d and order n by $\mathcal{U}_n^d$, and Δ_n^d denotes the class of unicyclic graphs of girth 3 with $n - d - 2(\geq 0)$ pendant edges and a path of length $\left\lfloor\frac{d}{2}\right\rfloor$ attached to one vertex of the cycle C_3, and a path of length $\left\lceil\frac{d}{2}\right\rceil$-1 attached to another vertex of C_3.

The following lemma proved in [24] is useful to prove our next result.

Lemma 3.4 [24] *Let $G \in \mathcal{U}_n^d$. Then $\lambda_1(G) \leq \lambda_1(\Delta_n^d)$.*

Lemma 3.5 *Let* $G \in \mathcal{U}_{3,n-3}$. *If diameter of* G *is* 3, *then* $\eta_1(G) < \dfrac{n-1}{\sqrt{n+1}}$ *for all* $n \geq 13$.

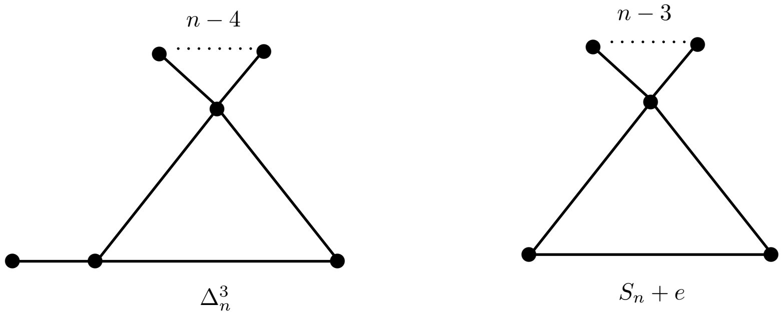
Proof: Since $d_i + d_j \leq n+1$ for all $1 \leq i, j \leq n$, we get $\mathcal{ABS}(G) \preceq \sqrt{\dfrac{n-1}{n+1}}\mathcal{A}(G)$. Thus, by Lemma 2.3, $\eta_1(G) < \sqrt{\dfrac{n-1}{n+1}}\lambda_1(G)$. Consequently, by Lemma 3.4, $\eta_1(G) < \sqrt{\dfrac{n-1}{n+1}}\lambda_1(\Delta_n^3)$.

Claim: $\lambda_1(\Delta_n^3) < \sqrt{n-1}$. The adjacency matrix of Δ_n^3 is as follows:

$$\mathcal{A}(\Delta_n^3) = \begin{bmatrix} 0 & 0 & \dots & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \dots & 0 & 1 & 0 & 0 & 0 \\ \vdots & & \ddots & & & & \vdots & \\ 0 & 0 & \dots & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & \dots & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & \dots & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & \dots & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 & 1 & 0 & 0 \end{bmatrix}.$$

Therefore, the characteristic polynomial of $\mathcal{A}(\Delta_n^3)$ is $(x^{n-5})f(x)$, where $f(x) := x^5 - nx^3 - 2x^2 - (7-2n)x$. It is straightforward to verify that $f(\sqrt{n-1}) > 0$ for all $n \geq 13$. Let $g(x) = f(x + \sqrt{n-1})$. Then $g'(x) = (-4 + 20x^3 + (14n-20)x)\sqrt{n-1} + 5x^4 + (27n-30)x^2 - 4x + 2n^2 - 5n - 2 > 0$ for all $x \geq 0$. Thus, $f(x)$ is increasing for all $x \geq \sqrt{n-1}$. So, $f(x)$ has no root in the interval $[\sqrt{n-1}, \infty)$. Proving, $\lambda_1(\Delta_n^3) < \sqrt{n-1}$. Hence, $\eta_1(G) < \sqrt{\dfrac{n-1}{n+1}}\lambda_1(\Delta_n^3) < \dfrac{n-1}{\sqrt{n+1}}$. That is, $\eta_1(G) < \dfrac{n-1}{\sqrt{n+1}}$. □

Let $S_n + e$ be the graph of order $n \geq 4$ obtained by attaching $n-3$ pendant vertices to one vertex of the triangle C_3.



Δ_n^3 $S_n + e$

Figure 4: The graphs Δ_n^3 and $S_n + e$.

Lemma 3.6 *We have* $\eta_1(S_n + e) > \dfrac{n-1}{\sqrt{n+1}}$.

Proof: The ABS matrix of $S_n + e$ is as follows:

$$\mathcal{ABS}(S_n+e) = \begin{bmatrix} 0 & 0 & \dots & 0 & \sqrt{\frac{n-2}{n}} & 0 & 0 \\ 0 & 0 & \dots & 0 & \sqrt{\frac{n-2}{n}} & 0 & 0 \\ \vdots & & \ddots & & & \vdots & \\ 0 & 0 & \dots & 0 & \sqrt{\frac{n-2}{n}} & 0 & 0 \\ \sqrt{\frac{n-2}{n}} & \sqrt{\frac{n-2}{n}} & \dots & \sqrt{\frac{n-2}{n}} & 0 & \sqrt{\frac{n-1}{n+1}} & \sqrt{\frac{n-1}{n+1}} \\ 0 & 0 & \dots & 0 & \sqrt{\frac{n-1}{n+1}} & 0 & \sqrt{\frac{1}{2}} \\ 0 & 0 & \dots & 0 & \sqrt{\frac{n-1}{n+1}} & \sqrt{\frac{1}{2}} & 0 \end{bmatrix}.$$

Therefore, characteristic polynomial of $\mathcal{ABS}(S_n+e)$ is $f(x) = x^{n-4} f(x)$, where $f(x) = x^4 - \frac{(2\,n^3 - 3\,n^2 - n + 12)\,x^2}{2\,(n+1)\,n} - \frac{(n-1)\,\sqrt{2}x}{n+1} + \frac{n^2 - 5\,n + 6}{2n}$. It is straightforward to verify that $f(\frac{n-1}{\sqrt{n+1}}) < 0$ and $f(n) > 0$. Since f is continuous, it follows that $f(x)$ has a root in $\left(\frac{n-1}{\sqrt{n+1}}, n\right)$. Hence $\eta_1(S_n+e) > \frac{n-1}{\sqrt{n+1}}$. □

Theorem 3.2 *Among all unicyclic graphs of order $n \geq 4$, the graph $S_n + e$ has the maximum ABS spectral radius.*

Proof: Let G be a unicyclic graph of order $n \geq 13$ with maximum ABS spectral radius. Then by Corollary 3.1, $G \in \mathcal{U}_{3,n-3}$. So, G is of diameter 2 or 3. If G is of diameter 2, then $G \cong S_n + e$, and thus by Lemma 3.6, $\eta_1(G) > \frac{n-1}{\sqrt{n+1}}$. Otherwise, G is of diameter 3. In this case, by Lemma 3.5, $\eta_1(G) < \frac{n-1}{\sqrt{n+1}}$. Thus, $S_n + e$ has the maximum ABS spectral radius among all unicyclic graphs of order $n \geq 13$. For $4 \leq n \leq 12$, it can be verified using Sage [28] that $S_n + e$ has the maximum ABS spectral radius. □

4. Conclusion

From our results on ABS spectral radius of trees, it can be observed that ordering of trees according the ABS spectral radius is different than the ordering of trees according to the ABC spectral radius [4,21] and extended adjacency spectral radius [15], see Table 1.

It is proved that among all unicyclic graphs on n vertices, the graph $S_n + e$ has maximum ABS spectral radius. Also, an upper bound for the ABS spectral radius of unicyclic graphs with girth at least 5 is obtained. The problem of ordering unicyclic graphs and bicyclic graphs with respect to ABS spectral radius would be an interesting problem for future research.

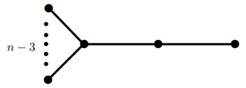
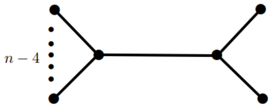
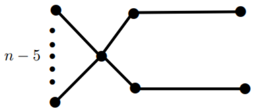
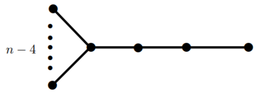
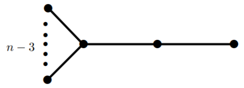
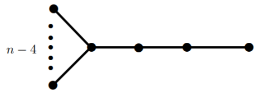
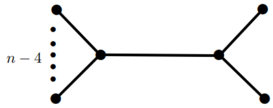
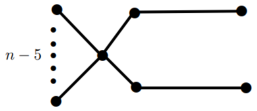
ABS spectral radius	ABC and extended adjacency spectral radius
   	   

Table 1: Ordering of trees based on ABS, ABC and extended adjacency spectral radius.

Conflict of interest

The authors declare that they have no conflicts of interest.

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