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Ordering Unicyclic Graphs by their ABS Spectral Radius

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Abstract

The ABS spectral radius of a graph G is the largest eigenvalue of the ABS matrix of G denoted by $\mathcal{ABS}(G)$, whose (i, j)- entry is $\sqrt{1 - \frac{2}{d_i + d_j}}$ if $ij \in E(G)$ and zero otherwise for $i, j \in V(G)$, where d_i is the degree of vertex i in G and $V(G)$ ($E(G)$) denotes the vertex (edge) set of G. In the present work, we extend the result of Lin and Liu [5] by determining the unicyclic graphs of order $n \geq 19$ with the second, third, and fourth largest ABS spectral radius.

Math. Subject Classification: 05C50, 05C35.
Key Words and Phrases: ABS matrix, ABS spectral radius, unicyclic graphs.

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1 Introduction

Let G be a simple, undirected graph with a non-empty set of vertices V of order n. The spectral radius, denoted by $\lambda_1(G)$, is the largest eigenvalue of the adjacency matrix $\mathcal{A}(G)$ of G. The atom-bond sum-connectivity index(ABS index) of a graph G was introduced by Ali et.al [1] as a degree-based topological index. It is defined as

$$ABS(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}},$$

where d_i and d_j denote the degrees of the adjacent vertices v_i and v_j, respectively. In recent years, the ABS index has attracted considerable attention due to its usefulness in both theoretical studies and chemical applications. A wide range of mathematical properties related to this index have been investigated in depth; a comprehensive account of these developments can be found in the survey article by Ali et. al. [2].

Recently, a new degree-based matrix, called the atom-bond sum-connectivity matrix $\mathcal{ABS}(G)$, was proposed in [7]. This matrix is defined as

$$(\mathcal{ABS}(G))_{ij} = \begin{cases} \sqrt{1 - \dfrac{2}{d_i + d_j}}, & \text{if } ij \in E(G), \\ 0, & \text{otherwise}, \end{cases}$$

where d_i denotes the degree of vertex v_i. The eigenvalues of $\mathcal{ABS}(G)$ are written as $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$, and the largest eigenvalue η_1 is called the ABS spectral radius. Several studies have begun to explore the spectral behavior of $\mathcal{ABS}(G)$. The ABS Estrada index and spectral radius of trees were investigated in [6, 7]. Subsequent research established bounds for the ABS spectral radius and the ABS energy [9], and more recently, ordering of trees based on spectral radius and extremal spectral radius of unicyclic graphs were reported in [8, 5]. Motivated by these studies, in the present

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work, we obtain the unicyclic graphs of order $n \geq 19$ that attain the second, third, and fourth maximum spectral radii. Further, we observe that the ordering of unicyclic graphs based on ABS spectral radius is different from that of the ABC spectral radius and arithmetic-geometric spectral radius. Our study indeed extends the following result obtained by Lin and Liu.

Theorem 1. *[5] Let G be a unicyclic graph with $n \geq 17$ vertices. Then $\rho_1(G) \leq \rho_1(U_n^1)$ with equality if and only if $G \cong U_n^1$. See Fig 1.*

2 Preliminaries

Let Λ_1 and Λ_2 be two real matrices of same order, we write $\Lambda_1 \preceq \Lambda_2$ if every entry in Λ_1 does not exceed the counterpart in Λ_2.

Lemma 2. *[4] Let Λ_1,Λ_2 be non-negative matrices of order n with spectral radius $\rho(\Lambda_1)$ and $\rho(\Lambda_2)$, respectively. If $\Lambda_1 \preceq \Lambda_2$, then $\rho(\Lambda_1) \leq \rho(\Lambda_2)$. Further, if Λ_1 is irreducible and $\Lambda_1 \neq \Lambda_2$, then $\rho(\Lambda_1) < \rho(\Lambda_2)$.*

Remark 3. *For any unicyclic graph $U_n \in \mathcal{U}_n$, the matrices $\mathcal{ABS}(U_n)$ and $\mathcal{A}(U_n)$ are irreducible with $\mathcal{ABS}(U_n) \preceq \sqrt{\frac{n-1}{n+1}}\mathcal{A}(U_n)$ and $\mathcal{ABS}(U_n) \neq \sqrt{\frac{n-1}{n+1}}\mathcal{A}(U_n)$. Thus, by Lemma 2, $\eta_1(U_n) < \sqrt{\frac{n-1}{n+1}}\lambda_1$.*

It is known that the first five largest values of the spectral radius of unicyclic graphs with n vertices are achieved by the graphs in Fig 1. That is, $\lambda_1(U_n^1) > \lambda_1(U_n^2) > \lambda_1(U_n^3) > \lambda_1(U_n^4) > \lambda_1(U_n^5)$ [3].

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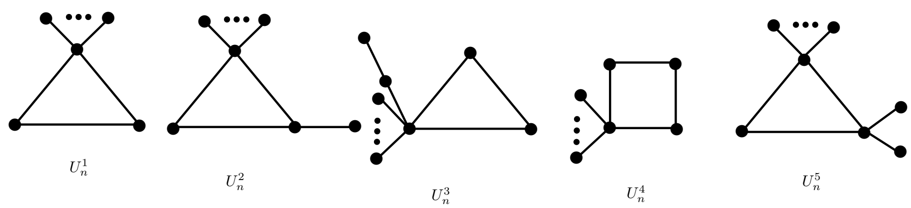

Figure 1: The unicyclic graphs U_n^1,U_n^2, U_n^3,U_n^4 and U_n^5.

3 Main results

In this section, we classify unicyclic graphs that have the second-largest, third-largest, and fourth-largest ABS spectral radius. We denote by $\mathcal{U}_n$ the class of unicyclic graphs on n vertices.

Lemma 4. *Let $U_n \notin \{U_n^1, U_n^2, U_n^3, U_n^4\}$. Then for $n \geq 19$,* $\eta_1(U_n) < \sqrt{\dfrac{(n-1)(10n-21)}{10(n+1)}}$.

Proof. If $U_n \notin \{U_n^1, U_n^2, U_n^3, U_n^4\}$, then by Remark 3, $\eta_1(U_n) < \sqrt{\dfrac{n-1}{n+1}}\lambda_1(U_n^5)$.
The characteristic polynomial of $\mathcal{A}(U_n^5)$ is given by $x^{n-4}\Phi(x)$, where $\Phi(x) = x^4 - nx^2 - 2x + 3n - 13$. It is straight-forward to verify that $\Phi\left(\sqrt{n - \dfrac{21}{10}}\right) > 0$ for all $n \geq 19$. Let $\Phi_1(x) = \Phi\left(x + \sqrt{n - \dfrac{21}{10}}\right)$. Then $\Phi_1'(x) = 4\left(x + \sqrt{n - \dfrac{21}{10}}\right)^3 - n\left(2x + 2\sqrt{n - \dfrac{21}{10}}\right) > 0$ for all $x \geq 0$. Thus, $\Phi(x)$ has no root in the interval $[\sqrt{n - \dfrac{21}{10}}, \infty)$. Proving, $\lambda_1(U_n^5) < \sqrt{n - \dfrac{21}{10}}$. That is, $\eta_1(U_n) < \sqrt{\dfrac{(n-1)(10n-21)}{10(n+1)}}$. □

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Lemma 5. *We have*

$$\sqrt{\frac{(n-1)(10n-21)}{10(n+1)}} < \eta_1(U_n^4) < \sqrt{\frac{(n-1)(n-2)}{n+1}},$$

the left side inequality valid for $n \geq 5$ and right side inequality valid for $n \geq 11$.

Proof. The characteristic polynomial of $\mathcal{ABS}(U_n^4)$ is

$$x^{n-4}\left(x^5 + \frac{-n^3+4n^2-5n-4}{n(n-1)}x^3 + \frac{n^3-7n^2+12n}{n(n-1)}x\right).$$

Thus,

$$\eta_1^2(U_n^4) = \frac{n^3-4n^2+5n+4+\sqrt{A}}{2n(n-1)},$$

where $A = n^6 - 12n^5 + 58n^4 - 108n^3 + 41n^2 + 40n + 16$.
Claim: $\eta_1^2(U_n^4) > \dfrac{(n-1)(10n-21)}{10(n+1)}$.
To prove this it suffices to prove that, $2n(n-1)^2(10n-21) < 10(n+1)[n^3-4n^2+5n+4+\sqrt{A}]$, where $A = n^6-12n^5+58n^4-108n^3+41n^2+40n+16$. Now, $100(n+1)^2A - 4(5n^4-26n^3+47n^2-66n-20)^2 = 4(10n^7-271n^6+2294n^5-4914n^4+88n^3+3024n^2+1760n+384)$. Since $\psi_1(x) = 4(10x^7-271x^6+2294x^5-4914x^4+88x^3+3024x^2+1760x+384)$ is an increasing function for $x \geq 5$ with $\psi_1(5) > 0$, $4(10n^7-271n^6+2294n^5-4914n^4+88n^3+3024n^2+1760n+384) > 0$. Therefore, $\eta_1(U_n^4) > \sqrt{\dfrac{(n-1)(10n-21)}{10(n+1)}}$.
Now, to prove the right side inequality, we claim that, $\eta_1^2(U_n^4) < \dfrac{(n-1)(n-2)}{n+1}$.
It is enough to show that, $(n+1)(n^3-4n^2+5n+4)+(n+1)\sqrt{A} < 2n(n-1)^2(n+2)$, where $A = n^6-12n^5+58n^4-108n^3+41n^2+40n+16$. Consider, $(n^4-5n^3+9n^2-13n-4)^2 - (n+1)^2A = 8n(n^5-14n^4+40n^3-26n^2-5n+4)$. Since $\psi_2(x) = 8x(x^5-14x^4+40x^3-26x^2-5x+4)$ is an increasing function for $x \geq 11$ with

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$\psi_2(11) > 0$, $8n(n^5 - 14n^4 + 40n^3 - 26n^2 - 5n + 4) > 0$. Therefore, $\eta_1(U_n^4) < \sqrt{\dfrac{(n-1)(n-2)}{n+1}}$. □

Lemma 6. *We have*

$$\sqrt{\frac{(n-1)(n-2)}{n+1}} < \eta_1(U_n^3) < \sqrt{\frac{(n-1)(n-2)}{n+1}} + \frac{100}{141n},$$

the left side inequality valid for $n \geq 5$ *and right side inequality valid for* $n \geq 11$. *Also,* $\eta_1(U_n^3) < \sqrt{\dfrac{(n-1)(n-2)}{n+1}} + \dfrac{100}{150n}$ *for* $n \in [12, 988]$.

Proof. The characteristic polynomial of $\mathcal{ABS}(U_n^3)$ is given by $x^{n-6}\varphi(x)$, where $\varphi(x) = x^6 - \dfrac{6n^3 - 25n^2 + 31n + 36}{6n(n-1)}x^4$
$- \dfrac{6\sqrt{2}n^2 - 18\sqrt{2}n + 12\sqrt{2}}{6n(n-1)}x^3 - \dfrac{-5n^3 + 32n^2 - 53n - 14}{6n(n-1)}x^2$
$- \dfrac{-2\sqrt{2}n^2 + 6\sqrt{2}n - 4\sqrt{2}}{6n(n-1)}x - \dfrac{n^3 - 8n^2 + 15n}{6n(n-1)}$.
It is straight forward to verify that, $\varphi\left(\sqrt{\dfrac{(n-1)(n-2)}{n+1}}\right) < 0$ and $f\left(\sqrt{n-1}\right) > 0$ for all $n \geq 5$. Since φ is continuous, it follows that φ has a root in $\left(\sqrt{\dfrac{(n-1)(n-2}{n+1}}, \sqrt{n-1}\right)$. Therefore, $\eta_1(U_n^3) > \sqrt{\dfrac{(n-1)(n-2)}{n+1}}$.
Also, one can directly verify that, $\varphi\left(\sqrt{\dfrac{(n-1)(n-2)}{n+1}} + \dfrac{100}{141n}\right) > 0$, for $n \geq 12$, and by first derivative test, $\varphi(x)$ strictly increases for $x \geq \sqrt{\dfrac{(n-1)(n-2)}{n+1}} + \dfrac{100}{141n}$. Therefore, $\eta_1(U_n^3) < \sqrt{\dfrac{(n-1)(n-2)}{n+1}} + \dfrac{100}{141n}$. Similarly using above argument we can prove that, $\eta_1(U_n^3) <$

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$\sqrt{\frac{(n-1)(n-2)}{n+1}} + \frac{100}{150n}$, for $12 \leq n \leq 988$. $\square$

Lemma 7. *We have* $\eta_1(U_n^2) > \sqrt{\frac{(n-1)(n-2)}{n+1}} + \frac{100}{150n}$, *for all* $n \geq 5$ *and* $\eta_1(U_n^2) > \sqrt{\frac{(n-1)(n-2)}{n+1}} + \frac{100}{141n}$ *for all* $n \geq 212$.

Proof. The characteristic polynomial of $\mathcal{ABS}(U_n^2)$ is given by $x^{n-4}\varrho(x)$, where $\varrho(x) = x^4 + \frac{-10n^4+29n^3-10n^2-109n-20}{10n(n-1)(n+1)}x^2 + \frac{4(n-n^3)\sqrt{15}\sqrt{\frac{n-1}{n+1}}\sqrt{\frac{n-2}{n}}}{10n(n-1)(n+1)}x + \frac{11n^4-61n^3+45n^2+127n+10}{10n(n-1)(n+1)}$. One can easily verify that, $\varrho\left(\sqrt{\frac{(n-1)(n-2)}{n+1}} + \frac{100}{150n}\right) < 0$ and $\varrho\left(\sqrt{n-1} + \frac{100}{150n}\right) > 0$ for all $n \geq 5$. Since ϱ is continuous, ϱ has a root in $\left(\sqrt{\frac{(n-1)(n-2)}{n+1}} + \frac{100}{150n}, \sqrt{n-1} + \frac{100}{150n}\right)$. Therefore, $\eta_1(U_n^2) > \sqrt{\frac{(n-1)(n-2)}{n+1}} + \frac{100}{150n}$. In similar way, one can prove, $\eta_1(U_n^2) > \sqrt{\frac{(n-1)(n-2)}{n+1}} + \frac{100}{141n}$ for all $n \geq 212$. $\square$

By Lemmas 4, 5, 6 and 7, we get the following result.

Theorem 8. *Among all unicyclic graphs of order* $n \geq 19$, *the graphs* U_n^1, U_n^2, U_n^3 *and* U_n^4 *are respectively, the unique unicyclic graphs with the first four largest* ABS *spectral radius.*

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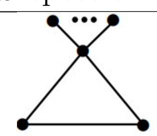
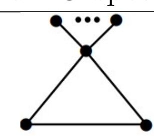
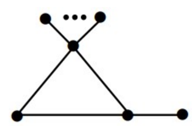
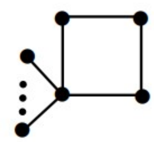
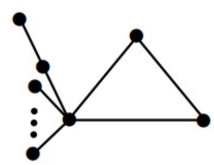
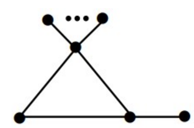
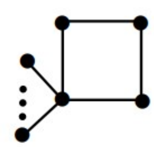
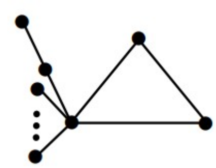
ABS spectral radius	ABC and AG spectral radius
	
	
	
	

Table 1: Ordering of trees based on ABS, ABC and arithmetic-geometric spectral radius.

Conclusion

From our results on ABS spectral radius of unicyclic graphs, it can be observed that, the ordering of unicyclic graph of order $n \geq 19$ based on ABS spectral radius is different from that of ABC spectral radius [10] and arithmetic-geometric spectral radius [11], see Table 1. Further study on ABS spectral radius may give some interesting results compared to other weighted adjacency matrices.

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