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Research Article

On the atom-bond sum-connectivity spectral radius of unicyclic graphs

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Abstract

Let G be a graph with n vertices. For $i = 1, 2, \dots, n$, let d_i be the degree of vertex v_i in G. The atom-bond sum-connectivity (ABS) matrix of G is an $n \times n$ matrix whose (i, j)-entry is equal to $\sqrt{(d_i + d_j - 2)/(d_i + d_j)}$ if the vertices v_i and v_j are adjacent, and 0 otherwise. The ABS spectral radius of G, denoted by $\rho_1(G)$, is the largest eigenvalue of the ABS matrix of G. Let C_n be the cycle graph with n vertices. Let U_n^1 be the unicyclic graph with n vertices and maximum degree $n - 1$. For a unicyclic graph G with $n \geq 17$ vertices, we prove that $\rho_1(C_n) \leq \rho_1(G) \leq \rho_1(U_n^1)$, where the left equality holds if and only if $G \cong C_n$ and the right equality holds if and only if $G \cong U_n^1$.

Keywords: ABS matrix; ABS spectral radius; unicyclic graph.

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1. Introduction

Let G be a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. Denote by $d_G(v_i)$ (or d_i for short) the degree of vertex v_i in G. The girth of a graph G, denoted by $g(G)$, is the length of the shortest cycle contained in G. The star, cycle, and path with n vertices are denoted by S_n, C_n, and P_n, respectively. A unicyclic graph is a simple connected graph with an equal number of vertices and edges. Clearly, a unicyclic graph contains a unique cycle. Let U_n^1 denote the unicyclic graph obtained from S_n by adding an edge. We use $G - u$ and $G - uv$ to denote the graphs that arise from G by deleting the vertex $u \in V(G)$ and the edge $uv \in E(G)$, respectively. The spectral radius, denoted by $\lambda_1(G)$, is the largest eigenvalue of the adjacency matrix $A(G)$ of G.

The atom-bond sum-connectivity (or ABS, for short) index of a graph G, introduced by Ali, Furtula, Redžepović, and Gutman [1] as a topological index, is defined as

$$ABS(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}}.$$

The study of the ABS index is a subject of increasing interest, both in pure and applied mathematics. The mathematical properties of the ABS index have been extensively studied; for example, see the survey paper [2].

Generally, a matrix keeps much more structural information about the graph than an index. Hence, extended adjacency matrices constructed by topological indices have been proposed and extensively studied, such as the Randić matrix [7], the geometric-arithmetic matrix [12], the harmonic matrix [8], the ABC matrix [5], the inverse sum indeg matrix [14] and etc. Naturally, the spectral properties (including energy, spectral radius, and Estrada index) of the extended adjacency matrices are among the popular topics in chemical graph theory.

In 2024, Lin et al. [9] introduced the atom-bond sum-connectivity matrix (ABS matrix, for short) from an algebraic viewpoint. The ABS matrix of a graph G, denoted by $\mathcal{A}(G)$, is an $n \times n$ matrix whose (i, j)-entry is equal to $\sqrt{(d_i + d_j - 2)/(d_i + d_j)}$ if $v_i v_j \in E(G)$, and 0 otherwise. The largest eigenvalue of the ABS matrix of G is called the ABS spectral radius, denoted by $\rho_1(G)$. Lin et al. [9] showed that the spectral radius of the ABS matrix is useful in predicting certain physicochemical properties of octane isomers. Moreover, they studied an extremal problem for the ABS spectral radius of trees and proved that $\rho_1(P_n) \leq \rho_1(T_n) \leq \rho_1(S_n)$, where the left equality (respectively, right equality) holds if and only if T_n is isomorphic to the path P_n (respectively, the star S_n). For research on other spectral properties of the ABS matrix, see [10, 11, 13]. Along this line, it is natural to study the ABS spectral radius of unicyclic graphs. In this paper, we determine the upper and lower bounds of the ABS spectral radius for unicyclic graphs, and characterize the respective extremal graphs.

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2. Preliminaries

Lemma 2.1 (see [3])**.** *Suppose that $A = (a_{i,j})$ and $B = (b_{i,j})$ are two $n \times n$ nonnegative symmetric matrices. If $A \geq B$, i.e., $a_{i,j} \geq b_{i,j}$ for all i, j, then $\lambda_1(A) \geq \lambda_1(B)$. Furthermore, if B is irreducible and $A \neq B$, then $\lambda_1(A) > \lambda_1(B)$.*

Lemma 2.2 (see [3])**.** *If M' is a principal sub-matrix of a real symmetric matrix M, then $\lambda_1(M) > \lambda_1(M')$.*

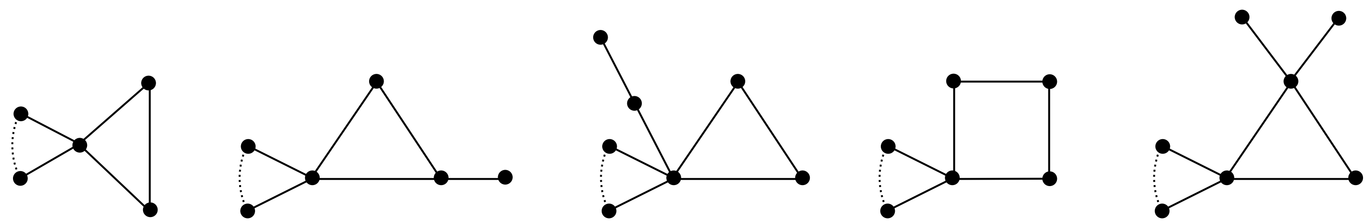
Lemma 2.3 (see [9])**.** *Let T_n be a tree with $n \geq 9$ vertices. Then*

$$\rho_1(P_n) < \rho_1(C_n) < \rho_1(T_n).$$

It is known that the first five largest values of the spectral radius of unicyclic graphs with n vertices are achieved by the graphs shown in Figure 2.1, and $\lambda_1(U_n^1) > \lambda_1(U_n^2) > \cdots > \lambda_1(U_n^5)$.

Lemma 2.4 (see [6])**.** *The characteristic polynomials of the adjacency matrices $A(U_n^3)$, $A(U_n^4)$, and $A(U_n^5)$ are given as follows:*

$$\begin{aligned} P_A(U_n^3) &= x^{n-6}[x^6 - nx^4 - 2x^3 + (2n-6)x^2 + 2x - n + 5], \\ P_A(U_n^4) &= x^{n-4}(x^4 - nx^2 + 2n - 8), \\ P_A(U_n^5) &= x^{n-4}(x^4 - nx^2 - 2x + 3n - 13). \end{aligned}$$



U_n^1 U_n^2 U_n^3 U_n^4 U_n^5

Figure 2.1: The unicyclic graphs U_n^1, U_n^2, U_n^3, U_n^4, and U_n^5.

3. Main results

Theorem 3.1. *Let $f(x, y)$ be an increasing function in both x and y for $x \geq 1$ and $y \geq 1$. Define a matrix $Af(G) = (w_{ij})$, called the weighted adjacency matrix of a connected graph G, whose (i, j)-entry is $w_{ij} = f(d_i, d_j)$ if $v_iv_j \in E(G)$ and $w_{ij} = 0$ otherwise. Let $\lambda_w(G)$ be the largest eigenvalue of $Af(G)$. Then $\lambda_w(G) > \lambda_w(G - v_iv_j)$ and $\lambda_w(G) > \lambda_w(G - v_i)$.*

Proof. Since $f(x, y)$ is increasing in both x and y for $x \geq 1$ and $y \geq 1$, we have $Af(G) \geq Af(G - v_iv_j)$. If $G - v_iv_j$ is connected, then $Af(G - v_iv_j)$ is irreducible. By Lemma 2.1, we have $\lambda_w(G) > \lambda_w(G - v_iv_j)$. If $G - v_iv_j$ is disconnected, then by Lemma 2.2, we have $\lambda_w(G) > \lambda_w(G - v_iv_j)$.

Consider a vertex $v_i \in V(G)$ and let $Af_{v_i}(G)$ be the principal submatrix of $Af(G)$ obtained by deleting the row and column related to v_i. Since $f(x, y)$ is increasing in both x and y for $x \geq 1$ and $y \geq 1$, we have $Af_{v_i}(G) \geq Af(G - v_i)$. By Lemma 2.2, we have $\lambda_w(G) > \lambda_w(Af_{v_i}(G)) \geq \lambda_w(G - v_i)$. This completes the proof. $\square$

Since $f(x, y) = \sqrt{1 - \frac{2}{x+y}}$ is strictly increasing in both x and y for $x \geq 1$ and $y \geq 1$. By Theorem 3.1, we obtain the following corollary:

Corollary 3.1. *Let G be a connected graph with n vertices. Then $\rho_1(G) > \rho_1(G - uv)$ and $\rho_1(G) > \rho_1(G - u)$.*

Theorem 3.2. *Let G be a connected graph with $n \geq 9$ vertices. If G is neither P_n nor C_n, then*

$$\rho_1(G) > \rho_1(C_n) > \rho_1(P_n).$$

Proof. Let T be a spanning tree of G. By Corollary 3.1, we have

$$\rho_1(G) \geq \rho_1(T).$$

Note that $\rho_1(C_n) = \sqrt{\frac{1}{2}}\,\lambda_1(C_n) = \sqrt{2}$. Since G is neither P_n nor C_n, by Lemma 2.3, we have

$$\rho_1(G) \geq \rho_1(T) > \sqrt{2} > \rho_1(P_n)$$

for $n \geq 9$. This completes the proof. $\square$

Theorem 3.3. *Let G be a unicyclic graph with $n \geq 5$ vertices. Then*

$$\rho_1(G) \geq \sqrt{2}$$

with equality if and only if $G \cong C_n$.

Proof. If $n \geq 9$, then by Theorem 3.2, the result holds. In what follows, assume that $5 \leq n \leq 8$. Let T_n be a tree with n vertices. If $\Delta(T_n) \geq 4$, then the star S_5 must be a subgraph of T_n. By Corollary 3.1, we have

$$\rho_1(T_n) \geq \rho_1(S_5) = \sqrt{\frac{12}{5}} > \sqrt{2}.$$

If $\Delta(T_n) = 3$, then we consider all trees for $n = 5, 6, 7, 8$, depicted in Figure 3.1 (taken from Table A4 of [4]). Table 1 gives the ABS spectral radius of these trees. Note that the ABS spectral radius of each of these trees except T^6, T^{11}, T^{12}, T^{23}, and T^{46}, is greater than $\sqrt{2}$. Let $\mathcal{U}^*$ be the set of graphs obtained from T^6, T^{11}, T^{12}, T^{23}, and T^{46}, by adding an edge. If $G \in \mathcal{U}^*$, then by simple numerical calculations, we have $\rho_1(G) > \sqrt{2}$. In summary, for $n \geq 5$, we have $\rho_1(G) \geq \sqrt{2}$ with equality if and only if $G \cong C_n$. $\square$

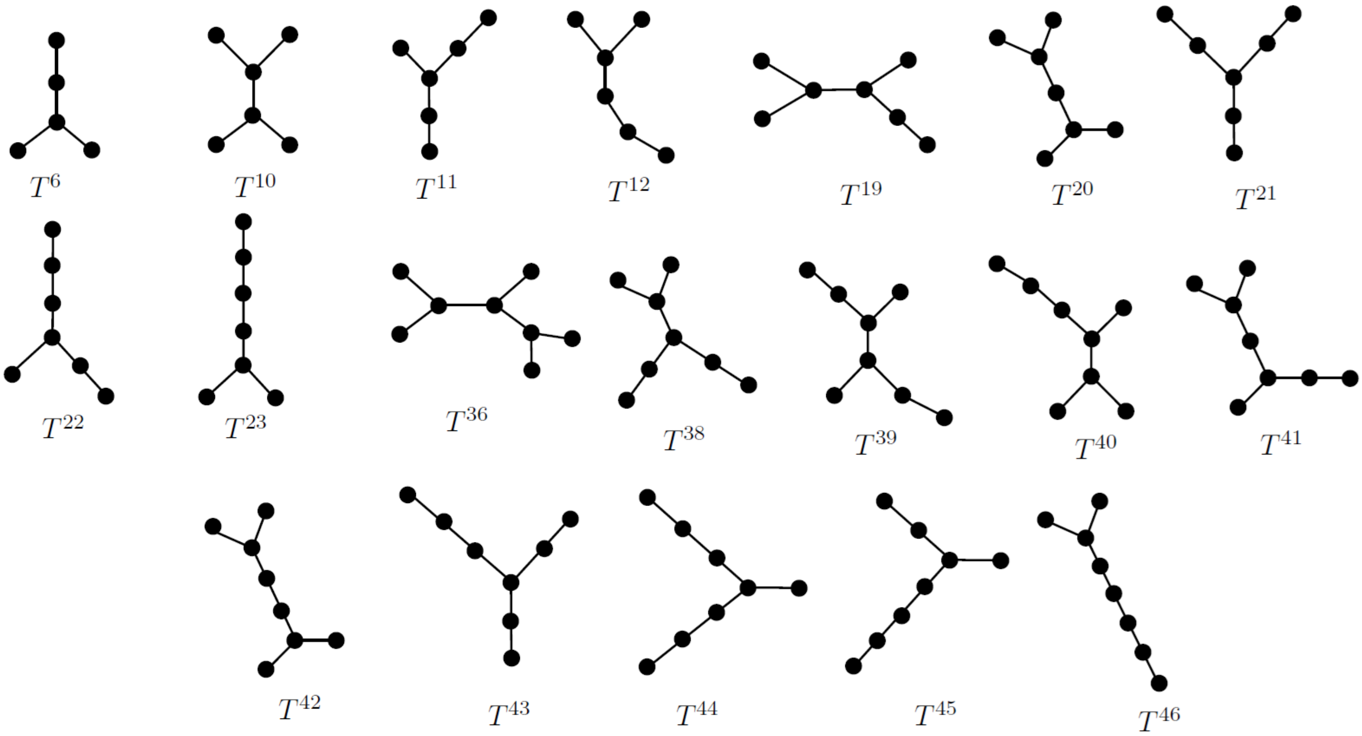


Figure 3.1: All trees with n vertices and $\Delta = 3$, where $5 \leq n \leq 8$.

Table 1: The spectral radius of $\mathcal{A}(T^i)$ for trees T^i depicted in Figure 3.1.

Trees	ρ_1	Trees	ρ_1	Trees	ρ_1	Trees	ρ_1
T^6	1.3198	T^{20}	1.4832	T^{38}	1.5802	T^{43}	1.4922
T^{10}	1.4884	T^{21}	1.4606	T^{39}	1.5744	T^{44}	1.4677
T^{11}	1.3956	T^{22}	1.4354	T^{40}	1.5568	T^{45}	1.4520
T^{12}	1.3730	T^{23}	1.3975	T^{41}	1.5195	T^{46}	1.4102
T^{19}	1.5352	T^{36}	1.6261	T^{42}	1.4687	-	-

Theorem 3.4. *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 Figure 2.1).

Proof. If $g(G) \geq 4$, then $d_i + d_j \leq n$ for $v_iv_j \in E(G)$. By Lemma 2.4, we have

$$P_A(U_n^4) = x^{n-4}(x^4 - nx^2 + 2n - 8).$$

Thus, we have

$$\lambda_1(G) \leq \lambda_1(U_n^4) \leq \sqrt{n-1}$$

for $n \geq 7$ and $g(G) \geq 4$, where U_n^4 is given in Figure 2.1. Since $f(x,y) = \sqrt{1 - \frac{2}{x+y}}$ is strictly increasing in both x and y for $x \geq 1$ and $y \geq 1$, by Lemma 2.1 and Corollary 3.1, we have

$$\rho_1(G) < \sqrt{\frac{n-2}{n}}\lambda_1(G) \leq \sqrt{\frac{n-2}{n}}\lambda_1(U_n^4) \leq \sqrt{\frac{(n-1)(n-2)}{n}} = \rho_1(S_n) < \rho_1(U_n^1)$$

for $n \geq 7$ and $g(G) \geq 4$.

If $g(G) = 3$, then $d_i + d_j \leq n+1$ for $v_iv_j \in E(G)$. Then, there are three cases.

Case 1. $g(G) = 3$ and $d_i + d_j \leq n$. By Lemma 2.4, we have

$$P_A(U_n^3) = x^{n-6}[x^6 - nx^4 - 2x^3 + (2n-6)x^2 + 2x - n + 5].$$

Thus, we have $\lambda_1(G) \leq \lambda_1(U_n^3) \leq \sqrt{n-1}$ for $n \geq 11$. Since $f(x,y) = \sqrt{1 - \frac{2}{x+y}}$ is strictly increasing in both x and y for $x \geq 1$ and $y \geq 1$, by Lemma 2.1 and Corollary 3.1, we have

$$\rho_1(G) < \sqrt{\frac{n-2}{n}}\lambda_1(G) \leq \sqrt{\frac{n-2}{n}}\lambda_1(U_n^3) \leq \sqrt{\frac{(n-1)(n-2)}{n}} = \rho_1(S_n) < \rho_1(U_n^1)$$

for $n \geq 11$.

Case 2. $g(G) = 3$, $d_i + d_j = n+1$, $G \ncong U_n^1$ and $G \ncong U_n^2$, where U_n^1 and U_n^2 are shown in Figure 2.1. By Lemma 2.4, we have

$$P_A(U_n^5) = x^{n-4}(x^4 - nx^2 - 2x + 3n - 13).$$

Thus, we have $\lambda_1(G) \leq \lambda_1(U_n^5) \leq \sqrt{n-2}$ for $n \geq 17$. Since $f(x,y) = \sqrt{1 - \frac{2}{x+y}}$ is strictly increasing in both x and y for $x \geq 1$ and $y \geq 1$, by Lemma 2.1 and Corollary 3.1, we have

$$\rho_1(G) < \sqrt{\frac{n-1}{n+1}}\lambda_1(G) \leq \sqrt{\frac{n-1}{n+1}}\lambda_1(U_n^5) \leq \sqrt{\frac{(n-1)(n-2)}{n+1}} < \rho_1(S_n) < \rho_1(U_n^1)$$

for $n \geq 17$.

Case 3. $G \cong U_n^2$. By direct computation, we obtain the characteristic polynomial of the ABS matrix $\mathcal{A}(U_n^2)$:

$$\begin{aligned} P_{ABS}(U_n^2, x) &= \det(xI_n - \mathcal{A}(U_n^2)) \\ &= \begin{vmatrix} x & -\sqrt{\frac{n-2}{n}} & -\sqrt{\frac{n-1}{n+1}} & 0 & -\sqrt{\frac{n-3}{n-1}} & \cdots & -\sqrt{\frac{n-3}{n-1}} \\ -\sqrt{\frac{n-2}{n}} & x & -\sqrt{\frac{3}{5}} & 0 & 0 & \cdots & 0 \\ -\sqrt{\frac{n-1}{n+1}} & -\sqrt{\frac{3}{5}} & x & -\sqrt{\frac{1}{2}} & 0 & \cdots & 0 \\ 0 & 0 & -\sqrt{\frac{1}{2}} & x & 0 & \cdots & 0 \\ -\sqrt{\frac{n-3}{n-1}} & 0 & 0 & 0 & x & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\sqrt{\frac{n-3}{n-1}} & 0 & 0 & 0 & 0 & \cdots & x \end{vmatrix} \\ &= \frac{x^{n-4}}{10n(n-1)(n+1)}\Big[(10n^3 - 10n)x^4 - (10n^4 - 29n^3 + 10n^2 + 109n + 20)x^2 \\ &\quad -4(n-1)\sqrt{15(n^4 - 2n^3 - n^2 + 2n)}x + 11n^4 - 61n^3 + 45n^2 + 127n + 10\Big]. \end{aligned}$$

Let $f(x) = (10n^3-10n)x^4-(10n^4-29n^3+10n^2+109n+20)x^2-4(n-1)\sqrt{15(n^4-2n^3-n^2+2n)}x+11n^4-61n^3+45n^2+127n+10$. We observe that $f'(x) > 0$ for $x \in [\sqrt{n-3}, +\infty)$. Thus, $f(x)$ is strictly increasing on $[\sqrt{n-3}, +\infty)$. Since

$$f\left(\sqrt{n-3}\right) = 10n^4 - \left(4\sqrt{\frac{15(n-1)(n-2)(n-3)}{n(n+1)}} + 78\right) n^3 + 26n^2 + \left(4\sqrt{\frac{15(n-1)(n-2)(n-3)}{n(n+1)}} + 344\right) n + 70 < 0$$

and

$$f\left(\sqrt{\frac{(n-1)(n-2)}{n}}\right) = \frac{1}{n}\left(10n^5 - \left(\frac{4n^2-12n+8}{n}\sqrt{\frac{15}{n+1}} + 58\right) n^4 - 36n^3 + \left(\frac{4n^2-12n+8}{n}\sqrt{\frac{15}{n+1}} + 324\right) n^2 - 28n - 80\right) > 0$$

for $n \geq 9$, it follows that

$$\sqrt{n-3} < \rho_1(U_n^2) < \sqrt{\frac{(n-1)(n-2)}{n}} = \rho_1(S_n).$$

By Corollary 3.1, we have $\rho_1(U_n^2) < \rho_1(S_n) < \rho_1(U_n^1)$.

Combining the conclusions of all three cases, we obtain $\rho_1(G) \leq \rho_1(U_n^1)$ with equality if and only if $G \cong U_n^1$. $\square$

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References

[1] A. Ali, B. Furtula, I. Redžepović, I. Gutman, Atom-bond sum-connectivity index, *J. Math. Chem.* **60** (2022) 2081–2093.

[2] A. Ali, I. Gutman, B. Furtula, I. Redžepović, T. Došlić, Z. Raza, Extremal results and bounds for atom-bond sum-connectivity index, *MATCH Commun. Math. Comput. Chem.* **92** (2024) 271–314.

[3] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs*, Academic Press, New York, 1980.

[4] D. Cvetković, P. Rowlinson, S. Simić, *An Introduction to the Theory of Graph Spectra*, Cambridge University Press, New York, 2010.

[5] E. Estrada, The ABC Matrix, *J. Math. Chem.* **55** (2017) 1021–1033.

[6] S. Guo, First six unicyclic graphs of order n with larger spectral radius, *Appl. Math. J. Chinese Univ. Ser. A* **18** (2003) 480–486 (in Chinese).

[7] I. Gutman, B. Furtula, S. B. Bozkurt, On Randić energy, *Linear Algebra Appl.* **442** (2014) 50–57.

[8] A. Jahanbani, New bounds for the harmonic energy and harmonic Estrada index of graphs, *Comput. Sci. J. Moldova* **26** (2018) 270–300.

[9] Z. Lin, Y. Liu, T. Zhou, On the atom-bond sum-connectivity spectral radius of trees, *Discrete Math. Lett.* **13** (2024) 122–127.

[10] Z. Lin, T. Zhou, Y. Liu, On ABS Estrada index of trees, *J. Appl. Math. Comput.* **70** (2024) 5483–5495.

[11] J. Liu, Y. Hu, X. Ren, Spectral properties of the atom-bond sum-connectivity matrix, *Contrib. Math.* **10** (2024) 1–10.

[12] J. M. Rodríguez, J. M. Sigarreta, Spectral study of the geometric-arithmetic index, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 121–135.

[13] S. Shetty, B. Rakshith, N. V. S. Udupa, On the ABS spectrum and energy of graphs, *arXiv*:2409.03287 [math.CO], (2024).

[14] B. Xu, S. Li, R. Yu, Q. Zhao, On the spectral radius and energy of the weighted adjacency matrix of a graph, *Appl. Math. Comput.* **340** (2019) 156–163.