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Research Article

Minimum atom-bond sum-connectivity index of unicyclic graphs with maximum degree

Palaniyappan Nithya[1], Suresh Elumalai[1,*], Selvaraj Balachandran[2]

[1]*Department of Mathematics, College of Engineering and Technology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu 603 203, India*
[2]*Department of Mathematics, School of Humanities and Sciences, SASTRA Deemed University, Thanjavur, India*

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Abstract

Let G be a graph with edge set $E(G)$. Denote by d_u the degree of a vertex u in G. The atom-bond sum-connectivity (ABS) index of G is defined as $ABS(G) = \sum_{xy\in E(G)} \sqrt{(d_x + d_y - 2)/(d_x + d_y)}$. In this article, we determine the minimum possible value of the ABS index of unicyclic graphs of order n and maximum degree Δ such that $3 \le \Delta \le n-2$. All the graphs that attain the obtained minimum value are also characterized.

Keywords: atom-bond sum-connectivity index; unicyclic graph; maximum degree.

2020 Mathematics Subject Classification: 05C07, 05C09, 05C35.

1. Introduction

Consider a connected and simple graph G, represented as $G = (V, E)$, with order n and size m. The graph G a c-cyclic graph when $m = n + c - 1$. Specifically, when $c = 1$, G is referred to as a unicyclic graph. Let P_n and S_n be respectively the path and star graphs with n vertices. The set of neighbors of a vertex y in G is represented by $N_G(y)$ (or simply by $N(y)$) and the degree of y in G is represented by $d_y(G)$ (or simply by d_y). The symbols $\delta = \delta(G)$ and $\Delta = \Delta(G)$ are used to represent the minimum and maximum degrees of G, respectively. A vertex of degree 1 in G is referred to as a leaf or an end-vertex, while a vertex adjacent to a leaf is known as a stem. On the other hand, a strong stem is a stem that is adjacent to two or more leaves. A stem having at most one non-leaf neighbor is called an end stem.

Consider two different subsets $\mathcal{U}$ and $\mathcal{V}$ of $V(G)$. A path P in G that begins at a vertex in $\mathcal{U}$ and ends at a vertex in $\mathcal{V}$ such that all other vertices of P do not belong to either of the sets $\mathcal{U}$ and $\mathcal{V}$ is known as an $(\mathcal{U}, \mathcal{V})$-path. If $\mathcal{V} = \{v\}$, we write $(\mathcal{U}, v)$-path instead of $(\mathcal{U}, \mathcal{V})$-path. The length of a shortest $(\mathcal{U}, \mathcal{V})$-path is referred to as the distance between the sets $\mathcal{U}$ and $\mathcal{V}$ in the graph G, denoted as $d_G(\mathcal{U}, \mathcal{V})$.

Chemical graph theory [22] is a fundamental branch of mathematical chemistry, which focuses on representing and analyzing chemical structures using mathematical models. In chemical graph theory, topological indices play a crucial role in establishing connections between the structures of molecules and their properties related to the development of computer-aided drug designs [10, 16]. Numerous topological indices based on vertex degrees have been discussed in [12, 15]. In this paper, we are concerned with the atom-bond sum-connectivity (ABS) index, which is a recently introduced topological index [5]. The ABS index of G is defined as follows:

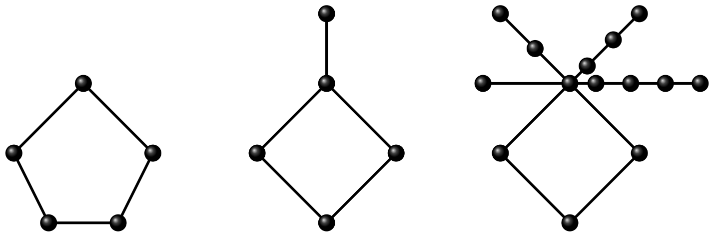
$$ABS(G) = \sum_{xy\in E(G)} \sqrt{\frac{d_x + d_y - 2}{d_x + d_y}}.$$

In [5], various basic mathematical properties of the ABS index were established. Ali et al. [6] examined the chemical applicability of the ABS index and identified its extremum values for unicyclic graphs. Gowtham and Gutman [14] formulated several inequalities between the ABS index and another existing connectivity index. In [8, 9], Alraqad et al. studied some extremal problems related to this index for certain classes of graphs. Noureen and Ali [20] solved the problem of determining the largest ABS index of trees of a given order with a fixed number of leaves. In [19], we determined the first four smallest values of the ABS index of unicyclic graphs of a given order with a specific girth and identified the graphs that achieve the obtained extremal values. For more details about the ABS index and its applications in the field of chemistry, additional information can be found in the references [1–3, 7, 13, 18, 19, 25].

*Corresponding author (sureshkako@gmail.com).

Recently, Hussain et al. [17] determined some sharp bounds for the ABS index in terms of other graph invariants. Among other things, a lower bound for the ABS index of trees in terms of their order and maximum degree was found in [17]. In this article, we extend this lower bound of Hussain et al. [17] to the one for unicyclic graphs.

Let $\mathbb{U}_n$ be the set of all unicyclic graphs on $n \geq 5$ vertices. Denote by $\mathbb{U}_{n,k}$ the subset of $\mathbb{U}_n$ that consists of those members of $\mathbb{U}_n$ that have a fixed girth k, $3 \leq k \leq n$. Certainly, $\mathbb{U}_n = \bigcup_{k=3}^{n} \mathbb{U}_{n,k}$ and $\mathbb{U}_{n,n} = \{\mathbf{C}_n\}$, where $\mathbf{C}_n$ is the cycle on n vertices. Let $\mathcal{U}^1_{n,n-1}$ be the unique unicyclic graph with n vertices and girth $n-1$. Thus, $\mathbb{U}_{n,n-1} = \{\mathcal{U}^1_{n,n-1}\}$. For k, with $3 \leq k \leq n-2$, denote by $\mathcal{U}^{k_1,k_2,\ldots,k_b}_{n,k} \in \mathbb{U}_{n,k}$ the unicyclic graph created by starting with the cycle $\mathbf{C}_k$ and then attaching b paths to a single vertex x of $\mathbf{C}_k$ such that the attached paths have lengths $k_1, k_2, \ldots, k_b$ provided that $\sum_{j=1}^{b} k_j = n-k$, see Figure 1.1.



$\mathbf{C}_5$ $\quad$ $\mathcal{U}^1_{5,4}$ $\quad$ $\mathcal{U}^{1,2,3,4}_{14,4}$

Figure 1.1: Some examples of unicyclic graphs.

The main objective of this study is to determine the minimum possible value of the ABS index of unicyclic graphs of order n and maximum degree Δ such that $3 \leq \Delta \leq n-2$, and characterize all the graphs that attain this minimum value. To prove some results of this paper, we utilize the following theorems:

Theorem 1.1. [19] *Consider a non-trivial connected graph H with a vertex x. Create a new graph G by adding 2 pendant paths P and Q to the vertex x. The paths are defined as $P := xx_1 \ldots x_a$ and $Q := xy_1 \ldots y_b$, where $a \geq b \geq 1$). Now, obtain a new graph G^* from G by adding an edge between vertices x_a and y_1 and removing the edge between x and y_1. Then $ABS(G) > ABS(G^*)$.*

Theorem 1.2. [19] *Consider a non-trivial connected graph H with 2 distinct vertices x and y such that both x and y have at least two neighbors. Additionally, suppose that when y (or x) has precisely two neighbors, the sum of these neighbors is at most 7 in H. Create a new graph G from H by adding two paths P and Q, to the vertices x and y, respectively, where $P := xx_1 \ldots x_a$ and $Q := yy_1 \ldots y_b (a \geq b \geq 1)$. Now, obtain a new graph G^* from G by adding an edge between y_b and x_1 and removing the edge between x and x_1.Then $ABS(G) > ABS(G^*)$.*

2. Main results

Throughout this section, we denote by G a unicyclic graph with n vertices, where $n \geq 5$. The unique cycle of the graph G is denoted as $\mathbf{C}$. Let $w \in V(G)$ be the vertex with maximum degree Δ such that its distance from the set of vertices of the cycle $\mathbf{C}$ (that is, $d_G(V(\mathbf{C}), w)$) is minimum. Take $N(w) = \{w_1, w_2, \ldots, w_\Delta\}$. In addition, $abs_w : E(G) \to \mathbb{R}$ is a function defined by

$$abs_w(xy) = \sqrt{\frac{d_x + d_y - 2}{d_x + d_y}}.$$

Hence, $ABS(G) = \sum_{xy \in E(G)} abs_w(xy)$. The next two results are direct consequences of Theorem 1.1 and Theorem 1.2.

Corollary 2.1. *Consider a unicyclic graph G with order n and maximum degree Δ such that $3 \leq \Delta \leq n-2$. If G possesses a strong stem (a stem with at least three neighbors) that is distinct from the vertex w, then there is a unicyclic graph G^* with order n and maximum degree Δ such that then $ABS(G) > ABS(G^*)$.*

Corollary 2.2. *Consider a unicyclic graph G with order n and maximum degree Δ such that $3 \leq \Delta \leq n-2$. Let $P := y_0y_1 \ldots y_k = w$ be the shortest path from a vertex $y_0 \in V(\mathbf{C})$ to w (i.e., $(V(\mathbf{C}), w)$-path), which may be of length zero. If G contains a vertex of degree at least three, excluding w and y_0, then there is a unicyclic graph G^* with order n and maximum degree Δ such that $ABS(G) > ABS(G^*)$.*

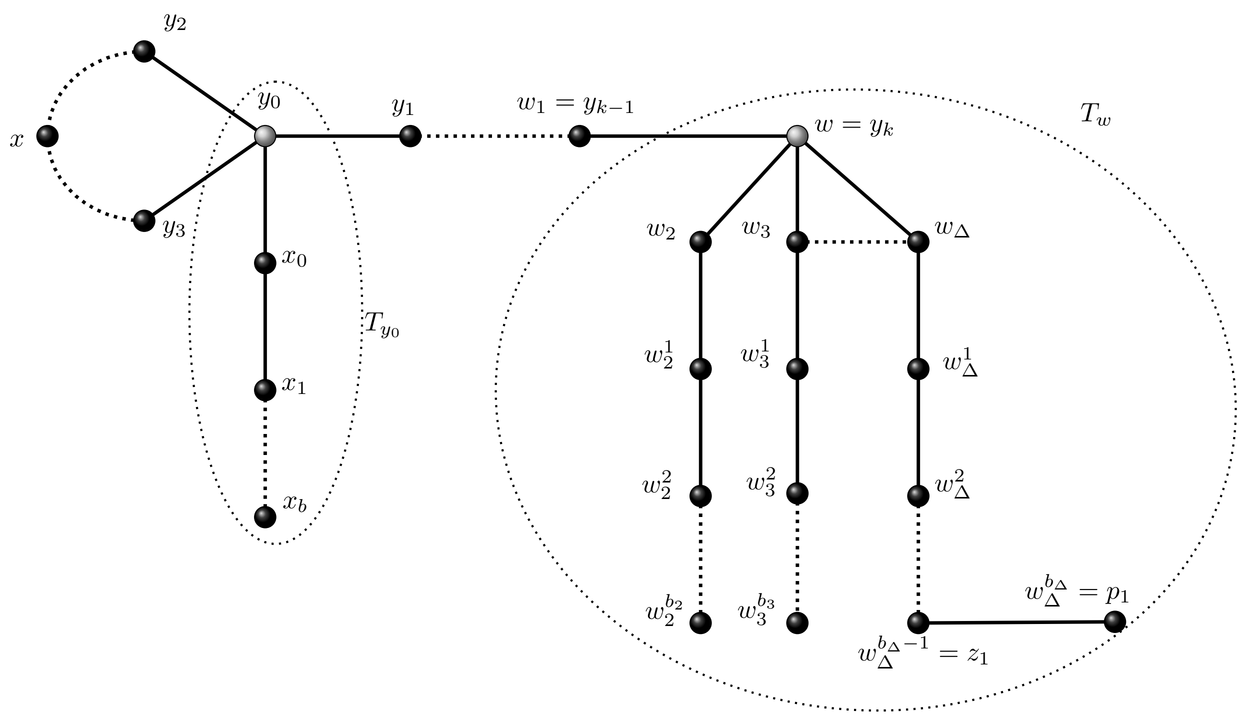


Figure 2.1: Unicyclic graph used in Lemma 2.1.

Lemma 2.1. *Consider a unicyclic graph G with order n and maximum degree Δ such that $3 \le \Delta \le n-2$. Let $P := y_0 y_1 \dots y_k = w$ be a shortest path from a vertex $y_0 \in V(\mathbf{C})$ to w (i.e., $(V(\mathbf{C}), w)$-path), which may be of length zero. If $k \ge 1$, then there is a unicyclic graph G^* with order n and maximum degree Δ such that $ABS(G) > ABS(G^*)$.*

Proof. By Corollary 2.2, we may assume that w and y_0 are the only vertices of degree at least 3 in G. Let w_1 be a vertex on the path P. For the sake of simplicity, we assume that $d(w_2) \le d(w_3) \le \cdots \le d(w_{\Delta-1}) \le d(w_\Delta)$, where $N(w) = \{w_1, w_2, \dots, w_\Delta\}$. Now, let T_w be the component of $G - ww_1$ containing w and within T_w, we have the longest path $ww_i{}^0 w_i{}^1 \dots w_i{}^{b_i}$, where $w_i = w_i{}^0$, for each $2 \le i \le \Delta$ (see Figure 2.1). Based on the selection of w and the assumption of $k \ge 1$, we can conclude that $\Delta \ge 4$ and $d(w) > d(y_0)$. Assume that $V(\mathbf{C}) \cap N(y_0) = \{y_2, y_3\}$ (see Figure 2.1).

First, consider the case when $d(y_0) \ge 4$. If y_0 is a stem of degree at least 3 and is different from w, then the result follows from Corollary 2.1. However, if y_0 is not a stem, let $x_0 \in N(y_0) - \{y_1, y_2, y_3\}$ and let T_{y_0} be the component of $G - \{y_0y_1, y_0y_2, y_0y_3\}$ containing y_0. The longest path in T_{y_0} is represented as $y_0 x_0 \dots x_b$. According to Corollary 2.2, assume that $d(x_0) = \cdots = d(x_{b-1}) = 2$ and $d(x_b) = 1$. Now, let $G^* = G - y_0x_0 + x_0 w_\Delta^{b_\Delta}$. It is evident that G^* remains a unicyclic graph with order n and $\Delta(G^*) = \Delta$. By Theorem 1.2, $ABS(G) > ABS(G^*)$.

Now, we consider the case when $d(y_0) = 3$. Let $p_1 = w_\Delta^{b_\Delta}$ and $p_2 = w_{\Delta-1}^{b_{\Delta-1}}$. Let z_1 and z_2 be the neighbors of p_1 and p_2, respectively. Assume that $G^* = G - y_0y_2 + p_1p_2$, and let $S = \{y_0y_1, y_0y_2, y_0y_3, p_1z_1, p_2z_2, y_2x\}$, where $x \in (V(\mathbf{C}) \cap N(y_2)) - \{y_0\}$. It is evident that G^* is a unicyclic graph with order n and $\Delta = \Delta(G^*)$. The assertion is that $ABS(G) > ABS(G^*)$.

Case 1: $d(w, y_0) = 1$ and $b_\Delta = b_{\Delta-1} = 0$.
Note that $y_0 = w_1, w = y_1, p_1 = w_\Delta$ and $p_2 = w_{\Delta-1}$. By the definition of the ABS index, we have

$$ABS(G) = \sum_{xy \notin S} abs_w(xy) + \sqrt{\frac{\Delta+1}{\Delta+3}} + 2\sqrt{\frac{3}{5}} + 2\sqrt{\frac{\Delta-1}{\Delta+1}} + \sqrt{\frac{1}{2}}, \tag{1}$$

$$ABS(G^*) = \sum_{xy \notin S} abs_w(xy) + 3\sqrt{\frac{\Delta}{\Delta+2}} + \sqrt{\frac{1}{3}} + 2\sqrt{\frac{1}{2}}. \tag{2}$$

Since $\Delta \ge 4$, it follows that

$$\sqrt{\frac{\Delta}{\Delta+2}} + \sqrt{\frac{1}{2}} < \sqrt{\frac{\Delta-1}{\Delta+1}} + \sqrt{\frac{3}{5}}. \tag{3}$$

By utilizing (3) along with Equations (1) and (2), we deduce that $ABS(G) > ABS(G^*)$.

Case 2: $d(w, y_0) \geq 2$ and $b_\Delta = b_{\Delta-1} = 0$.
We observe that $p_1 = w_\Delta$ and $p_2 = w_{\Delta-1}$. By the definition of the ABS index, we have

$$ABS(G) = \sum_{xy \notin S} abs_w(xy) + 2\sqrt{\frac{\Delta-1}{\Delta+1}} + 3\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}},$$

$$ABS(G^*) = \sum_{xy \notin S} abs_w(xy) + 2\sqrt{\frac{\Delta}{\Delta+2}} + 3\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{3}}.$$

By employing (3), we deduce that $ABS(G) > ABS(G^*)$.

Case 3: $d(w, y_0) = 1$, $b_\Delta \geq 1$, $b_{\Delta-1} = 0$.
In this case, $y_0 = w_1, w = y_1, p_2 = w_{\Delta-1}$. By the definition of the ABS index, we have

$$ABS(G) = \sum_{xy \notin S} abs_w(xy) + \sqrt{\frac{\Delta+1}{\Delta+3}} + 2\sqrt{\frac{3}{5}} + \sqrt{\frac{\Delta-1}{\Delta+1}} + \sqrt{\frac{1}{3}} + \sqrt{\frac{1}{2}}, \tag{4}$$

$$ABS(G^*) = \sum_{xy \notin S} abs_w(xy) + 2\sqrt{\frac{\Delta}{\Delta+2}} + \sqrt{\frac{1}{3}} + 3\sqrt{\frac{1}{2}}. \tag{5}$$

By employing (4) and (5), along with (3), we deduce that $ABS(G) > ABS(G^*)$.

Case 4: $d(w, y_0) \geq 2$, $b_\Delta \geq 1$, $b_{\Delta-1} = 0$.
Note that $p_2 = w_{\Delta-1}$ and hence

$$ABS(G) = \sum_{xy \notin S} abs_w(xy) + \sqrt{\frac{\Delta-1}{\Delta+1}} + 3\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{3}} + \sqrt{\frac{1}{2}},$$

$$ABS(G^*) = \sum_{xy \notin S} abs_w(xy) + \sqrt{\frac{\Delta}{\Delta+2}} + 4\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{3}}.$$

By employing (3), we deduce that $ABS(G) > ABS(G^*)$.

Case 5: $d(w, y_0) = 1$, $b_\Delta \geq 1$, and $b_{\Delta-1} \geq 1$.
In this case, we have

$$ABS(G) = \sum_{xy \notin S} abs_w(xy) + \sqrt{\frac{\Delta+1}{\Delta+3}} + 2\sqrt{\frac{3}{5}} + 2\sqrt{\frac{1}{3}} + \sqrt{\frac{1}{2}}, \tag{6}$$

$$ABS(G^*) = \sum_{xy \notin S} abs_w(xy) + \sqrt{\frac{\Delta}{\Delta+2}} + \sqrt{\frac{1}{3}} + 4\sqrt{\frac{1}{2}}. \tag{7}$$

Using (6) and (7), along with (3), we deduce that $ABS(G) > ABS(G^*)$.

Case 6: $d(w, y_0) \geq 2$, $b_\Delta \geq 1$, $b_{\Delta-1} \geq 1$.
By the definition of the ABS index, we have

$$ABS(G) = \sum_{xy \notin S} abs_w(xy) + 3\sqrt{\frac{3}{5}} + 2\sqrt{\frac{1}{3}} + \sqrt{\frac{1}{2}},$$

$$ABS(G^*) = \sum_{xy \notin S} abs_w(xy) + 5\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{3}}.$$

It is clear that $ABS(G) > ABS(G^*)$.

In all cases, we arrive at the desired inequality. □

By Corollary 2.2 and Lemma 2.1, we may make the assumption that w is a vertex on the cycle **C** and it is the only vertex in G having a degree greater than two.

Contracting an edge e in a graph G gives a new graph G/e obtained from G by removing e and then merging its end vertices into a single vertex.

Lemma 2.2. *Consider a unicyclic graph G with order n and maximum degree Δ such that $3 \leq \Delta \leq n-2$. If w is a stem and the girth of G is $k \geq 4$, then there is a unicyclic graph G^* with order n and $\Delta(G^*) = \Delta$ such that $ABS(G) > ABS(G^*)$.*

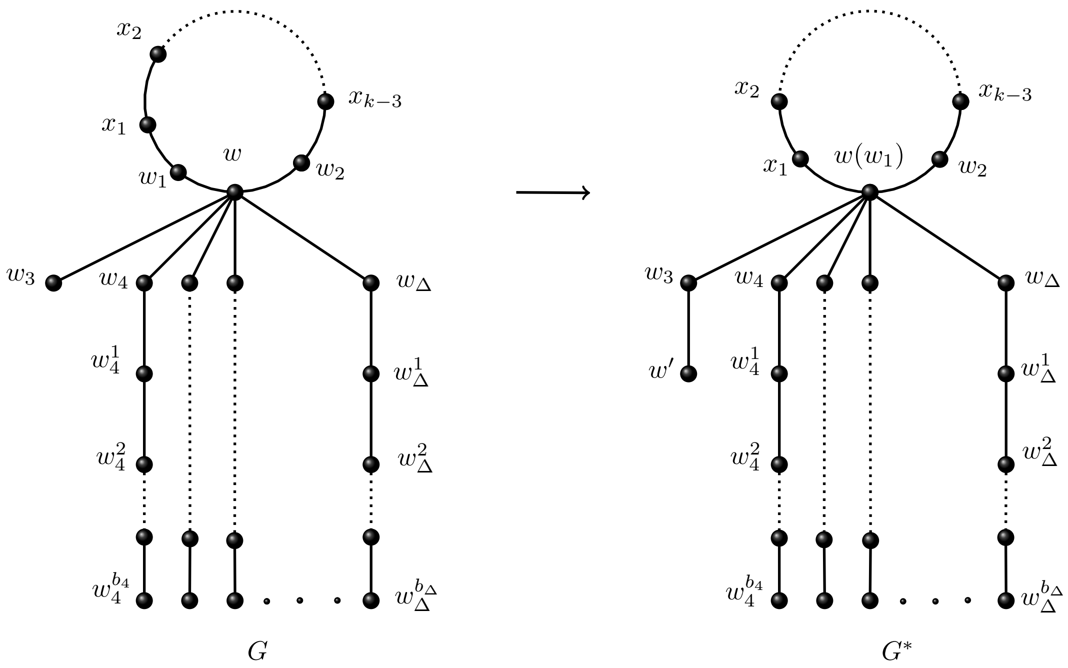


Figure 2.2: Unicyclic graphs used in Lemma 2.2.

Proof. Let $N(w) \cap V(\mathbf{C}) = \{w_1, w_2\}$ and $V(\mathbf{C}) = \{w, w_1, x_1, \ldots, x_{k-3}, w_2\}$. Now, choose $w_3 \in N(w)$ such that $d(w_3) = 1$. Create a new graph G^* obtained from G by identifying the vertices w and w_1 and adding a new pendant edge w_3w' (see Figure 2.2). It is clear that G^* is a unicyclic graph with order n and $\Delta(G^*) = \Delta$. Now, let $S = \{ww_1, w_1x_1, ww_3\}$. Using the definition of the ABS index, we have

$$ABS(G) = \sum_{xy \notin S} abs_w(xy) + \sqrt{\frac{\Delta}{\Delta+2}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{\Delta-1}{\Delta+1}}, \tag{8}$$

$$ABS(G^*) = \sum_{xy \notin S} abs_w(xy) + 2\sqrt{\frac{\Delta}{\Delta+2}} + \sqrt{\frac{1}{3}}. \tag{9}$$

Since $\Delta \geq 3$, from (8) and (9), it follows that $ABS(G) > ABS(G^*)$. □

Lemma 2.3. *Consider a unicyclic graph G with order n and maximum degree Δ such that $4 \leq \Delta \leq n-2$. If w is a stem, w_3 is a leaf adjacent to w, and there exists an end vertex y with $d(y, w_3) \geq 4$, then there is a unicyclic graph G^* with order n and $\Delta(G^*) = \Delta$ such that $ABS(G) > ABS(G^*)$.*

Proof. Suppose that $N(w) \cap V(\mathbf{C}) = \{w_1, w_2\}$. Consider the component T_w of $G - E(\mathbf{C})$ containing w and within T_w, there exists a longest path $ww_i^0w_i^1 \ldots w_i^{b_i}$, where $w_i = w_i^0$, for each $4 \leq i \leq \Delta(G)$. In this path $d\left(w_i^{b_i}\right) = 1$ for each i and $d\left(w_i^j\right) = 2$ otherwise. Assuming that $b_4 \geq 2$. Create a new graph $G^* = G - w_4^{b_4}w_4^{b_4-1}w_3w_4^{b_4}$ as illustrated in Figure 2.3. Additionally, take $S = \left\{ww_3, w_4^{b_4}w_4^{b_4-1}, w_4^{b_4-1}w_4^{b_4-2}\right\}$. It is clear that G^* is a unicyclic graph with n vertices and $\Delta(G^*) = \Delta$. Using the definition of the ABS index, we have

$$ABS(G) = \sum_{xy \notin S} abs_w(xy) + \sqrt{\frac{\Delta-1}{\Delta+1}} + \sqrt{\frac{1}{3}} + \sqrt{\frac{1}{2}}, \tag{10}$$

$$ABS(G^*) = \sum_{xy \notin S} abs_w(xy) + \sqrt{\frac{\Delta}{\Delta+2}} + 2\sqrt{\frac{1}{3}}. \tag{11}$$

From (10) and (11), it is evident that $ABS(G) > ABS(G^*)$. □

Recall the structure of the graph $\mathcal{U}_{n,k}^{k_1,k_2,\ldots,k_b}$ defined in the introduction section. For $3 \leq \Delta \leq n-2$, let

$$\mathfrak{F}_1(n,\Delta) = \left\{\mathcal{U}_{n,3}^{b_1,\ldots,b_{\Delta-2}} : 1 \leq b_1, \ldots, b_{\Delta-2} \leq 2\right\} \quad \text{and} \quad \mathfrak{F}_2(n,\Delta) = \left\{\mathcal{U}_{n,k}^{b_1,\ldots,b_{\Delta-2}} : k \geq 3 \text{ and } b_1, \ldots, b_{\Delta-2} \geq 2\right\}.$$

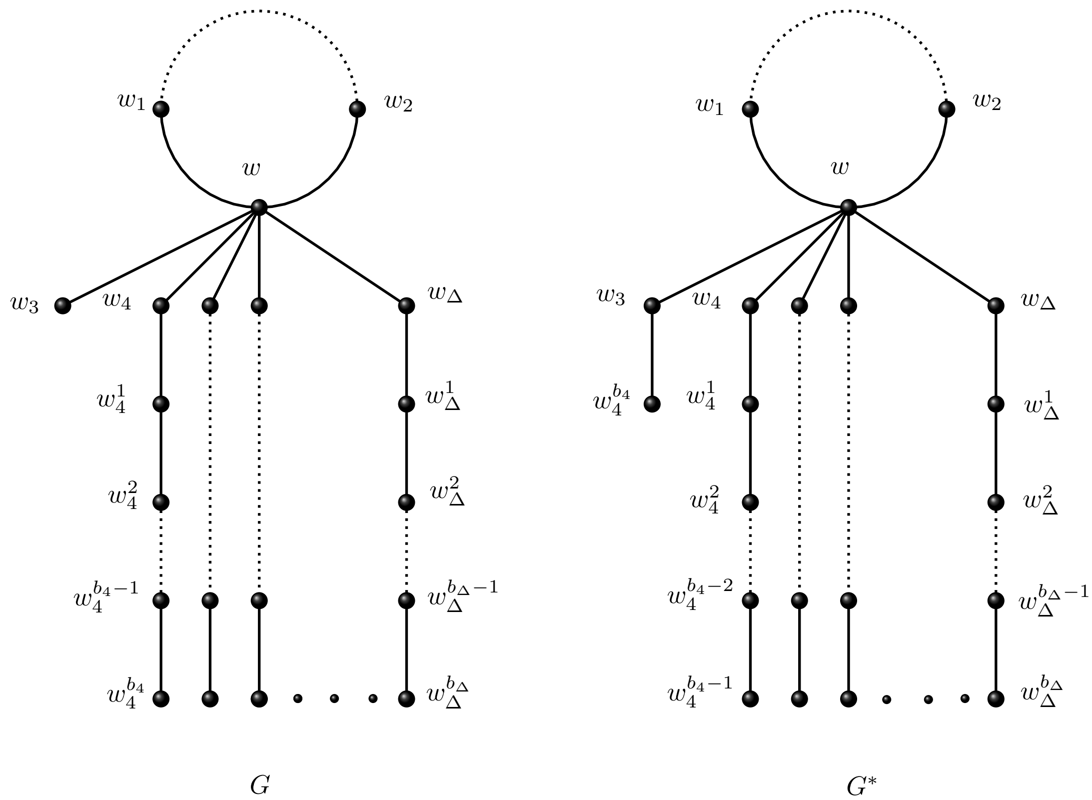


Figure 2.3: Unicyclic graphs used in Lemma 2.3.

We are now prepared to present the proof of our main result.

Theorem 2.1. *Consider a unicyclic graph G with order n and maximum degree Δ such that $3 \leq \Delta \leq n-2$, then*

$$ABS(G) \geq \begin{cases} (2\Delta - n - 1)\sqrt{\dfrac{\Delta-1}{\Delta+1}} + (n-\Delta+1)\sqrt{\dfrac{\Delta}{\Delta+2}} + (n-\Delta-1)\sqrt{\dfrac{1}{3}} + \sqrt{\dfrac{1}{2}} & \text{if } \Delta \geq \dfrac{n+2}{2}, \\ \Delta\sqrt{\dfrac{\Delta}{\Delta+2}} + (n-2\Delta+2)\sqrt{\dfrac{1}{2}} + (\Delta-2)\sqrt{\dfrac{1}{3}} & \text{if } \Delta \leq \dfrac{n+1}{2}. \end{cases}$$

Equality is achieved if and only if $G \in \mathfrak{F}_1 \cup \mathfrak{F}_2$.

Proof. Let $\mathbb{U}_n^\Delta$ be the collection of unicyclic graphs with n vertices and maximum degree Δ such that $3 \leq \Delta \leq n-2$. Consider $G \in \mathbb{U}_n^\Delta$ such that

$$ABS\,(G) = \min\left\{ABS\,(G_1) : G_1 \in \mathbb{U}_n^\Delta\right\}.$$

Consider a vertex $w \in V(G)$ with maximum degree Δ. By Corollary 2.2 and Lemma 2.1, it is concluded that $w \in V(\mathbf{C})$ and it is the only vertex with a degree exceeding two in G. With the help of Lemma 2.2 and Lemma 2.3 along with our choice of G, we conclude that $G \in \mathfrak{F}_1(n,\Delta) \cup \mathfrak{F}_2(n,\Delta)$.

First, consider the case when $G \in \mathfrak{F}_2(n,\Delta)$. In this case $n \geq 2\Delta - 1$, which implies $\Delta \leq \dfrac{n+1}{2}$. Using the definition of the ABS index, we have

$$ABS(G) = \Delta\sqrt{\frac{\Delta}{\Delta+2}} + (n-2\Delta+2)\sqrt{\frac{1}{2}} + (\Delta-2)\sqrt{\frac{1}{3}}. \tag{12}$$

Now, assume that $G \in \mathfrak{F}_1(n,\Delta)$. Let γ be the number of leaves adjacent to w. If $\gamma = 0$, then $G \in \mathfrak{F}_2(n,\Delta)$ and we already determined $ABS(G)$ in (12). However, if $\gamma \geq 1$, then $n-3 = 2\Delta - \gamma - 4$ and $\gamma = 2\Delta - n - 1$. Given that $\gamma \geq 1$, it follows that $\Delta \geq \dfrac{n+2}{2}$. Using the definition of the ABS index, we have

$$ABS(G) = \gamma\sqrt{\frac{\Delta-1}{\Delta+1}} + (\Delta-\gamma)\sqrt{\frac{\Delta}{\Delta+2}} + (\Delta-\gamma-2)\sqrt{\frac{1}{3}} + \sqrt{\frac{1}{2}}$$

$$ABS(G) = (2\Delta-n-1)\sqrt{\frac{\Delta-1}{\Delta+1}} + (n-\Delta+1)\sqrt{\frac{\Delta}{\Delta+2}} + (n-\Delta-1)\sqrt{\frac{1}{3}} + \sqrt{\frac{1}{2}}.$$

This completes the proof. $\square$

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