Iranian Journal of Mathematical Chemistry

IJMC

DOI: 10.22052/IJMC.2024.255486.1909
Vol. 16, No. 2, 2025, pp. 93-108
Research Paper

Harmonic-Arithmetic Index of Unicyclic Graphs

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Keywords:
Harmonic-arithmetic index,
Extremal graph,
Unicyclic graph

AMS Subject Classification (2020):

05C05; 05C35; 05C69

Article History:
Received: 21 September 2024
Accepted: 9 December 2024

Abstract

Let $G = (V(G), E(G))$ be a graph. The harmonic-arithmetic index of G is defined as $HA(G) = \sum_{uv\in E(G)} \frac{4d_G(u)d_G(v)}{(d_G(u)+d_G(v))^2}$, where $d_G(u)$ is the degree of a vertex $u \in V(G)$. In this paper, we consider the upper and lower bounds of the harmonic-arithmetic index of unicyclic graphs with a fixed order. Furthermore, the graphs attaining the extremal values are also characterised.

1 Introduction

Let $G = (V(G), E(G))$ be a simple connected graph, where $V(G)$ and $E(G)$ are its vertex set and edge set, respectively. G is a unicyclic graph if it contains exactly one cycle. In this paper, we only consider unicyclic graphs of order $n(n \geqslant 3)$.

For two simple connected graphs $F_1 = (V_1, E_1)$ and $F_2 = (V_2, E_2)$, if $V_1 \subseteq V_2$ and $E_1 \subseteq E_2$, then F_1 is a subgraph of F_2, written as $F_1 \subseteq F_2$. Furthermore, if $F_1 \subseteq F_2$ and E_1 contains all the edges $uv \in E_2$ with $u, v \in V_1$, then F_1 is an induced graph of F_2, written as $F_1 = F_2[V_1]$.

For a vertex $u \in V(G)$, we define $N_G(u) = \{v \in V(G)|uv \in E(G)\}$, and $d_G(u) = |N_G(u)|$ is the degree of u. In a unicyclic graph G, if the vertex u (edge e) lies on the cycle of G, then we call it a cycle vertex (a cycle edge). For a cycle vertex u, if $d_G(u)$ is no less than the degree of any other cycle vertices, then it is called a maximum degree cycle vertex. If $d_G(u)$ is no less than the degree of two cycle vertices adjacent to itself, then it is called a local maximum degree cycle vertex. Similarly, we define (local) minimum degree cycle vertex. Let T_1 be a component of $G - u$, where u is a cycle vertex. If T_1 contains cycle edges of G, we define $T_u = T[V(G) - V(T_1)]$, then T_u is a tree rooted at u.

Identifying non-adjacent vertices u and v of a graph G is to replace these two vertices by a single vertex, which is incident with all the edges that are incident with either u or v in G. For more basic definitions about graph theory, one may refer to [1].

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Academic Editor: Boris Furtula

If the output of a function based on the graphs is same under graph isomorphisms, then we call this function a graph invariant. Graph invariants that only take numerical qualities are usually called topological indices, which are heavily employed in chemical graph theory. They can reflect biological and physico-chemical properties of organic compounds on the molecular graphs. Some applications of topological indices in predicting particular properties of compounds are shown in [2].

Randić index (also known as connectivity index), defined as $R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}$, was introduced by Randić [3]. It is one of the most frequently investigated and widely applied topological indices. In fact, different from any other topological indices, Randić index is the first topological index that has being designed for specific goals. The idea behind it is to use available information on some molecular properties for their construction. For example, the relative values of the boiling points of smaller alkanes are used in construction of Randić index. Zhang and Wu [4] found a lower bound of Randić index of line graphs of trees.

A well-known modification of Randić index is geometric-arithmetic index first introduced by Vukičević and Furtula [5] and it is defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$. The summand of GA index is the ratio between the geometric and arithmetic means of $d_G(u)$ and $d_G(v)$. The upper and lower bounds of simple graphs, simple connected graphs, trees and molecular trees are all presented in [5], respectively. Besides, Vukičević and Furtula showed that the prediction ability of GA index for physico-chemical properties such as entropy, enthalpy of vaporization, and acentric factor, is at least 2.5% better than that of Randić index. Moon and Park [6] established that the maximum and minimum values of GA index of unicyclic graphs are attained by C_n and S_n^*, respectively, where S_n^* is obtained by attaching $n-3$ pendant edges to a single vertex of C_3. If we replace each summand by its reverse, we can get a new index called arithmetic-geometric index [7]: $AG(G) = \sum_{uv \in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}}$. Vukićević et al. [8] proved that the extremal situations of AG index of unicyclic graphs are exactly opposite to that of GA index of unicyclic graphs. For more recent papers about GA index and AG index, one may refer to [9–19].

Harmonic-arithmetic index is defined in same way by taking the ratio between harmonic and arithmetic means of $d_G(u)$ and $d_G(v)$ into consideration, where $HA(G) = \sum_{uv \in E(G)} \frac{4d_G(u)d_G(v)}{(d_G(u)+d_G(v))^2}$. Albalahi et al. [20] determined the upper and lower bounds of HA index of trees and molecular trees. The HA index of molecular trees with a fixed-order and a given number of leaves was studied in [21]. In [22], Albalahi et al. reported a lower bound on the HA index for molecular graphs in terms of graphs' order, size and maximum degree. Some inequalities about HA index was derived in [23].

Since the extremal situations of GA and AG index over unicyclic graphs are already known, we intend to investigate the extremal values of HA index of unicyclic graphs and characterize the corresponding extremal graphs. It would be interesting for others to investigate the application of HA index in predicting certain properties of chemical compounds.

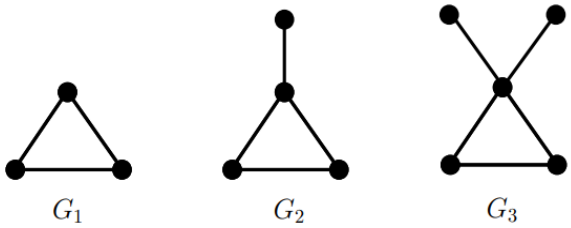
2 Bounds for harmonic-arithmetic index of unicyclic graphs

Consider an arbitrary edge $e = uv \in E(G)$ such that $d_G(u) \geq d_G(v)$, we define $w_G(e) = \frac{4d_G(u)d_G(v)}{(d_G(u)+d_G(v))^2}$ as the weight of edge e. Let $r_G(e) = \frac{d_G(u)}{d_G(v)}$ and $h(x) = \frac{4x}{(x+1)^2}$, where $h(x)$ is strictly decreasing for $x \geq 1$. Then $w_G(e) = h(\frac{d_G(u)}{d_G(v)}) = h(r_G(e))$. It is easy to see that if $r_G(e)$ is increased, then $w_G(e)$ or the weight of edge e will be subsequently decreased.

Since $1 \leq r_G(e) \leq n-1$, then $\frac{4(n-1)}{n^2} \leq w_G(e) \leq 1$. It is distinct that the upper bound n

of HA index of G is only obtained by the cycle C_n. By the way, it is clear that n and C_n are also the maximum value and the corresponding extremal graph of molecular unicyclic graphs, respectively. In the following part of this section, we mainly study the lower bound of HA index of unicyclic graphs.

When $n = 3, 4, 5$, we can list all the possible graphs directly and compare their values of HA index, respectively. The graphs which obtain the lower bound of HA index are shown in Figure 1, respectively. Hence, next we let $n \geq 6$.



(a) n=3 (b) n=4 (c) n=5

Figure 1: the extremal unicyclic graphs for $n = 3, 4, 5$.

Proposition 2.1. *Let G be a unicyclic graph of order n with the minimum value of HA index. If u is a local maximum degree cycle vertex of G, then T_u is a star with center u.*

Proof. When $d_G(u) = 2$ or $d_G(u) = 3$, T_u is a star with center u. Next we let $d_G(u) \geqslant 4$. Suppose that T_u is not a star with center u. We replace T_u by a star of the same set of vertices, with center u, and define this new graph as $G^{'}$(see Figure 2).

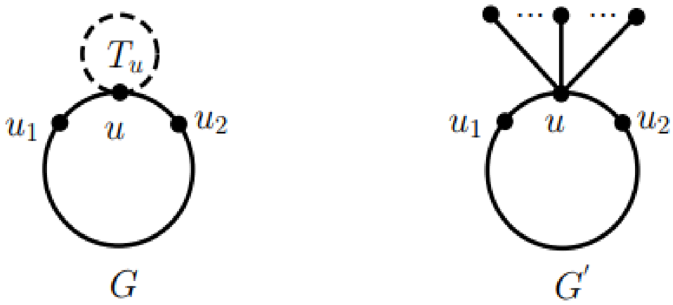


Figure 2: $G \longrightarrow G^{'}$.

For each edge $e \in E_G(T_u)$, it is replaced by appropriate pendant edge $e^{'}$ under this transformation. Then

$$r_G(e) < \frac{|E_G(T_u)| + 2}{1} = \frac{d_{G'}(u)}{1} = r_{G'}(e^{'}).$$

So $w_G(e) > w_{G'}(e^{'})$.

Suppose that u_1 and u_2 are two cycle vertices adjacent to u in G. The degree of u_1 and u_2

remain unchanged under this transformation and $d_G(u) < d_{G'}(u)$, hence

$$\frac{d_G(u)}{d_G(u_i)} < \frac{d_{G'}(u)}{d_{G'}(u_i)} \quad \text{for} \quad i = 1, 2.$$

Then $w_G(uu_i) > w_{G'}(uu_i)$ for $i = 1, 2$.
The weight of other edges of G remain unchanged under this transformation. Hence, $HA(G) > HA(G^{'})$. This is a contradiction to the fact that G has minimum value of HA index. ■

Proposition 2.2. *Let G be a unicyclic graph of order n. u and v are its local maximum degree cycle vertex and local minimum degree cycle vertex, respectively. $d_G(u) \geq 3$, $d_G(v) \geq 3$ and T_u is a star with center u. If G^* is obtained by replacing each edge of T_v by a pendant edge incident with u(see Figure 3), then $HA(G^*) < HA(G)$.*

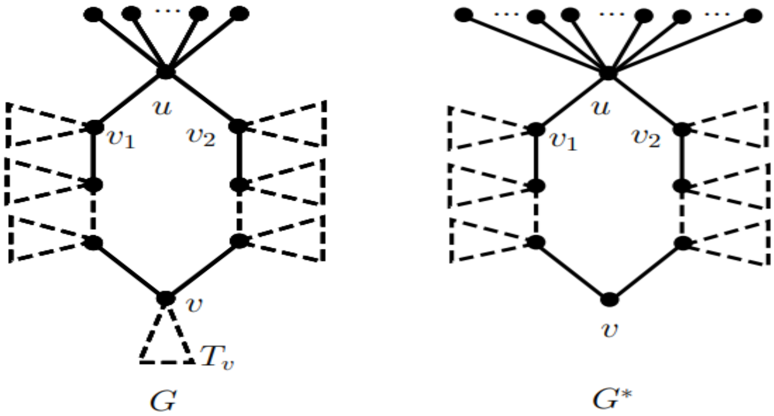


Figure 3: $G \longrightarrow G^*$.

Proof. For each edge $e_1 \in E_G(T_v)$, it is replaced by appropriate pendant edge $e_1^{'}$ under this transformation. So we have

$$r_G(e_1) \leq \frac{|E_G(T_v)| + 2}{1} < \frac{d_{G^*}(u)}{1} = r_{G^*}(e_1^{'}).$$

Thus $w_G(e_1) > w_{G^*}(e_1^{'})$.
For each pendant edge e_2 incident with u in G, we have

$$r_G(e_2) = \frac{d_G(u)}{1} < \frac{d_{G^*}(u)}{1} = r_{G^*}(e_2).$$

Then $w_G(e_2) > w_{G^*}(e_2)$.
Suppose that v_1 and v_2 are two cycle vertices adjacent to u in G. If $v_i = v$ for some $i = 1, 2$, then $d_G(u) < d_{G^*}(u)$ and $d_G(v_i) \geq d_{G^*}(v_i)$. If $v_i \neq v$ for any $i = 1, 2$, then $d_G(u) < d_{G^*}(u)$ and $d_G(v_i) = d_{G^*}(v_i)$. In both cases, $r_G(uv_i) < r_{G^*}(uv_i)$, then $w_G(uv_i) > w_{G^*}(uv_i)$ for $i = 1, 2$.
For another cycle edge v_3v_4 in G with $v_3, v_4 \neq u$, we consider two cases.
If $v_3, v_4 \neq v$, the degree of v_3 and v_4 remain unchanged under this transformation. Then $w_G(v_3v_4) = w_{G^*}(v_3v_4)$.
If $v_i = v$ for $i = 3$ or 4, for example $v_3 = v$, we have $r_G(v_3v_4) = \frac{d_G(v_4)}{d_G(v_3)} \leq \frac{d_G(v_4)}{3} < \frac{d_G(v_4)}{2} =$

$r_{G^*}(v_3v_4)$. Then $w_G(v_3v_4) > w_{G^*}(v_3v_4)$.
The weight of other edges of G remain unchanged. Hence, $HA(G^*) < HA(G)$. ∎

Let x, y be two non-adjacent cycle vertices, and let e be a cycle edge of G. We write (x, y)-arc containing the edge e as xey. Then the xey-transformation is defined as follows:
(i) For every cycle vertex z on xey, replace each edge of T_z by a pendant edge incident with y.
(ii) Let x_1 be a cycle vertex adjacent to x on xey. For every cycle edge on xey, except for xx_1, replace it by a pendant edge incident with y.
(iii) identify x_1 and y, and we still use y to name this new vertex.
We denote by G_{xey} the new graph obtained by above transformation.

Proposition 2.3. *Let G be a unicyclic graph of order n. u is a local maximum degree cycle vertex of G and T_u is a star with center u. If e is an arbitrary cycle edge and v is a cycle vertex which is not adjacent to u and has degree two, then $HA(G_{veu}) < HA(G)$(see Figure 4).*

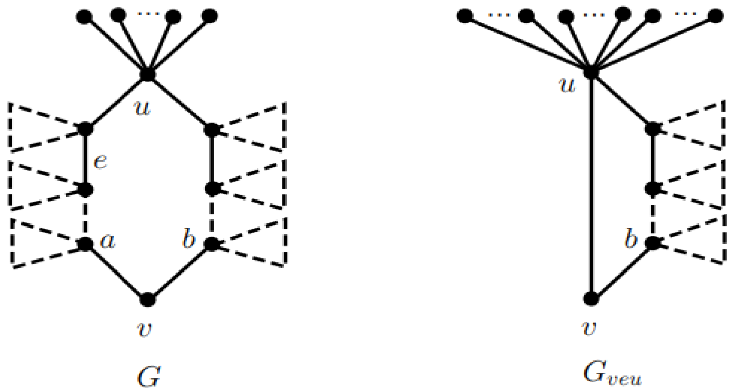


Figure 4: $G \longrightarrow G_{veu}$.

Proof. Let a, b be two cycle vertices, which are adjacent to v, and va lies on the veu. Let w be a cycle vertex lying on the veu. For each edge $e_1 \in T_w$, it is replaced by appropriate pendant edge $e_1^{'}$ under this transformation, then we have

$$r_G(e_1) \leq \frac{|E_G(T_w)| + 2}{1} < \frac{d_{G_{veu}}(u)}{1} = r_{G_{veu}}(e_1^{'}).$$

Thus $w_G(e_1) > w_{G_{veu}}(e_1^{'})$.
For each cycle edge e_2 on the veu except for va, it is replaced by appropriate pendant edge $e_2^{'}$. Suppose that $e_2 = x_1x_2$ such that $d_G(x_2) \geq d_G(x_1)$, we have

$$r_G(e_2) = \frac{d_G(x_2)}{d_G(x_1)} < \frac{d_{G_{veu}}(u)}{1} = r_{G_{veu}}(e_2^{'}).$$

Then $w_G(e_2) > w_{G_{veu}}(e_2^{'})$.
For edge va, we have

$$r_G(va) = \frac{d_G(a)}{2} < \frac{d_{G_{veu}}(u)}{2} = r_{G_{veu}}(vu).$$

Then $w_G(va) > w_{G_{veu}}(vu)$.
For the edge e_3 which is incident with u in G and does not lie on the veu, since the degree of u is increased and the degree of the other endvertex remains unchanged under this transformation, $r_G(e_3) < r_{G_{veu}}(e_3)$, that is, $w_G(e_3) > w_{G_{veu}}(e_3)$.
The weight of the other edges remain unchanged. Hence, $HA(G_{veu}) < HA(G)$. ■

From the three propositions above, we can get the next Lemma:

Lemma 2.4. *Assume that G is a unicyclic graph of order n with maximum degree cycle vertex u. If G has a minimum HA index, then T_u is a star with center u, and G has at least one but no more than two cycle vertices of degree two. Moreover, the cycle vertex of degree two must be the neighbour of u.*

Then, we use several propositions to explore the structure of G which attains the minimum value of HA index.

Proposition 2.5. *Assume that G contains exactly one cycle vertex of degree two. If G has minimum HA index among all the unicyclic graphs of order n, then the length of cycle of G must be three and each nontrival tree rooted at a cycle vertex must be a star whose center is a cycle vertex.*

Proof. Assume that there exists a unicyclic graph G with minimum HA index. u and v_1 are maximum degree cycle vertex and the cycle vertex with degree two, respectively. Then u and v_1 are pairwise adjacent and T_u is a star with center u by Lemma 2.4. We will take two steps to prove this proposition.
Step 1: Firstly we are going to prove the length of cycle of G is three.
Suppose that the girth of G is greater than three. Let $S = \{s_1, s_2, \cdots, s_k\}$, $k \geq 2$, be the set of remaining cycle vertices, where s_1 and s_k are adjacent to v_1 and u, respectively (see Figure 5). Let s be a maximum degree vertex among all the vertices in S.

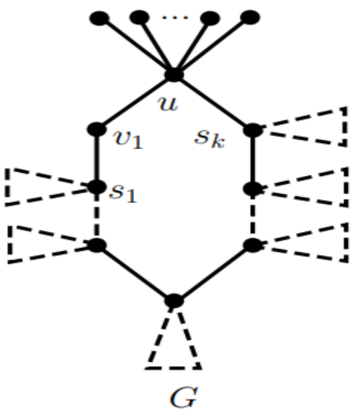


Figure 5: the graph G whose girth is greater than three.

Case 1: If $s = s_1$, then s is a local maximum degree cycle vertex and T_s is a star with center s. Firstly we replace v_1u by a pendant edge incident with u and replace v_1s by a pendant edge incident with s. Then we identify the vertices u and s. Define by $\widetilde{G}$ the resulting graph. Analogy with the proof of Proposition 2.1, we can get that $HA(\widetilde{G}) < HA(G)$, which is a contradiction

to the fact that G has minimum value of HA index.
Case 2: If $s \neq s_1, s_k$, then s is a local maximum degree cycle vertex and T_s is a star with center s. Let $e = v_1 s_1$ and perform the $v_1 es$-transformation. We can get that $HA(G_{v_1 es}) < HA(G)$ by Proposition 2.3, which is also a contradiction.
Case 3: If $s = s_k$, we let $e = v_1 u$ and perform the $v_1 es_k$-transformation. Analogy with the proof of Proposition 2.3, we can get that $HA(G_{v_1 es_k}) < HA(G)$, which is also a contradiction. Hence, the length of cycle of G is three.
Step 2: We need to prove that each nontrival pendant tree rooted at a cycle vertex is a star whose center is a cycle vertex when the length of cycle is three.
Suppose that v_2 is another cycle vertex adjacent to u, and T_{v_2} is not a star with center v_2. Let v^* be an arbitrary vertex in $N_G(v_2) - \{u, v_1\}$ and T'_{v^*} be the maximal tree rooted at v^* that does not contain edge $v_2 v^*$.
Case 1: For every v^*, it satisfies that $d_G(v^*) \leq d_G(v_2)$.
We replace all the edges of every T'_{v^*} by the pendant edges incident with u(see Figure 6). Define the resulting graph by G_1.

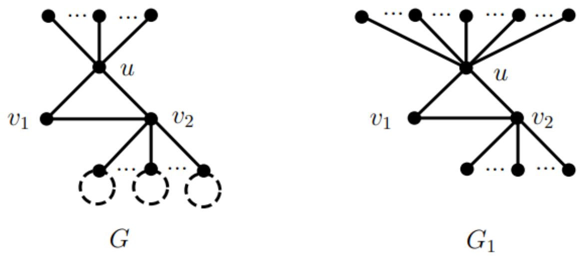


Figure 6: $G \longrightarrow G_1$.

For every pendant edges $e_1 \in G$ incident with u, we have

$$r_G(e_1) = \frac{d_G(u)}{1} < \frac{d_{G_1}(u)}{1} = r_{G_1}(e_1).$$

Then $w_G(e_1) > w_{G_1}(e_1)$.
For cycle edges $uv_i (i = 1, 2)$, the degree of u is increased and the degree of v_i remain unchanged under this transformation, so the weight of $uv_i (i = 1, 2)$ is decreased. For edge $v_1 v_2$, the weight of it is unchanged.
For the edge $e_2 \in E_G(T_{v_2})$ incident with v_2, we have

$$r_G(e_2) = \frac{d_G(v_2)}{d_G(v^*)} \leq \frac{d_G(v_2)}{1} = \frac{d_{G_1}(v_2)}{1} = r_{G_1}(e_2).$$

Thus $w_G(e_2) \geq w_{G_1}(e_2)$.
For the edge $e_3 \in E_G(T'_{v^*})$, it is replaced by appropriate pendant edge e'_3 incident with u. Since

$$d_{G_1}(u) - 2 = |E_G(T_u)| + |E_G(T_{v_2})| - (d_G(v_2) - 2) \geq 1 + |E_G(T_{v_2})| - (d_G(v_2) - 2),$$

we have

$$r_G(e_3) \leq \frac{|E_G(T_{v_2})| - (d_G(v_2) - 2) + 1}{1} < \frac{d_{G_1}(u)}{1} = r_{G_1}(e'_3).$$

Then $w_G(e_3) > w_{G_1}(e'_3)$.
Hence, $HA(G) > HA(G_1)$, which is a contradiction to the fact that G has a minimum HA

index.
Case 2: There exist a v^* such that $d_G(v^*) > d_G(v_2)$.
We take three steps to transform G into G_2. First, we delete the edge v_1v_2 and add an edge v_1v^* in G. Next, replace all the edges in $E_G(T_{v_2}) \setminus (E_G(T'_{v^*}) \cup v_2v^*)$ by the pendant edges incident with u. Then, we relocate the edges in T'_{v*} to the pendant edges incident with v^*(see Figure 7). Define the resulting graph by G_2.

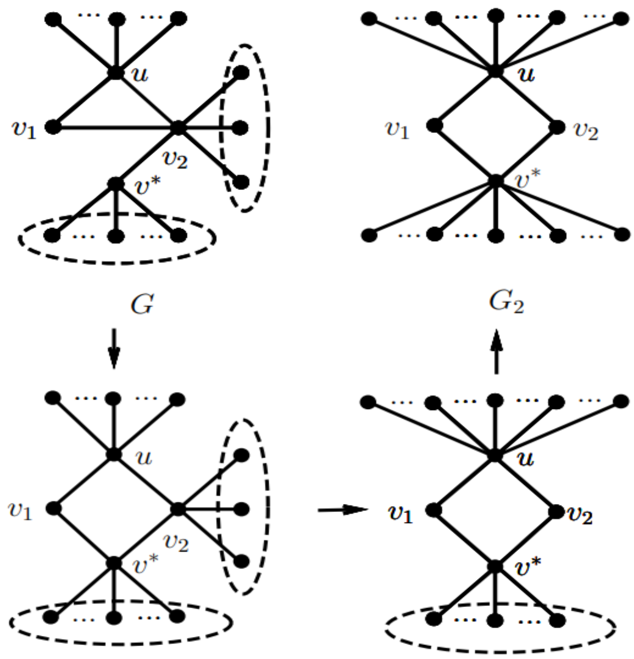


Figure 7: $G \longrightarrow G_2$.

For the pendant edges incident with u in G, since $d_G(u) < d_{G_2}(u)$, the weight of these edges are decreased under this transformation.
Let $e_1 \in E_G(T'_{v^*})$, then it is replaced by appropriate pendant edge e'_1 incident with v^*. Since $|E_G(T'_{v^*})| + 2 = d_{G_2}(v^*)$, we have

$$r_G(e_1) \leq \frac{|E_G(T'_{v^*})| + 1}{1} < \frac{d_{G_2}(v^*)}{1} = r_{G_2}(e'_1).$$

Then $w_G(e_1) > w_{G_2}(e'_1)$.
For each e_2 in $E_G(T_{v_2}) \setminus (E_G(T'_{v^*}) \cup v_2v^*)$, it is replaced by appropriate pendant edge e'_2 incident with u. Since

$$d_{G_2}(u) - 2 = |E_G(T_u)| + |E_G(T_{v_2})| - (|E_G(T'_{v^*})| + 1) \geq 1 + |E_G(T_{v_2})| - (|E_G(T'_{v^*})| + 1),$$

we have

$$r_G(e_2) \leq \frac{|E_G(T_{v_2})| - (|E_G(T'_{v^*})| + 1) + 3}{1} \leq \frac{d_{G_2}(u)}{1} = r_{G_2}(e'_2).$$

Thus $w_G(e_2) \geq w_{G_2}(e'_2)$.
Since $d_G(u) \leq d_{G_2}(u)$ and the degree of v_1, v_2 are unchanged and decreased under this transformation, respectively, then we have $w_G(uv_1) \geq w_{G_2}(uv_1)$ and $w_G(uv_2) > w_{G_2}(uv_2)$.

For the edge $v_1v_2 \in G$, we have

$$r_G(v_1v_2) = \frac{d_G(v_2)}{2} < \frac{d_G(v^*)}{2} < \frac{d_{G_2}(v^*)}{2} = r_{G_2}(v_1v^*).$$

Then $w_G(v_1v_2) > w_{G_2}(v_1v^*)$.
For the edge v_2v^*, since $d_G(v^*) < d_{G_2}(v^*)$ and $d_G(v_2) > d_{G_2}(v_2) = 2$, we have

$$r_G(v_2v^*) = \frac{d_G(v^*)}{d_G(v_2)} < \frac{d_{G_2}(v^*)}{2} = r_{G_2}(v_2v^*).$$

Then $w_G(v_2v^*) > w_{G_2}(v_2v^*)$.
Hence, $HA(G) > HA(G_2)$, which is also a contradiction. ■

Thus, the possible extremal graph which attains the minimum HA index among all the unicyclic graphs of order n is $S_{r,k;3}$, which is obtained by attaching r and k pendent vertices, respectively, to two vertices of C_3. And $r + k = n - 3$, $r \geq 1$, $k \geq 1$. Graph $S_{r,k;3}$ is just like the G_1 shown in Figure 6.

Proposition 2.6. *Assume that G contains exactly two cycle vertex of degree two. If G has minimum HA index among all the unicyclic graphs of order n, then the length of cycle of G must be no more than four and each nontrival tree rooted at a cycle vertex must be a star whose center is a cycle vertex.*

Proof. Assume that there exists a unicyclic graph G with minimum HA index. u is maximum degree cycle vertex. v_1 and v_2 are two cycle vertices of degree two. Then by Lemma 2.4, T_u is a star with center u, and $uv_i \in E(G)(i = 1, 2)$. We will take two steps to prove this proposition.
Step 1: Firstly, we are going to prove the length of cycle of G is no more than four.
Suppose that the girth of G is greater than four. Let $S = \{s_1, s_2, \cdots, s_k\}$, $k \geq 2$, be the set of remaining cycle vertices, where s_1 and s_k are adjacent to v_1 and v_2, respectively (see Figure 8). Let s be the maximum degree vertex among all the vertices in S.

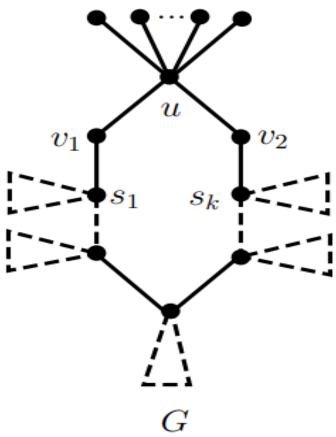


Figure 8: the graph G whose girth is greater than four.

Case 1: If $s = s_1$, then s is a local maximum degree cycle vertex and T_s is a star with center s.
Let $e = v_2s_k$ and perform the v_2es-transformation. We can get $HA(G_{v_2es}) < HA(G)$ by

Proposition 2.3, which is a contradiction to the fact that G has minimum HA index.
Case 2: If $s \neq s_1$, then s is a local maximum degree cycle vertex and T_s is a star with center s. Let $e = v_1 s_1$ and perform the $v_1 es$-transformation. We can get that $HA(G_{v_1 es}) < HA(G)$ by Proposition 2.3, which is also a contradiction.
Step 2: We need to prove that each nontrival tree rooted at a cycle vertex is a star whose center is a cycle vertex when the length of cycle is no more than four.
When the length of cycle is three, the proof is already completed.
When the length of cycle is four, suppose that v_3 is the remaining cycle vertex not adjacent to u. If T_{v_3} is not a star with center v_3, replace all the edges of T_{v_3} by the pendent edges incident with v_3 and then we can get a unicyclic graph with a smaller HA index than G by Proposition 2.1, which is a contradiction. ■

Thus, the possible extremal graph which attains the minimum HA index among all the unicyclic graphs of order n is one of two graphs shown in Figure 9, in which $S_{r,k;4}$ is obtained by attaching r and k pendent vertices, respectively, to two non-adjacent vertices of C_4, where $r + k = n - 4$, $r \geq 1$, $k \geq 1$, and graph S_n^* is obtained by attaching $n - 3$ pendant vertices to a single vertex of C_3.

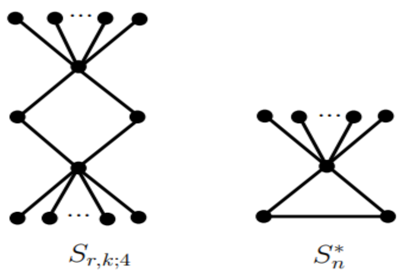


Figure 9: $S_{r,k;4}, r + k = n - 4$, and S_n^*.

Proposition 2.7. *For the graphs $S_{r,k;3}$ and S_n^*, $r + k = n - 3$, we have $HA(S_n^*) < HA(S_{r,k;3})$.*

Proof. For the graphs $S_{r,k;3}$ and S_n^*, we have

$$HA(S_n^*) = \frac{4(n-1)(n-3)}{n^2} + \frac{16(n-1)}{(n+1)^2} + 1,$$
$$HA(S_{r,k;3}) = \frac{4r(r+2)}{(r+3)^2} + \frac{4k(k+2)}{(k+3)^2} + \frac{8(r+2)}{(r+4)^2} + \frac{8(k+2)}{(k+4)^2} + \frac{4(r+2)(k+2)}{(r+k+4)^2}.$$

Since $n = r + k + 3$, we have

$$HA(S_n^*) = \frac{4(r+k)(r+k+2)}{(r+k+3)^2} + \frac{16(r+k+2)}{(r+k+4)^2} + 1.$$

Let $g(x) = \frac{8x}{(x+2)^2}$ and assume that $r \geq k \geq 1$, then

$$\begin{aligned} HA(S_{r,k;3}) - HA(S_n^*) &= rh(r+2) + kh(k+2) + g(r+2) + g(k+2) + \frac{4(r+2)(k+2)}{(r+k+4)^2} \\ &\quad - (r+k)h(r+k+2) - 2g(r+k+2) - 1 \\ &= r[h(r+2) - h(r+k+2)] + k[h(k+2) - h(r+k+2)] \\ &\quad + g(r+2) + g(k+2) - 2g(r+k+2) + \frac{4(r+2)(k+2)}{(r+k+4)^2} - 1. \end{aligned}$$

Let

$$\begin{aligned} A(r,k) &= r[h(r+2) - h(r+k+2)] + k[h(k+2) - h(r+k+2)], \\ B(r,k) &= g(r+2) + g(k+2) - 2g(r+k+2) + \frac{4(r+2)(k+2)}{(r+k+4)^2}. \end{aligned}$$

Since $h(x)$ is strictly decreasing for $x \geq 1$ and $g(x)$ is strictly decreasing for $x \geq 2$, it is easy to get that $A(r,k) > 0$ and $B(r,k) > 0$. In the following, we just need to prove $A(r,k)+B(r,k) > 1$ for $r \geq k \geq 1$.
For the function $A(r,k)$, the partial derivative with respective to r is

$$\begin{aligned} \frac{\partial}{\partial r} A(r,k) &= h(r+2) - h(r+k+2) + r[h^{'}(r+2) - h^{'}(r+k+2)] - kh^{'}(r+k+2) \\ &= \frac{4(r+2)}{(r+3)^2} - \frac{4(r+k+2)}{(r+k+3)^2} - \frac{4r(r+1)}{(r+3)^3} + \frac{4r(r+k+1)}{(r+k+3)^3} + \frac{4k(r+k+1)}{(r+k+3)^3} \\ &= 4\Big[\frac{4r+6}{(r+3)^3} - \frac{4(r+k)+6}{(r+k+3)^3}\Big]. \end{aligned}$$

Since the function $\frac{2x+3}{(x+3)^3}$ is strictly decreasing for $x \geq 1$, then $\frac{\partial}{\partial r} A(r,k) > 0$, that is, for any fixed $k \geq 1$, $A(r,k)$ is increasing with respect to r.
Case 1: $k = 1$. We have $A(r,1) \geq A(1,1) = h(3) - h(4) + h(3) - h(4) = 2(\frac{12}{16} - \frac{16}{25}) = \frac{22}{100}$ and

$$\begin{aligned} B(r,1) &= g(r+2) + g(3) - 2g(r+3) + \frac{12(r+2)}{(r+5)^2} \\ &> g(3) - g(r+3) + \frac{12(r+2)}{(r+5)^2} \\ &= \frac{24}{25} - \frac{8(r+3)}{(r+5)^2} + \frac{12(r+2)}{(r+5)^2} > \frac{24}{25}, \end{aligned}$$

so $A(r,1) + B(r,1) > 1$ for $r \geq k = 1$. Hence, $HA(S_n^*) < HA(S_{r,k;3})$ for $r \geq k = 1$. When $k \geq 2$, some values of $A(r,k)$ and $B(r,k)$ are shown in Table 1.
Case 2: $k = 2$. Since $A(r,2)$ is increasing with respect to r and $A(6,2) > 1$, then $A(r,2) > 1$ for $r \geq 6$. If $r \leq 5$, $B(r,2) > 1$. So $A(r,2) + B(r,2) > 1$ for $r \geq k = 2$. Hence, $HA(S_n^*) < HA(S_{r,k;3})$ for $r \geq k = 2$.
Case 3: Similarly, we can get that $HA(S_n^*) < HA(S_{r,k;3})$ for $r \geq k = 3$.
Case 4: $k \geq 4$. Since $A(r,k)$ is increasing with respect to r for any fixed $k \geq 4$, if $A(k,k) > 1$ for $k \geq 4$, then $A(r,k) > 1$ for $r \geq k \geq 4$, that is $A(r,k) + B(r,k) > 1$.
When $k = 4$, $A(4,4) = 1.2737 > 1$. Let $k \geq 5$, then $A(k,k) = 2k[h(k+2) - h(2k+2)]$. By mean value theorem, there exist $\alpha \in (k+2, 2k+2)$ such that $h(k+2) - h(2k+2) = -kh^{'}(\alpha)$,

Table 1: Some values of $A(r,k)$ and $B(r,k)$.

r	$A(r,2)$	$B(r,2)$	$A(r,3)$	$B(r,3)$	$A(r,4)$	$B(r,4)$
2	0.6008	1.2778	-	-	-	-
3	0.7592	1.3102	0.9630	1.3527	-	-
4	0.8688	1.3189	1.1059	1.3680	1.2737	1.3889
5	0.9475	1.3158	1.2095	1.3688	1.3967	1.3940
6	1.0057	1.3067	1.2870	1.3617	1.4893	1.39
7	1.05	1.2946	1.3464	1.3501	1.5608	1.3806

thus $A(k,k) = -2k^2h^{'}(\alpha)$.
Since $h^{'}(x)$ is a negative increasing function for $x \geq 2$, then

$$A(k,k) = -2k^2h^{'}(\alpha) > -2k^2h^{'}(2k+2) = -2k^2\frac{-4(2k+1)}{(2k+3)^3} = \frac{8k^2(2k+1)}{(2k+3)^3}.$$

Because the function $\frac{8k^2(2k+1)}{(2k+3)^3}$ is increasing, we have $A(k,k) \geq \frac{8\times25\times11}{13^3} > 1$. So, $A(k,k) > 1$ for $k \geq 5$, that is, $A(r,k) > 1$ for $r \geq k \geq 5$. Hence, $HA(S_n^*) < HA(S_{r,k;3})$ for $r \geq k \geq 5$. ■

Proposition 2.8. *For the graphs $S_{r,k;4}$ and S_n^*, $r+k = n-4$, we have $HA(S_n^*) < HA(S_{r,k;4})$.*

Proof. For the graphs $S_{r,k;4}$ and S_n^*, we have

$$HA(S_n^*) = \frac{4(n-1)(n-3)}{n^2} + \frac{16(n-1)}{(n+1)^2} + 1,$$
$$HA(S_{r,k;4}) = \frac{4r(r+2)}{(r+3)^2} + \frac{4k(k+2)}{(k+3)^2} + \frac{16(r+2)}{(r+4)^2} + \frac{16(k+2)}{(k+4)^2}.$$

Since $n = r+k+4$, we have

$$HA(S_n^*) = \frac{4(r+k+1)(r+k+3)}{(r+k+4)^2} + \frac{16(r+k+3)}{(r+k+5)^2} + 1,$$

then

$$\begin{aligned} HA(S_{r,k;4}) - HA(S_n^*) &= rh(r+2) + kh(k+2) + 2g(r+2) + 2g(k+2) \\ &\quad - (r+k+1)h(r+k+3) - 2g(r+k+3) - 1 \\ &= r[h(r+2) - h(r+k+3)] + k[h(k+2) - h(r+k+3)] \\ &\quad + 2g(r+2) + 2g(k+2) - 2g(r+k+3) - h(r+k+3) - 1. \end{aligned}$$

Let

$$\begin{aligned} C(r,k) &= r[h(r+2) - h(r+k+3)] + k[h(k+2) - h(r+k+3)], \\ D(r,k) &= 2g(r+2) + 2g(k+2) - 2g(r+k+3) - h(r+k+3). \end{aligned}$$

Since $h(x)$ is strictly decreasing for $x \geq 1$, $g(x)$ is strictly decreasing for $x \geq 2$ and $g(x) \geq h(x)$ when $x \geq 2$, it is easy to get that $C(r,k) > 0$ and $D(r,k) > 0$. In the following, we just need to prove $C(r,k) + D(r,k) > 1$ for $r \geq k \geq 1$.

For the function $C(r,k)$, the partial derivative with respective to r is

$$\begin{aligned}\frac{\partial}{\partial r}C(r,k) &= h(r+2) - h(r+k+3) + r[h^{'}(r+2) - h^{'}(r+k+3)] - kh^{'}(r+k+3)\\ &= \frac{4(r+2)}{(r+3)^2} - \frac{4(r+k+3)}{(r+k+4)^2} - \frac{4r(r+1)}{(r+3)^3} + \frac{4r(r+k+2)}{(r+k+4)^3} + \frac{4k(r+k+2)}{(r+k+4)^3}\\ &= 4\Big[\frac{4r+6}{(r+3)^3} - \frac{5(r+k)+12}{(r+k+4)^3}\Big].\end{aligned}$$

For any fixed $k \geq 1$, the graph of $\frac{\partial}{\partial r}C(r,k)$ with respect to r is shown in Figure 10. From Figure 10, we can see that for any fixed $k \geq 1$, $\frac{\partial}{\partial r}C(r,k)$ only have one root on $r \geq k$, let it be r_0, and when $k \leq r < r_0$, $\frac{\partial}{\partial r}C(r,k) > 0$, when $r > r_0$, $\frac{\partial}{\partial r}C(r,k) < 0$. Hence, for any fixed $k \geq 1$, $C(r,k)$ is strictly increasing with respect to r on $[k, \lfloor r_0 \rfloor]$ and decreasing with respect to r on $[\lceil r_0 \rceil, \infty)$.

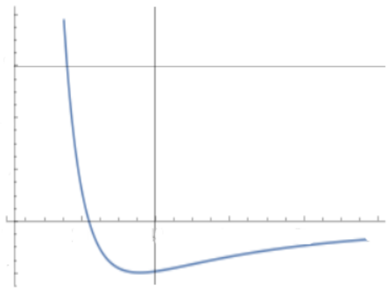


Figure 10: the graph of $C(r,k)$ with respect to r when k is a fixed integer.

Case 1: $k = 1$.

$$\begin{aligned}D(r,1) &= 2g(r+2) + 2g(3) - 2g(r+4) - h(r+4)\\ &= 2[g(r+2) - g(r+4)] + 2g(3) - h(r+4)\\ &> 2g(3) - h(5)\\ &= \frac{307}{225} > 1.\end{aligned}$$

Hence, $HA(S_n^*) < HA(S_{r,k;4})$ for $r \geq k = 1$.

When $k \geq 2$, since $\lim_{r\to\infty} C(r,k) = \lim_{r\to\infty}[\frac{4r(r+2)}{(r+3)^2} - \frac{4r(r+k+3)}{(r+k+4)^2} + \frac{4k(k+2)}{(k+3)^2} - \frac{4k(r+k+3)}{(r+k+4)^2}] = \frac{4k(k+2)}{(k+3)^2}$, and $[\frac{4k(k+2)}{(k+3)^2}]' = \frac{2(k+2)}{(k+3)^3} > 0$, then $\lim_{r\to\infty} C(r,k) = \frac{4k(k+2)}{(k+3)^2} \geq \frac{32}{25} > 1$. Because $C(r,k)$ is strictly decreasing with respect to r on $[\lceil r_0 \rceil, \infty)$, we can get that for any fixed $k \geq 2$, $C(r,k) > 1$ for $r \in [\lceil r_0 \rceil, \infty)$. When $k \geq 2$, some values of $C(r,k)$ and $D(r,k)$ are shown in Table 2.

Case 2: $k = 2$, $C(r,2)$ is increasing on $[2, \lfloor r_0 \rfloor]$ and decreasing on $[\lceil r_0 \rceil, \infty)$. Since $C(4,2) = 1.0792 > 1$ and $2 < 4 < \lfloor r_0 \rfloor$, then $C(r,2) > 1$ for $r \geq 4$. And if $r \leq 3$, we have $D(r,2) > 1$. So, $C(r,k) + D(r,k) > 1$ for $r \geq k = 2$. Hence, $HA(S_n^*) < HA(S_{r,k;4})$ for $r \geq k = 2$.

Case 3: $k \geq 3$. Since for any fixed $k \geq 3$, $C(r,k)$ is strictly increasing with respect to r on $[k, \lfloor r_0 \rfloor]$, decreasing with respect to r on $[\lceil r_0 \rceil, \infty)$ and $C(r,k) > 1$ for $r \in [\lceil r_0 \rceil, \infty)$, if $C(k,k) > 1$ for $k \geq 3$, then $C(r,k) > 1$ for $r \geq k \geq 3$, that is $C(r,k) + D(r,k) > 1$.

When $k = 3, 4$, $C(3,3) > 1, C(4,4) > 1$. Let $k \geq 5$, then $C(k,k) = 2k[h(k+2) - h(2k+3)]$. By

Table 2: Some values of $C(r,k)$ and $D(r,k)$.

r	$C(r,2)$	$D(r,2)$	$C(r,3)$	$D(r,3)$	$C(r,4)$	$D(r,4)$
2	0.81	1.7353	-	-	-	-
3	0.9714	1.7354	1.1733	1.7152	-	-
4	1.0792	1.7277	1.3118	1.6910	1.4739	1.6530
5	1.1535	1.7188	1.4097	1.6684	1.5905	1.6191

mean value theorem, there exists $\beta \in (k+2, 2k+3)$ such that $h(k+2)-h(2k+3) = (-k-1)h^{'}(\beta)$, thus $C(k,k) = -2k(k+1)h^{'}(\beta)$.
Since $h^{'}(x)$ is a negative increasing function for $x \geq 2$, then

$$C(k,k) = -2k(k+1)h^{'}(\beta) > -2k(k+1)h^{'}(2k+3) = \frac{8k(k+1)(2k+2)}{(2k+4)^3} = \frac{2k(k+1)^2}{(k+2)^3}.$$

Because the function $\frac{2k(k+1)^2}{(k+2)^3}$ is increasing, we have $C(k,k) \geq \frac{2\times5\times36}{7^3} = \frac{360}{343} > 1$. So, $C(k,k) > 1$ for $k \geq 5$, that is, $C(r,k) > 1$ for $r \geq k \geq 5$. Hence, $HA(S_n^*) < HA(S_{r,k;4})$ for $r \geq k \geq 5$. ■

By the results above, we can get the following theorem.

Theorem 2.9. *If G is a unicyclic graph of order n $(n \geq 3)$, then*

$$\frac{4(n-1)(n-3)}{n^2} + \frac{16(n-1)}{(n+1)^2} + 1 \leq HA(G) \leq n.$$

The lower bound is attained only by the graph S_n^*, which is obtained by attaching $n-3$ pendant vertices to a single vertex of the cycle C_3. The upper bound is only attained by the cycle C_n.

3 Concluding remarks

The purpose of this paper is to find the extremal values of a harmonic-arithmetic index over unicyclic graphs. We provide the upper and lower bounds of a harmonic-arithmetic index over unicyclic graphs and characterize the unicyclic graphs that attain the extremal situation, respectively.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

Acknowledgment. This research was supported by the National Science Foundation of China (No. 12171239).

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