

Extremal Unicyclic and Bicyclic Graphs with Respect to Harary Index

¹KEXIANG XU AND ²KINKAR CH. DAS

¹College of Science, Nanjing University of Aeronautics Astronautics, Nanjing, P. R. China
²Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea
¹xukexiang0922@yahoo.cn, ²kinkardas2003@googlegmail.com

Abstract. The Harary index is defined as the sum of reciprocals of distances between all pairs of vertices of a connected graph. In this paper, we determined the extremal (maximal and minimal) unicyclic and bicyclic graphs with respect to Harary index.

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1. Introduction

The Harary index of a graph G , denoted by $H(G)$, has been introduced independently by Plavšić *et al.* [25] and by Ivanciuc *et al.* [20] in 1993. It has been named in honor of Professor Frank Harary on the occasion of his 70th birthday. The Harary index is defined as follows:

$$H = H(G) = \sum_{v_i, v_j \in V(G)} \frac{1}{d_G(v_i, v_j)},$$

where the summation goes over all pairs of vertices of G and $d_G(v_i, v_j)$ denotes the distance of the two vertices v_i and v_j in the graph G (i.e., the number of edges in a shortest path connecting v_i and v_j). Mathematical properties and applications of H are reported in [4, 10, 11, 22, 32].

Another distance-based topological indices of a graph G is the Wiener index $W(G)$. As an oldest topological index, the Wiener index of a graph G , first introduced by Wiener [27] in 1947, was defined as

$$W(G) = \sum_{v_i, v_j \in V(G)} d_G(v_i, v_j)$$

with the summation going over all pairs of vertices of G . Mathematical properties and applications of Wiener index is extensively reported in the literature [2, 6–9, 11–17, 21, 23, 24, 26, 33, 34].

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Let $\gamma(G, k)$ be the number of vertex pairs of the graph G that are at distance k . Then

$$(1.1) \quad H(G) = \sum_{k \geq 1} \frac{1}{k} \gamma(G, k).$$

Note that, in any disconnected graph G , the distance is infinite of any two vertices from two distinct components. Therefore its reciprocal can be viewed as 0. Thus we can define validly the Harary index of disconnected graph G as follows:

$$H(G) = \sum_{i=1}^k H(G_i),$$

where G_1, G_2, \dots, G_k are all the components of G .

All graphs considered in this paper are finite, simple and connected. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. For a vertex $v_i \in V(G)$, the *degree* of v_i , denoted by $d_G(v_i)$ (or written as $d(v_i)$ for short) is the number of vertices in G adjacent to v_i . In particular, $\Delta = \Delta(G)$ is called the maximum degree of vertices of G . A vertex v_i of degree 1 is called pendent vertex. An edge $e = v_i v_j$ incident with the pendent vertex v_i is a pendent edge. For a subset W of $V(G)$, let $G - W$ be the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, for a subset E' of $E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E' . If $W = \{v_i\}$ and $E' = \{v_j v_k\}$, the subgraphs $G - W$ and $G - E'$ will be written as $G - v_i$ and $G - v_j v_k$ for short, respectively. For any two nonadjacent vertices v_i and v_j in graph G , we use $G + v_i v_j$ to denote the graph obtained from adding a new edge $v_i v_j$ to graph G . A connected graph G is called unicyclic graph if $|E(G)| = |V(G)|$. Similarly a connected graph G is bicyclic graph when $|E(G)| = |V(G)| + 1$. In the following we denote by P_n , C_n and S_n the path graph, the cycle graph and the star graph with n vertices, respectively. For other undefined notations and terminology from graph theory, the readers are referred to [1].

Let $\mathcal{U}(n)$ and $\mathcal{B}(n)$ be the set of connected unicyclic graphs of order n and the set of connected n -vertex bicyclic graphs, respectively. A graph with maximum degree at most 4 is called molecular graph, which models the skeleton of an molecule in chemistry [26]. Gutman [16] first determined the extremal (minimal and maximal) trees with respect to Harary index (which are path and star, respectively). For more mathematical properties or chemical applications of Harary index, the readers can refer to [4, 5, 10, 11, 16, 18, 19, 30–33]. In particular, one of the present authors, Zhou and Trinajstić [4], Zhou, Cai, Trinajstić [32] gave some nice bounds on Harary index. Moreover, Theorem 2.1 of [18] has also been reported in [16]. In this paper we determined the extremal graphs in $\mathcal{U}(n)$ and $\mathcal{B}(n)$, respectively, at which the maximal and minimal Harary index are attained.

2. Some lemmas

In this section we list or prove some lemmas as basic but necessary preliminaries, which will be used in the subsequent proofs.

First, for a connected graph G with $v_i \in V(G)$, we define $Q_G(v_i) = \sum_{v_j \in V(G)} \frac{d_G(v_i, v_j)}{d_G(v_i, v_j) + 1}$. For convenience, sometimes we write $Q_G(v_i)$ as $Q_{V(G)}(v_i)$. Note that the function $f(x) = \frac{x}{x+1}$ is strictly increasing for $x \geq 1$.

Lemma 2.1. [28] *Let G be a graph of order n and v_i be a pendent vertex of G with $v_i v_j \in E(G)$. Then we have $H(G) = H(G - v_i) + n - 1 - Q_{G-v_i}(v_j)$.*

Proof. By the definitions of Harary index and $Q_G(u)$, we have

$$\begin{aligned} H(G) &= \sum_{v_s, v_t \in V(G-v_i)} \frac{1}{d_G(v_s, v_t)} + \sum_{x \in V(G-v_i)} \frac{1}{d_G(x, v_i)} \\ &= H(G - v_i) + \sum_{x \in V(G-v_i)} \frac{1}{d_G(x, v_j) + 1} \\ &= H(G - v_i) + \sum_{x \in V(G-v_i)} \left(1 - \frac{d_G(x, v_j)}{d_G(x, v_j) + 1}\right) \\ &= H(G - v_i) + n - 1 - Q_{G-v_i}(v_j), \end{aligned}$$

completing the proof of this lemma. ▮

Lemma 2.2. [30] *Let G be a graph with v_i, v_j as its two nonadjacent vertices and $e \in E(G)$. Then*

- (1) $H(G + v_i v_j) > H(G)$;
- (2) $H(G - e) < H(G)$.

From Lemma 2.1 and Lemma 2.2 (2), the following corollary is obvious.

Corollary 2.1. *Let G be a graph of order n and $v_i v_j \in E(G)$. Then*

$$H(G) \geq H(G - v_i) + n - 1 - Q_{G-v_i}(v_j)$$

with equality holding if and only if v_i is a pendent vertex of G .

Let $T_n(n_1, n_2, \dots, n_m)$ (see in Fig. 1(a)) be a starlike tree of order n obtained from the star S_{m+1} by replacing its m edges by m paths $P_{n_1}, P_{n_2}, \dots, P_{n_m}$ with $\sum_{i=1}^m n_i = n - 1$. For convenience, if the number of n_k in $T_n(n_1, n_2, \dots, n_m)$ is $l_k > 1$, we write it as $n_k^{l_k}$ in the following. For example, $T_{11}(2, 2, 3, 3)$ will be written as $T_{11}(2^2, 3^2)$ for short. A broom of order n with k leaves is just written as $B_{n,k} = T_n(1^{k-1}, (n-k)^1)$ (see Fig. 1(b)). A leaf adjacent to the unique vertex of maximum degree k in $B_{n,k}$ is called *unit leaf*. Obviously, $B_{n,k}$ has $k - 1$ unit leaves. Suppose $B'_{n,k} \supseteq B_{n,k}$, where $B'_{n,k}$ is a graph of order n obtained by adding some edges (if exists) between unit leaves in $B_{n,k}$. If v_i is the pendent vertex of $B'_{n,k}$ with the distance $n - k$ from that vertex of maximum degree k , then

$$Q_{B'_{n,k}}(v_i) = \frac{n(n-k+1)}{n-k+2} - \sum_{t=1}^{n-k+1} \frac{1}{t+1}.$$

Lemma 2.3. *Let G be a connected graph of order n with diameter $d \leq k$ ($k < n$). For any vertex $v \in V(G)$,*

$$(2.1) \quad Q_G(v) \leq \frac{nk}{k+1} - \sum_{t=1}^k \frac{1}{t+1}$$

with equality holding in (2.1) if and only if G is isomorphic to $B'_{n,n-k+1}$ and v is the unique vertex of $B'_{n,n-k+1}$ with the distance $k - 1$ from that vertex of maximum degree $n - k + 1$.

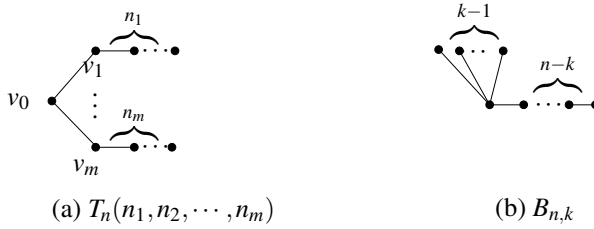


Fig. 1 The graphs $T_n(n_1, n_2, \dots, n_m)$ and $B_{n,k}$

Proof. Suppose that $P_{d+1} : v_1 v_2 \dots v_d v_{d+1}$ is a path, where the vertices v_i and v_{i+1} are adjacent for $i = 1, 2, \dots, d$ in G .

Then we have

$$\begin{aligned}
 Q_G(v) &= \sum_{v_j \in V(G)} \frac{d_G(v, v_j)}{d_G(v, v_j) + 1} = n - 1 - \sum_{v_j \in V(G)} \frac{1}{d_G(v, v_j) + 1} \\
 (2.2) \quad &\leq n - 1 - \sum_{j=1}^d \frac{1}{j+1} - \frac{n-d-1}{d+1} \text{ as } d_G(v, v_j) \leq d.
 \end{aligned}$$

If $k = d$, then from (2.2), we get the required result (2.1). Otherwise, $k > d$. In this case we have to prove that

$$n - 1 - \sum_{j=1}^d \frac{1}{j+1} - \frac{n-d-1}{d+1} < n - 1 - \sum_{j=1}^k \frac{1}{j+1} - \frac{n-k-1}{k+1},$$

that is,

$$\sum_{j=1}^k \frac{1}{j+1} + \frac{n-k-1}{k+1} < \sum_{j=1}^d \frac{1}{j+1} + \frac{n-d-1}{d+1},$$

that is,

$$\sum_{j=1}^k \frac{1}{j+1} - \sum_{j=1}^d \frac{1}{j+1} = \sum_{j=d+1}^k \frac{1}{j+1} < \frac{n(k-d)}{(k+1)(d+1)},$$

that is,

$$\sum_{j=d+1}^k \frac{1}{j+1} \leq \frac{k-d}{d+2} < \frac{n(k-d)}{(k+1)(d+1)},$$

which, evidently, is always obeyed as $d < k < n$. First part of the proof is over.

Suppose that the equality holds in (2.1). Then the equality holds in (2.2) and we must have $d = k$. From equality in (2.2), we get

$$v = v_1, \quad d_G(v, v_j) = d \text{ for } j = d+2, d+3, \dots, n.$$

Since $d = k$, obviously, G is isomorphic to a graph obtained from $B_{n,n-k+1}$ by adding some edges (if exists) between unit leaves in it. Thus $G \cong B'_{n,n-k+1}$ and v_i is the pendent vertex of $B'_{n,n-k+1}$ with the distance $k - 1$ from that vertex of maximum degree $n - k + 1$.

Conversely, one can see easily that the equality holds in (2.1) for $B'_{n,n-k}$ and v_i is the pendent vertex of $B'_{n,n-k+1}$ with the distance $k - 1$ from that vertex of maximum degree $n - k + 1$. ■

Let K'_4 be a graph obtained by deleting an edge from K_4 . Using $B_n^{(0)}$ we denote the graph obtained by identifying a pendent vertex of P_{n-3} with a vertex in K'_4 of degree 2. Denote by $B_n^{(0,s)}$ a graph of order n which is obtained by attaching paths P_{n-s-4} and P_s at each of two 2-degree vertices of K'_4 , $0 \leq s \leq \lceil \frac{n-4}{2} \rceil$. In particular, $B_n^{(0)} = B_n^{(0,0)}$. One can see easily that

$$(2.3) \quad Q_{B_n^{(0,s)}}(v_j) < \dots < Q_{B_n^{(0,1)}}(v_j) < Q_{B_n^{(0,0)}}(v_i) = Q_{B_n^{(0)}}(v_i) \text{ with } s = \lceil \frac{n-4}{2} \rceil,$$

where v_i is the only pendent vertex in $B_n^{(0)}$ and v_j is one pendent vertex farthest from K'_4 in $B_n^{(0,s)}$.

Lemma 2.4. *Let G be a connected bicyclic graph of order n with diameter $n - 2$. Then $G \cong B_n^{(0,s)}$ with $0 \leq s \leq \lceil \frac{n-4}{2} \rceil$.*

Proof. Since the diameter of bicyclic graph G is $n - 2$, we have an induced path P_{n-1} in G . Suppose that $P_{n-1} : v_1 v_2 \dots v_{n-2} v_{n-1}$ is a path, where the vertices v_i and v_{i+1} are adjacent for $i = 1, 2, \dots, n - 2$ in G . Considering that G is bicyclic, we claim that the remaining vertex v_n must be adjacent to three vertices of $v_1, v_2, \dots, v_{n-2}, v_{n-1}$. Notice that the diameter of G is $n - 2$, again, the three vertices adjacent to v_n must be consecutive. Thus we find that $G \cong B_n^{(0,s)}$ with $0 \leq s \leq \lceil \frac{n-4}{2} \rceil$, which completes the proof of this lemma. ■

Lemma 2.5. *Let G be a connected bicyclic graph of order n . For any vertex $v_i \in V(G)$,*

$$(2.4) \quad Q_G(v_i) \leq \frac{n^2 - 3n + 1}{n - 2} - \sum_{t=1}^{n-2} \frac{1}{t + 1}$$

with equality holding in (2.4) if and only if G is isomorphic to $B_n^{(0)}$ and v_i is the unique pendent vertex of $B_n^{(0)}$.

Proof. Since there is only one connected graph of order n with diameter $d = n - 1$, which is just path P_n , any bicyclic graph G of order n has diameter $d \leq n - 2$. Now we consider two cases (i) $d \leq n - 3$, (ii) $d = n - 2$.

Case (i) : $d \leq n - 3$. By Lemma 2.3, we have

$$(2.5) \quad Q_G(v_i) \leq \frac{n(n-3)}{n-2} - \sum_{t=1}^{n-3} \frac{1}{t+1}$$

with equality holding in (2.5) if and only if G is isomorphic to $B'_{n,4}$ and v_i is the unique vertex of $B'_{n,4}$ with the distance $n - 4$ from that vertex of maximum degree 4.

Case (ii) : $d = n - 2$. Since G is bicyclic graph, we have

$$G \cong B_n^{(0,s)}, \quad 0 \leq s \leq \lceil \frac{n-4}{2} \rceil, \text{ by Lemma 2.4.}$$

By (2.3), we have

$$(2.6) \quad Q_G(v_i) \leq Q_{B_n^{(0,0)}}(v_i) = Q_{B_n^{(0)}}(v_i) = \frac{n^2 - 3n + 1}{n - 2} - \sum_{t=1}^{n-2} \frac{1}{t + 1}$$

with equality holding in (2.6) if and only if G is isomorphic to $B_n^{(0)}$ and v_i is the unique pendent vertex of $B_n^{(0)}$.

Set

$$M = \left(\frac{n^2 - 3n + 1}{n - 2} - \sum_{t=1}^{n-2} \frac{1}{t + 1} \right) - \left(\frac{n(n - 3)}{n - 2} - \sum_{t=1}^{n-3} \frac{1}{t + 1} \right).$$

Then we have

$$M = \frac{1}{n - 2} - \frac{1}{n - 1} = \frac{1}{(n - 1)(n - 2)} > 0.$$

By the above arguments, the result (2.4) follows immediately. Moreover, the equality in (2.4) holds if and only if $G \cong B_n^{(0)}$ and v_i is the unique pendent vertex of $B_n^{(0)}$. ■

3. Main results

In [31], Yu and Feng characterized the extremal graph with maximal Harary index among all connected bicyclic graphs of order n and with two edge disjoint cycles. In [3], Chen first gave a formula for the Harary index of any unicyclic graph, and then calculated the first three greatest Harary indices of graphs in $\mathcal{U}(n)$ and with given girth (this result was obtained by Yu and Feng [31] with a different method). By the above results, Chen [3] determined the first three greatest Harary indices of graphs in $\mathcal{U}(n)$ and characterized these corresponding extremal graphs. Moreover, Chen [3] conjectured that the extremal graph in $\mathcal{U}(n)$ with minimal Harary index is probably a graph obtained by identifying a pendent vertex of P_{n-2} with one vertex of C_3 . In this section we will determine completely the extremal (maximal and minimal) unicyclic and bicyclic graphs with respect to Harary index, one of which confirms this conjecture of Chen.

Before obtaining our main results, we first introduce some new graphs below. Denote by $C_k(1^{n-k})$ the graph obtained by attaching $n - k$ pendent edges to one vertex of C_k . Let $C_k((n - k)^1)$ be a graph obtained by identifying one pendent vertex of P_{n-k+1} with one vertex of C_k . We use $C_{3,3}$ to denote the graph obtained by adding two nonadjacent edges to a star S_5 . Let $B_n^{(1)}$ be the graph obtained by attaching $n - 4$ pendent edges to one vertex in K'_4 of degree 3 and also let $B_n^{(2)}$ be a graph obtained by attaching $n - 5$ pendent edges to the unique vertex in $C_{3,3}$ of degree 4 (see Fig. 2).

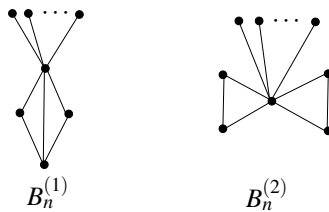


Fig. 2. The graphs $B_n^{(1)}$ and $B_n^{(2)}$.

If $n = 4$, $\mathcal{U}(n)$ contains only two graphs C_4 and $C_3(1^1)$. By a simple calculation, we have $H(C_4) = H(C_3(1^1)) = 5$. So in the following we always assume that $n \geq 5$ in $\mathcal{U}(n)$.

For $n = 4$, there exists only one graph K'_4 in $\mathcal{B}(n)$. So in the following we only need to consider the set $\mathcal{B}(n)$ with $n \geq 5$.

In the following two theorems the extremal graphs in $\mathcal{U}(n)$ and $\mathcal{B}(n)$ with maximal Harary index are completely determined, respectively. In particular, compared with that of [3], we give a different but short proof in Theorem 3.1.

Theorem 3.1. [3] *Let $G \in \mathcal{U}(n)$. Then we have $H(G) \leq \frac{n^2+n}{4}$ with equality holding if and only if $G \cong C_3(1^{n-3})$ for $n \geq 6$ and $G \cong C_n$ or $G \cong C_3(1^{n-3})$ for $n = 5$.*

Proof. There are $\binom{n}{2}$ vertex pairs (at distance at least one) in any unicyclic graph G , the number of vertex pairs at distance one is n , i.e., the number of edges in G . By (1.1), we have

$$(3.1) \quad H(G) \leq n + \frac{1}{2} \left(\binom{n}{2} - n \right) = \frac{n^2 + n}{4}.$$

It is easy to see that equality in (3.1) holds if and only if G has diameter 2. Obviously, unicyclic graph G has diameter 2 if and only if $G \cong C_3(1^{n-3})$ for $n \geq 5$ and there is one more graph C_n for $n = 5$, which implies the result in this theorem. ■

When $n = 5$, there are only five graphs in $\mathcal{B}(n)$ which are shown in Fig. 3. We can easily check that

$$(3.2) \quad H(B_5^{(1)}) = H(B_5^{(2)}) = H(B_5^{(3)}) = H(B_5^{(4)}) = 8 > 7 + \frac{1}{2} + \frac{1}{3} = H(B_5^{(5)}).$$

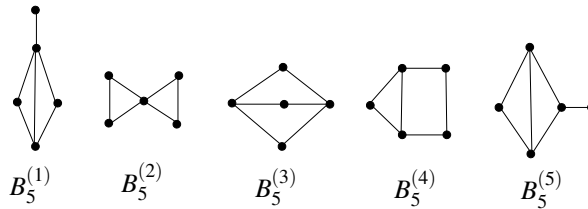


Fig. 3. All the graphs in $\mathcal{B}(5)$.

Theorem 3.2. *For any graph $G \in \mathcal{B}(n)$ with $n \geq 6$, we have $H(G) \leq \frac{n^2+n+2}{4}$ with equality holding if and only if $G \cong B_n^{(1)}$ or $G \cong B_n^{(2)}$, and G is isomorphic to an exceptional graph B'_6 when $n = 6$ obtained from $B_5^{(4)}$ (see Fig. 3) by subdividing the edge connecting two vertices of degree 3 in it.*

Proof. Again, by a similar reasoning to that in Theorem 3.1, we conclude that, for any graph $G \in \mathcal{B}(n)$, $H(G) \leq \frac{n^2+n+2}{4}$ with the equality holding if and only if G has diameter $d = 2$. To obtain our main result, now we will prove the following claim.

Claim 1. Any bicyclic graph G , except the graph B'_6 , with diameter 2 has the maximum degree $\Delta = n - 1$.

Proof of Claim 1. There is no bicyclic graph with maximum degree 2. Obviously, except the graph B'_6 , any bicyclic G of order $n \geq 6$ with maximum degree 3 has diameter more

than 2. Thus, to the contrary, we have $4 \leq \Delta \leq n - 2$. Any bicyclic graph G contains $T = T_{\Delta+2}(1^{\Delta-1}, 2^1)$ as a subgraph because of the fact that $\Delta \leq n - 2$. Now we assume that $V(T) = \{u, v_1, v_2, \dots, v_{\Delta-1}, w_1, w_2\}$ where $d(u) = \Delta$ with $v_1, v_2, \dots, v_{\Delta-1}, w_1$ as all of its neighbors and w_2 is a neighbor of w_1 different from u . Considering the definition of bicyclic graph and $\Delta - 1 \geq 3$, we find that, in G , the distance from vertex w_2 to one of vertices $v_1, v_2, \dots, v_{\Delta-1}$ is 3, which is a contradiction to the fact that G has diameter 2. This completes the proof of this claim.

Combining Claim 1 and the definition of bicyclic graph, we claim that, except the graph B'_6 , $G \cong B_n^{(1)}$ or $G \cong B_n^{(2)}$ immediately, finishing the proof of this theorem. ■

Furthermore Theorems 3.1 and 3.2 can be viewed as particular cases of Proposition 2 in [32]. From Theorem 3.2, the following corollary can be easily obtained.

Corollary 3.1. [31] *Let $G \in \mathcal{B}(n)$ with two edge disjoint cycles. Then $H(G) \leq \frac{n^2+n+2}{4}$ with equality holding if and only if $G \cong B_n^{(2)}$.*

We now turn to the minimal Harary index of graphs in $\mathcal{U}(n)$. To do it, we first list two useful lemmas below.

Lemma 3.1. [25] $H(P_n) = n \sum_{i=1}^{n-1} \frac{1}{i} - n + 1$.

Lemma 3.2. [30] *Let G be a (connected) graph with a cut vertex u such that G_1 and G_2 are two connected subgraphs of G having u as the only common vertex and $G_1 \cup G_2 = G$. Let $|V(G_i)| = n_i$ for $i = 1, 2$. Then $H(G) = H(G_1) + H(G_2) + \sum_{x \in V(G_1) \setminus u, y \in V(G_2) \setminus u} \frac{1}{d_{G_1}(x, u) + d_{G_2}(u, y)}$.*

Lemma 3.3. $H(C_3((n-3)^1)) = n \sum_{i=2}^{n-3} \frac{1}{i} + \frac{2}{n-2} + 4$.

Proof. Applying Lemma 3.1 to the unique 3-degree vertex of $C_3((n-3)^1)$, we have

$$\begin{aligned} H(C_3((n-3)^1)) &= H(C_3) + H(P_{n-2}) + 2 \sum_{i=1}^{n-3} \frac{1}{i+1} \\ &= 3 + (n-2) \sum_{i=1}^{n-3} \frac{1}{i} - n + 3 + 2 \sum_{i=2}^{n-2} \frac{1}{i} \text{ by Lemma 3.2} \\ &= n \sum_{i=2}^{n-3} \frac{1}{i} + \frac{2}{n-2} + 4. \end{aligned}$$

■

Theorem 3.3. *Let $G \in \mathcal{U}(n)$. Then we have*

$$(3.3) \quad H(G) \geq n \sum_{i=2}^{n-3} \frac{1}{i} + \frac{2}{n-2} + 4$$

with equality holding if and only if $G \cong C_3((n-3)^1)$.

Proof. We prove this result by induction on n . When $n = 5$, there are only five graphs in $\mathcal{U}(5)$. They are $C_5, C_4(1^1), C_3(2^1), C_3(1^2)$ and $C_3(1, 1)$, and the last one is obtained by attaching

an edge at each of two vertices of C_3 . With a simple calculation, we have

$$H(C_3(1^2)) = H(C_5) > H(C_3(1, 1)) = H(C_4(1^1)) > H(C_3(2^1)) = 6 + \frac{1}{2} + \frac{2}{3}.$$

Therefore the result holds for $n = 5$.

Now we assume that $n \geq 6$. Note that any unicyclic graph of order $n - 1$ has diameter $d \leq n - 3$. By Corollary 2.1, Lemmas 2.3, 3.3 and induction hypothesis, we have

$$\begin{aligned} H(G) &\geq H(G - v_i) + n - 1 - Q_{G - v_i}(v_j) \\ &\geq (n - 1) \sum_{i=2}^{n-4} \frac{1}{i} + \frac{2}{n-3} + 4 + n - 1 - \frac{(n-1)(n-3)}{n-2} + \sum_{i=1}^{n-3} \frac{1}{i+1} \\ &= n \sum_{i=2}^{n-3} \frac{1}{i} + \frac{2}{n-2} + 4. \end{aligned}$$

Therefore the result (3.3) holds by induction. Both equalities hold if and only if v_i is a pendent vertex of G with v_j as only one neighbor and $G \cong C_3((n - 3)^1)$, by Corollary 2.1 and Lemma 2.3. This completes the proof of this theorem. ■

Lemma 3.4. $H(B_n^{(0)}) = n \sum_{i=1}^{n-4} \frac{1}{i} - n + \frac{19}{2} - \sum_{i=1}^{n-4} (\frac{3}{i} - \frac{2}{i+1} - \frac{1}{i+2})$.

Proof. Applying Lemma 3.1 to the 3-degree vertex of $B_n^{(0)}$, at which a pendent path P_{n-3} is attached, from Lemma 3.2, we have

$$\begin{aligned} H(B_n^{(0)}) &= H(K'_4) + H(P_{n-3}) + 2 \sum_{i=1}^{n-4} \frac{1}{i+1} + \sum_{i=1}^{n-4} \frac{1}{i+2} \\ &= \frac{11}{2} + (n - 3) \sum_{i=1}^{n-4} \frac{1}{i} - n + 4 + 2 \sum_{i=1}^{n-3} \frac{1}{i+1} + \sum_{i=1}^{n-2} \frac{1}{i+2} \\ &= n \sum_{i=1}^{n-4} \frac{1}{i} - n + \frac{19}{2} - \sum_{i=1}^{n-4} (\frac{3}{i} - \frac{2}{i+1} - \frac{1}{i+2}). \end{aligned}$$

Theorem 3.4. For any graph $G \in \mathcal{B}(n)$, we have

$$(3.4) \quad H(G) \geq n \sum_{i=1}^{n-4} \frac{1}{i} - n + \frac{19}{2} - \sum_{i=1}^{n-4} (\frac{3}{i} - \frac{2}{i+1} - \frac{1}{i+2})$$

with equality holding if and only if $G \cong B_n^{(0)}$.

Proof. We will prove this result by induction on n . Note that $B_5^{(5)} \cong B_5^{(0)}$ as shown in Fig. 2. From (3.2), we claim that this result holds for $n = 5$.

Now we consider the case when $n \geq 6$. By Corollary 2.1, Lemmas 2.5, 3.4 and induction hypothesis, we have

$$\begin{aligned} H(G) &\geq H(G - v_i) + n - 1 - Q_{G - v_i}(v_j) \\ &\geq (n - 1) \sum_{i=1}^{n-5} \frac{1}{i} - (n - 1) + \frac{19}{2} - \sum_{i=1}^{n-5} (\frac{3}{i} - \frac{2}{i+1} - \frac{1}{i+2}) \end{aligned}$$

$$\begin{aligned}
& + n - 1 - \left[\frac{(n-1)(n-4) + 1}{n-3} - \sum_{t=1}^{n-3} \frac{1}{t+1} \right] \\
& = n \sum_{i=1}^{n-4} \frac{1}{i} - n + \frac{19}{2} - \sum_{i=1}^{n-4} \left(\frac{3}{i} - \frac{2}{i+1} - \frac{1}{i+2} \right).
\end{aligned}$$

Therefore the result (3.4) holds by induction. Both equalities hold if and only if v_i is a pendent vertex of G with v_j as only one neighbor and $G \cong B_n^{(0)}$, by Corollary 2.1 and Lemma 2.5. This completes the proof of this theorem. ■

4. Conclusion

By applying certain advanced proof techniques of graph theory, we obtain the extremal (maximal and minimal) unicyclic and bicyclic graphs with respect to Harary index.

In $\mathcal{U}(n)$, the graph $C_3(1^{n-3})$ has the maximal Harary index with one more graph C_4 when $n = 4$, and one more graph C_5 when $n = 5$; and the extremal graph with minimal Harary index is uniquely $C_3((n-3)^1)$. In $\mathcal{B}(n)$, the maximal Harary index is attained at $B_n^{(1)}$ or $B_n^{(2)}$, with an exceptional graph B_6' when $n = 6$, and the minimal Harary index is uniquely attained at $B_n^{(0)}$.

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