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Minimal Harary index of unicyclic graphs with diameter at most 4

Lihua Feng[a], Ziyuan Li[a], Weijun Liu[a], Lu Lu[a,*], Dragan Stevanović[a,b]

[a] School of Mathematics and Statistics, Central South University, Changsha 410083, China
[b] Mathematical Institute, Serbian Academy of Science and Arts, Kneza Mihaila 36, Belgrade 11000, Serbia

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A B S T R A C T

The Harary index of a graph G is defined as $H(G)=\sum_{\{u,v\}\subseteq V(G)}\frac{1}{d_G(u,v)}$, where $d_G(u, v)$ is the distance between the vertices u and v. In this paper, we respectively determine the minimal Harary index among all unicyclic graphs with diameter 3 and all unicyclic graphs with diameter 4.

1. Introduction

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The *distance* of two vertices $u, v \in V(G)$ is the length of a shortest path from u to v, denoted by $d_G(u, v)$. The *neighborhood* $N_G(v)$ of the vertex $v \in V(G)$ is the set of vertices having distance 1 between v, that is, $N_G(v)=\{u\in V(G)\mid d_G(u,v)=1\}$. The cardinality of $N_G(v)$ is the *degree* of v, denoted by $d_G(v)=|N_G(v)|$. For a pair of vertices $u, v \in V(G)$ with $uv\notin E(G)$, denote by $G+uv$ the graph obtained from G by adding an edge connecting u and v. We always use $P(u)$ to denote the set of pendent vertices adjacent to u. If there is no confusion aroused, we alway delete the subscript G in the notions like $d_G(v)$.

In the fields of chemical graph theory, molecular topology and mathematical chemstry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound [26]. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariants. There are various topological indices based on various parameters of the graph, such as the Hosoya index [10], the Wiener polarity index [21,22], the Randić index [17,25], the Balaban index [1] and so on. As one of the oldest and most popular topological indices, the *Wiener index* of a graph G is defined as

$$W(G)=\sum_{\{u,v\}\in V(G)} d_G(u,v),$$

which has been studied adequately and many elegant results are obtained [6,9,24,27].

* Corresponding author.
E-mail address: lulugdmath@163.com (L. Lu).

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Because of the success in investigating the Wiener index, many other topological indices of chemical graphs, based on the distances of the graph, have been developed. As one of them, the *Harary index* of a graph G is defined as

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

which was introduced by Plavšić et al. [23] and by Ivanciuc et al. [11] independently in 1993. It can be viewed as the "reciprocal analogue" of the Wiener index. As the Wiener index $W(G)$ is just the half-sum of the distance matrix of G, it is natural to construct a matrix such that $H(G)$ is the half-sum of this matrix. Such matrix is the so-called *reciprocal distance matrix* (also called the Harary matrix [15]), which is defined as $H=(h_{u,v})_{n\times n}$ where $h_{uv}=\frac{1}{d_G(u,v)}$. The Harary index and its related molecular descriptors as well as various modifications have shown somewhat success in structure property correlations [3–5,12,19,20]. Recently, it is found that the Harary index has a number of interesting chemical physics properties [13].

The upper and lower bounds and the corresponding extremal graphs of topological indices are very important in studying them. Gutman [9] showed that the path and the star are respectively the graphs with minimal and maximal Harary index among all trees. In [2,7,30,33], the authors presented several upper and lower bounds for the Harary index of connected graphs, triangle-free, quadrangle-free graphs, graphs with given diameter, matching number. Ilić et al. [14] investigated the Harary index of trees with various parameters. There are also many results concerning the Harary index of graph classes with several constraints, like connectivity [16], trees with given degree sequence [28], unicyclic graphs [31], bicyclic graphs [32], the ordering [29]. Other results related to distance and its invariants, one can see [18]. One may find that there are so many results on upper bound of Harary index but there are few results on lower bound of Harary index. In fact, to determine the lower bound of Harary index and find the extremal graph is much more complex. Recently, Feng et al. [8] investigated the minimal Harary index of trees with small diameters. It is natural to consider the unicyclic graphs with small diameters. Since there is only one unicyclic graph of order greater than 5 with diameter 2, which is obtained from $K_{1,n-1}$ by adding an edge connecting two pendent vertices, we start the investigation from the unicyclic graphs with diameter 3. In this paper, we determine the graphs minimizing the Harary index among unicyclic graphs with diameter 3 and 4, respectively.

2. Preliminaries

In this part, we will present some old and new results which will be used latter. Firstly, we recall the graphs that minimize the Harary index among trees with diameter 3 and 4, respectively. For a graph G and two vertices $u,\ v\in V(G)$, let $G(u,\ a;\ v,\ b)$ be the graph obtained from G by attaching a pendent vertices to u and b pendent vertices to v. For a graph G and $v\in V(G)$, throughout this paper, we would like to denote by $P(v)$ the set of pendent vertices adjacent to v. A automorphism f of a graph G is a bijection $f\colon V(G)\to V(G)$ such that $u\sim v$ if and only if $f(u)\sim f(v)$. The set of all automorphisms of G forms the automorphism group of G, denoted by $\mathrm{Aut}(G)$. By observations, the following result is obtained.

Lemma 1. *Let G be a connected graph and let $u,\ v\in V(G)$ be two vertices such that there exists $\sigma\in\mathrm{Aut}(G)$ satisfying $\sigma(u)=v$. For a positive integer t, it holds that $H(G(u,\ a;\ v,\ b))\geq H(G(u,\ \lfloor t/2\rfloor;\ v,\ \lceil t/2\rceil))$ for any $a+b=t$, where the equality holds if and only if $\{a,b\}=\{\lfloor t/2\rfloor,\lceil t/2\rceil\}$.*

Proof. Without loss of generality, assume that $a\leq b$ in $G(u,\ a;\ v,\ b)$. It suffices to show that $H(G(u,a;v,b))>H(G(u,a+1;v,b-1))$ whenever $b-a\geq 2$. By calculations, we have

$$\begin{cases} H(G(u,a;v,b))=H(G)+a\sum\limits_{x\in V(G)}\dfrac{1}{d_G(u,x)+1}+b\sum\limits_{x\in V(G)}\dfrac{1}{d_G(v,x)+1}\\ \qquad +\dfrac{1}{2}\left(\binom{a}{2}+\binom{b}{2}\right)+\dfrac{ab}{d_G(u,v)+2},\\ H(G(u,a+1;v,b-1))=H(G)+(a+1)\sum\limits_{x\in V(G)}\dfrac{1}{d_G(u,x)+1}+(b-1)\sum\limits_{x\in V(G)}\dfrac{1}{d_G(v,x)+1}\\ \qquad +\dfrac{1}{2}\left(\binom{a+1}{2}+\binom{b-1}{2}\right)+\dfrac{(a+1)(b-1)}{d_G(u,v)+2}. \end{cases}$$

It leads to that

$$\begin{aligned} &H(G(u,a;v,b))-H(G(u,a+1;v,b-1))\\ =\ &\sum_{x\in V(G)}\frac{1}{d_G(v,x)+1}-\sum_{x\in V(G)}\frac{1}{d_G(u,x)+1}+\frac{d_G(u,v)(b-a-1)}{2(d_G(u,v)+2)}. \end{aligned}$$

Since $\sigma(u)=v,$ we have

$$\begin{aligned} &\sum_{x\in V(G)}\frac{1}{d_G(v,x)+1}=\sum_{x\in V(G)}\frac{1}{d_G(v,\sigma(x))+1}\\ =\ &\sum_{x\in V(G)}\frac{1}{d_G(\sigma(u),\sigma(x))+1}=\sum_{x\in V(G)}\frac{1}{d_G(u,x)+1}. \end{aligned}$$

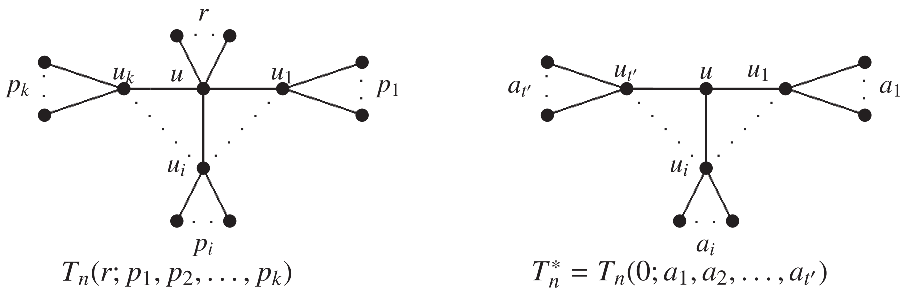

Fig. 1. Trees with diameter 4.

Thus, $H(G(u, a; v, b)) - H(G(u, a+1; v, b-1)) = \dfrac{d_G(u, v)(b-a-1)}{2(d_G(u, v)+2)} > 0$ whenever $b - a \geq 2$. The result follows. □

Clearly, the double star $S(a, b)$, which is obtained from two stars $K_{1,a}$ and $K_{1,b}$ by adding an edge connecting their non-pendent vertex, is the only tree with diameter three on $n = a + b + 2$ vertices. Note that $S(a, b) = K_2(u, a; v, b)$ if the two endpoints of K_2 are u and v. Therefore, the following result follows from Lemma 1 immediately.

Lemma 2. *For any positive integer $n \geq 4$, it holds that*

$$H(S(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)) \leq H(S(a, b)),$$

where the equality holds if and only if $S(a, b) = S(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)$.

It is clear that any tree on n vertices with diameter 4 has the form shown in the left side of Fig. 1 and denoted by $T_n(r; p_1, p_2, \dots, p_k)$. The vertex u is called the center, the non-pendent vertices $u_1, u_2, \dots, u_k$ adjacent to u are called pseu-centers. Therefore, $|P(u)| = r$, $|P(u_i)| = p_i$ and $n = r + 1 + k + \sum_{i=1}^{k} p_i$. Feng et al. [8] proved that the graph with minimal Harary index among all trees on n vertices with diameter 4 is the graph $T(0; p_1, p_2, \dots, p_{k(n)})$ with $p_1, p_2, \dots, p_{k(n)}$ being almost equal where $k(n)$ is uniquely determined by n.

Theorem 1 (Feng et al.[8]). *For any tree $T = T_n(r; p_1, p_2, \dots, p_k)$ on $n = r + 1 + k + \sum_{i=1}^{k} p_i$ vertices with diameter 4, it holds that*

$$H(T) \geq \min\{H(T_n(0; a_1, a_2, \dots, a_t)) \mid k_0 - 1 \leq t \leq k_0\},$$

where k_0 is the largest root of cubic equation $2x^3 + x^2(2n-3) - 3(n-1)^2 = 0$ and $k_0 \in \left[\sqrt{\frac{4n}{3}}, \sqrt{\frac{3n}{2}}\right]$, and $|a_i - a_j| \leq 1$ for any i, j.

Throughout this paper, we always use $T_n^* = T(0; a_1, a_2, \dots, a_{k(n)})$ to denote the tree minimizing the Harary index among all trees on n vertices with diameter 4.

To end up this part, we give the following basic but useful result.

Lemma 3. *If $G' = G + uv$ for a connected graph G and $uv \notin E(G)$, then it holds that*

$$H(G') \geq H(G) + 1/2,$$

where the equality holds if and only if u and v are pendent vertices sharing the same neighbor.

Proof. It is clear that $d_{G'}(x, y) \leq d_G(x, y)$ for any pair of vertices $\{x, y\} \in V(G)$. Note that $d_G(u, v) \geq 2$ and $d_{G'}(u, v) = 1$. It follows that

$$\begin{aligned} H(G') &= \textstyle\sum_{\{x,y\} \in V(G), \{x,y\} \neq \{u,v\}} \frac{1}{d_{G'}(x, y)} + \frac{1}{d_{G'}(u, v)} \\ &\geq \textstyle\sum_{\{x,y\} \in V(G), \{x,y\} \neq \{u,v\}} \frac{1}{d_G(x, y)} + 1 \\ &\geq \textstyle\sum_{\{x,y\} \in V(G), \{x,y\} \neq \{u,v\}} \frac{1}{d_G(x, y)} + \frac{1}{d_G(u, v)} + \frac{1}{2} \\ &= H(G) + \frac{1}{2}. \end{aligned}$$

Clearly, $H(G') = H(G) + \frac{1}{2}$ if and only if all the inequalities above are equalities. That is, $d_{G'}(x, y) = d_G(x, y)$ for any $\{x, y\} \neq \{u, v\}$ and $d_G(u, v) = 2$. It means that u, v are two pendent vertices sharing the same neighbor. □

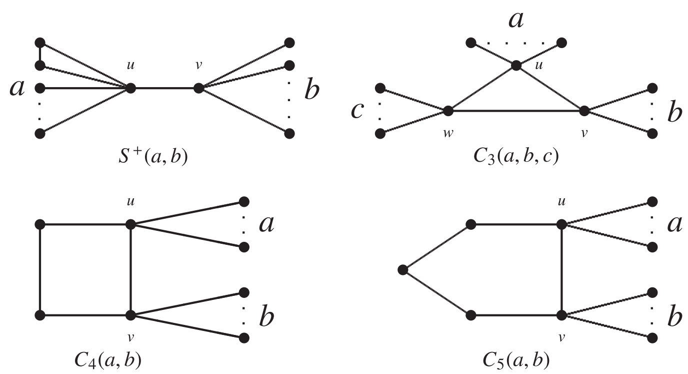

Fig. 2. Unicyclic graphs with diameter 3.

3. Unicyclic graphs with diameter 3

In this part, we will determine the graph minimizing the Harary index among all unicyclic graphs with diameter 3. Denote by $\mathcal{C}_n^3$ be the set of unicyclic graphs on n vertices with diameter 3. By observations, each graph in $\mathcal{C}_n^3$ must have one of the forms shown in Fig. 2. The graph $S^+(a,b)$ is obtained from $S(a, b)$ by adding an edge in $P(u)$; the graph $C_3(a, b, c)$ is obtained from C_3 by attaching a pendent vertices to u, b pendent vertices to v and c pendent vertices to w; the graphs $C_4(a, b)$ and $C_5(a, b)$ are respectively obtained from C_4 and C_5 by attaching a pendent vertices to u and b pendent vertices to v for two adjacent vertices u and v in C_4 and C_5. To insure the diameter to be 3, the graphs in Fig. 2 should satisfy the following conditions.

- The graph $S^+(a,b)$ should satisfy that both a and b are non-zero.
- The graph $C_3(a, b, c)$ should satisfy that at least two of a, b and c are non-zero.
- The graph $C_4(a, b)$ and $C_5(a, b)$ should satisfy that at least one of a and b is non-zero.

To find the graph minimizing the Haray index among $\mathcal{C}_n^3$, we should investigate all the four types of unicyclic graphs above. We first consider the graph $S^+(a,b)$.

Lemma 4. *For a positive integer $n \geq 5$ and two integers a, b satisfying $a+b=n-2$, it holds that*

$$H(S^+(a,b)) \geq H(S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)),$$

where the equality holds if and only if $\{a,b\} = \{\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil\}$.

Proof. Since $G = S^+(a,b)$ is obtained from $S(a, b)$ by adding an edge connecting two pendent vertices with a common neighbor, Lemmas 3 and 2 indicate that

$$\begin{aligned} H(G) &= H(S(a,b)) + 1/2 \geq H(S(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)) + 1/2 \\ &= H(S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)) \\ &= H(S^+(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)), \end{aligned}$$

where the equality holds if and only if $\{a,b\} = \{\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil\}$. The result follows. □

Since $S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)$ is obtained from $S(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)$ by adding an edge connecting two pendent vertices with a common neighbor, Lemma 3 implies that

$$\begin{aligned} &H(S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)) = H(S(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)) + 1/2 \\ = &\begin{cases} \frac{5}{24}n^2 + \frac{5}{12}n - \frac{1}{6} & \text{if } n \text{ is even,} \\ \frac{5}{24}n^2 + \frac{5}{12}n - \frac{1}{8} & \text{if } n \text{ is odd.} \end{cases} \end{aligned} \tag{1}$$

Next we consider the graph $C_4(a, b)$.

Lemma 5. *If $G = C_4(a,b)$ with $n = a+b+4 \geq 5$, then $H(G) > H(S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil))$.*

Proof. Since G is obtained from $S(a+1, b+1)$ by adding an edge connecting two pendent vertices with distinct neighbors, Lemmas 3 and 2 indicate that

$$\begin{aligned} H(G) &> H(S(a+1,b+1)) + 1/2 \geq H(S(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)) + 1/2 \\ &= H(S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)). \end{aligned}$$

It yeilds the result. □

In what follows, we consider the graph $C_3(a, b, c)$. Let $C_3^*(n) = C_3(p_1, p_2, p_3)$ with $p_1 \leq p_2 \leq p_3$, $p_1 + p_2 + p_3 = n - 3$ and $p_3 - p_1 \leq 1$. From Lemma 1, we get the following result.

Lemma 6. *For a positive integer $n \geq 5$ and three non-negative integers a, b, c satisfying $a + b + c = n - 3$, it holds that*

$$H(C_3(a, b, c)) \geq H(C_3^*(n)),$$

where the equality holds if and only if $C_3(a, b, c) = C_3^*(n)$.

Proof. Let $C_3(p_1, p_2, p_3)$ be the graph minimizing the Harary index among the graph set $\{C_3(a, b, c) \mid a + b + c = n - 3\}$. Without loss of generality, assume that $p_1 \leq p_2 \leq p_3$. It suffices to show that $p_3 - p_1 \leq 1$. Suppose to the contrary that $p_3 - p_1 \geq 2$. Let G' be the graph obtained from the triangle $K_3 = uvw$ by attaching p_2 pendent vertices to v. Therefore, $C_3(p_1, p_2, p_3) = G'(u, p_1; w, p_3)$. Let $\sigma: V(G') \to V(G')$ be the map defined by $\sigma(u) = w$, $\sigma(w) = u$ and $\sigma(x) = x$ for $x \notin \{u, w\}$. It is easy to see that $\sigma \in \mathrm{Aut}(G')$. Therefore, Lemma 1 indicates that

$$H(C_3(p_1, p_2, p_3)) = H(G'(u, p_1; w, p_3)) > H(G'(u, \lfloor (p_1 + p_3)/2 \rfloor; w, \lceil (p_1 + p_3)/2 \rceil)),$$

a contradiction. □

By immediate calculations, we have

$$H(C_3^*(n)) = \begin{cases} \frac{7}{36}n^2 + \frac{7}{12}n - \frac{1}{2} & \text{if } n \equiv 0 \pmod 3, \\ \frac{7}{36}n^2 + \frac{7}{12}n - \frac{4}{9} & \text{if } n \not\equiv 0 \pmod 3. \end{cases} \tag{2}$$

At last, we consider the graph $C_5(a, b)$. The following result is immediate from Lemma 1, and we present it without proof.

Lemma 7. *For a positive integer $n \geq 6$ and two integers a, b satisfying $a + b = n - 5$, it holds that*

$$H(C_5(a, b)) \geq H(C_5(\lfloor (n-5)/2 \rfloor, \lceil (n-5)/2 \rceil)),$$

where the equality holds if and only if $\{a, b\} = \{\lfloor (n-5)/2 \rfloor, \lceil (n-5)/2 \rceil\}$.

By immediate calculations, we have

$$H(C_5(\lfloor (n-5)/2 \rfloor, \lceil (n-5)/2 \rceil)) = \begin{cases} \frac{5}{24}n^2 + \frac{n}{3} + \frac{2}{3} & \text{if } n \text{ is even}, \\ \frac{5}{24}n^2 + \frac{n}{3} + \frac{5}{8} & \text{if } n \text{ is odd}. \end{cases} \tag{3}$$

Now we are in the position to give the main result of this part.

Theorem 2. *Let $\mathcal{C}_n^3$ be the set of unicyclic graphs on n vertices with diameter 3 and $G \in \mathcal{C}_n^3$. Then the followings hold.*

(i) *If $5 \leq n \leq 8$ then*

$$H(G) \geq \begin{cases} \frac{5}{24}n^2 + \frac{5}{12}n - \frac{1}{6} & \text{if } n \text{ is even}, \\ \frac{5}{24}n^2 + \frac{5}{12}n - \frac{1}{8} & \text{if } n \text{ is odd}, \end{cases}$$

with equality if and only if $G \cong S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)$.

(ii) *If $n = 9$ then $H(G) \geq 20.5$ with equality if and only if $G \in \{S^+(3, 4), C_3^*(9), C_5(2, 2)\}$.*

(iii) *If $n = 10$ then $H(G) \geq 149/6$ with equality if and only if $G \in \{S^+(4, 4), C_3^*(10), C_5(2, 3)\}$.*

(iv) *If $n = 11$ then $H(G) \geq 29.5$ with equality if and only if $G \in \{C_3^*(11), C_5(3, 3)\}$.*

(v) *If $n \geq 12$ then*

$$H(G) \geq \begin{cases} \frac{7}{36}n^2 + \frac{7}{12}n - \frac{1}{2} & \text{if } n \equiv 0 \pmod 3, \\ \frac{7}{36}n^2 + \frac{7}{12}n - \frac{4}{9} & \text{if } n \not\equiv 0 \pmod 3, \end{cases}$$

with equality if and only if $G \cong C_3^*(n)$.

Proof. Let G_0 be the graph minimize the Harary index among $\mathcal{C}_n^3$. Lemmas 4–7 imply that $G_0 \in \{S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil), C_3^*(n), C_5(\lfloor (n-5)/2 \rfloor, \lceil (n-5)/2 \rceil)\}$. In what follows, we campare $H(S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil))$, $H(C_3^*(n))$ and $H(C_5(\lfloor (n-5)/2 \rfloor, \lceil (n-5)/2 \rceil))$ according to Eqs. (1)–(3).

Note that, for even n, $\frac{5}{24}n^2 + \frac{5}{12}n - 1/6 \geq \frac{5}{24}n^2 + \frac{n}{3} + \frac{2}{3}$ if and only if $n \geq 10$, and for odd n, $\frac{5}{24}n^2 + \frac{5}{12}n - 1/8 \geq \frac{5}{24}n^2 + \frac{n}{3} + \frac{5}{8}$ if and only if $n \geq 9$. Therefore, Eqs. (1) and (3) imply that $H(S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)) < H(C_5(\lfloor (n-5)/2 \rfloor, \lceil (n-5)/2 \rceil))$ if $n \leq 8$, and $H(S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)) > H(C_5(\lfloor (n-5)/2 \rfloor, \lceil (n-5)/2 \rceil))$ if $n \geq 11$.

If $n \leq 8$, we have $\frac{5}{24}n^2 + \frac{5}{12}n - 1/8 < \frac{7}{36}n^2 + \frac{7}{12}n - 1/2$. Therefore, Eqs. (1) and (2) indicate that $H(S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)) < H(C_3^*(n))$, and thus $G_0 \cong S^+(\lfloor (n-2)/2 \rfloor, \lceil (n-2)/2 \rceil)$. The statement (i) is obtained.

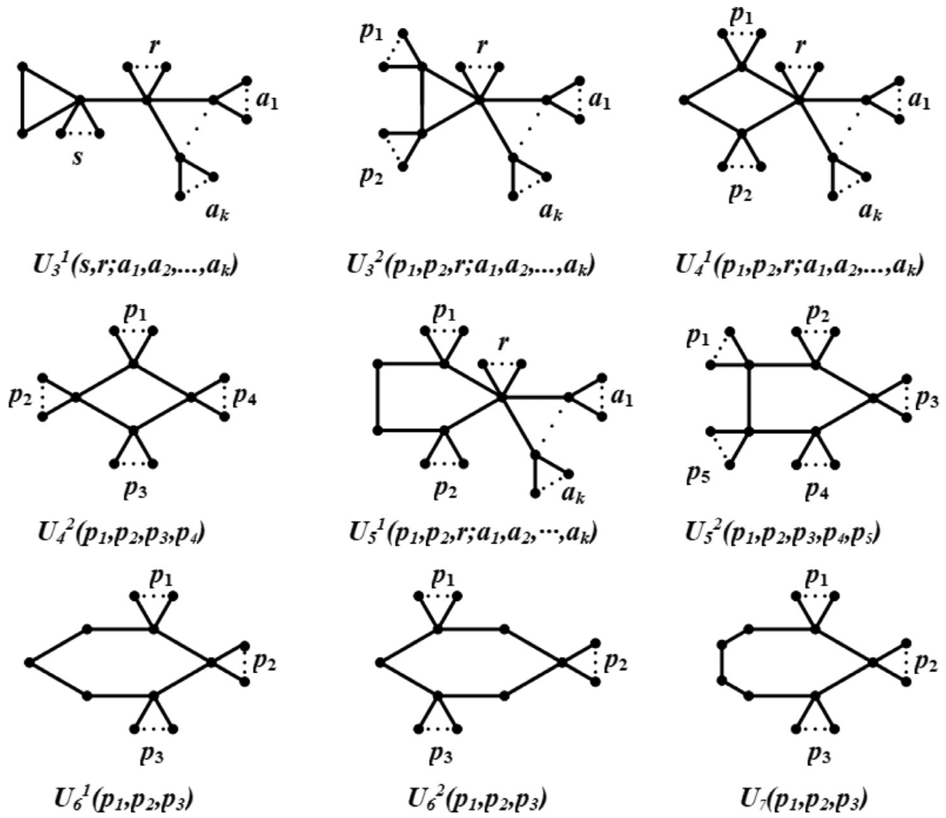

Fig. 3. Unicyclic graphs with diameter 4..

If $n \geq 12$, we have $\frac{5}{24}n^2 + \frac{n}{3} + \frac{5}{8} > \frac{7}{36}n^2 + \frac{7}{12}n - 4/9$. Therefore, Eqs. (2) and (3) mean that $H(C_3^*(n)) < H(C_5(\lfloor (n-5)/2 \rfloor, \lceil (n-5)/2 \rceil))$. The statement (v) is obtained.

If $9 \leq n \leq 11$, we obtain the statements (ii) (iii) and (iv) by immediate calculations.

This completes the proof. □

4. Unicyclic graphs with diameter 4

Denote by $\mathcal{U}_n^4$ the set of unicyclic graphs on n vertices with diameter 4. By simple observations, every graph in $\mathcal{U}_n^4$ has one of the forms shown in Fig. 3. Note that, in the graphs in Fig. 3, we say $a_i = 0$ means that the corresponding structure is vanished. In detail, the graph $U_3^1(s, r; a_1, 0)$ is obtained from $U_3^1(s, r; a_1, a_2)$ by deleting the corresponding a_2 pendent vertices and their common neighbor. Usually, we do not write such zeros in the notions. For example, we write $U_3^1(s, r; 1, 2)$ for $U_3^1(s, r; 1, 2, 0, 0)$ though they represent the same graph. However, if $a_1 = a_2 = \ldots = a_k = 0$ then we remain one 0 in the notions. For example, we write $U_3^1(s, r; 0)$ for $U_3^1(s, r;)$. To ensure the diameter to be 4, the parameters of the graphs given in Fig. 3 should satisfy some conditions.

- The graph $U_3^1(s, r; a_1, a_2, \ldots, a_k)$ satisfies that there exists $i \in \{1, 2, \ldots, k\}$ such that $a_i \geq 1$.
- The graph $U_3^2(p_1, p_2, r; a_1, a_2, \ldots, a_k)$ satisfies one of the followings: (1) at least one of p_1 and p_2 is not zero and there exists $i \in \{1, 2, \ldots, k\}$ such that $a_i \geq 1$; (2) $p_1 = p_2 = 0$ and there exists $\{i, j\} \in \{1, 2, \ldots, k\}$ such that $a_i, a_j \geq 1$.
- The graph $U_4^1(p_1, p_2, r; a_1, a_2, \ldots, a_k)$ satisfies that there exists $i \in \{1, 2, \ldots, k\}$ such that $a_i \geq 1$ when $p_1 = p_2 = 0$.
- The graph $U_4^2(p_1, p_2, p_3, p_4)$ satisfies $p_1p_3 \neq 0$ or $p_2p_4 \neq 0$.
- The graph $U_5^1(p_1, p_2, r; a_1, a_2, \ldots, a_k)$ satisfies that there exists $i \in \{1, 2, \ldots, k\}$ such that $a_i \geq 1$ when $p_1 = p_2 = 0$.
- The graph $U_5^2(p_1, p_2, \ldots, p_5)$ satisfies one of the conditions: $p_1p_3 \neq 0$, $p_1p_4 \neq 0$, $p_2p_4 \neq 0$, $p_2p_5 \neq 0$ and $p_3p_5 \neq 0$.
- The graphs $U_6^1(p_1, p_2, p_3)$, $U_6^2(p_1, p_2, p_3)$ and $U_7(p_1, p_2, p_3)$ satisfy that there exists $i \in \{1, 2, 3\}$ such that $p_i \geq 1$.

Recall that $T_n^* = T_n(0; a_1, \ldots, a_{k(n)})$ is the unique tree minimize the Harary index among all trees on n vertices with diameter 4. Assume that u is the center of T_n^* and $u_1, u_2, \ldots, u_{k(n)}$ are pseu-centers of T_n^*. For each $1 \leq i \leq k(n)$, denote by $T_n^*(i, +)$ the graph obtained from T_n^* by adding an edge in $P(u_i)$, where $P(u_i)$ is the set of pendent vertices adjacent to u_i. Lemma 3 implies that $H(T_n^*(i, +)) = H(T_n^*) + \frac{1}{2}$ for any $1 \leq i \leq k(n)$. This fact will be used frequently. Now we are ready to present the main result of this part.

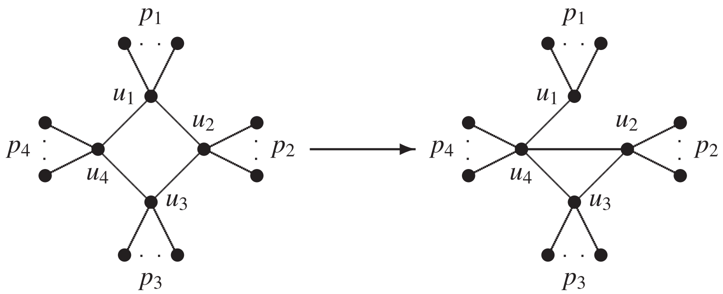

Fig. 4. The figure used in Lemma 10.

Theorem 3. *If $G \in \mathcal{U}_n^4$, then $H(G) \geq H(T_n^*(i,+))$ for $1 \leq i \leq k(n)$ with equality if and only if $G = T_n^*(j,+)$ for some $1 \leq j \leq k(n)$.*

To prove this result, we need to consider all the nine forms of unicyclic graphs shown in Fig. 3. For convenience, we write such as U_3^1 for $U_3^1(s, r; a_1, a_2, \ldots, a_k)$ when it does not arouse confusion.

Lemma 8. *If $G \in \mathcal{U}_n^4$ has the form of U_3^1, then $H(G) \geq H(T_n^*(i,+))$ for $1 \leq i \leq k(n)$ with equality if and only if $G = T_n^*(j,+)$ for some $1 \leq j \leq k(n)$.*

Proof. Assume that $G = U_3^1(s, r; a_1, a_2, \ldots, a_k)$ with $n = s + 3 + r + 1 + \sum_{i=1}^{k}(a_i + 1)$. Let $T = T_n(r; a_1, a_2, \ldots, a_k, s + 2)$ be the tree with center u and pseu-centers $u_1, u_2, \ldots, u_k, u_{k+1}$. It means that $d_T(u_i) = a_i + 1$ for $1 \leq i \leq k$ and $d_T(u_{k+1}) = s + 3$. For two vertices $v_1, v_2 \in P(u_{k+1})$, we have $G = T + v_1v_2$. Lemma 3 implies that $H(G) \geq H(T) + \frac{1}{2}$. Thus, we have

$$H(G) \geq H(T) + \frac{1}{2} \geq H(T_n^*) + \frac{1}{2} = H(T_n^*(i,+)).$$

It is clear that $H(G) = H(T_n^*(i,+))$ if and only if $T = T_n^*$ and v_1, v_2 are two pendent vertices sharing the same neighbor. It follows the result. □

Lemma 9. *If $G \in \mathcal{U}_n^4$ has the form of U_3^2, U_4^1 or U_5^1, then $H(G) > H(T_n^*(i,+))$.*

Proof. Assume that $G = U_3^2(p_1, p_2, r; a_1, a_2, \ldots, a_k)$ with $n = p_1 + 1 + p_2 + 1 + r + 1 + \sum_{i=1}^{k}(a_i + 1)$. Let $T = T_n(r; a_1, a_2, \ldots, a_k, p_2, p_1)$ be the tree with center u and pseu-centers $u_1, u_2, \ldots, u_k, u_{k+1}, u_{k+2}$. It means that $d_T(u_i) = a_i + 1$ for $1 \leq i \leq k$, $d_T(u_{k+1}) = p_2 + 1$ and $d_T(u_{k+2}) = p_1 + 1$. It is clear that $G = T + u_{k+1}u_{k+2}$. Lemma 3 indicates that

$$H(G) \geq H(T) + \frac{1}{2} \geq H(T_n^*) + \frac{1}{2} = H(T_n^*(i,+)).$$

Since u_{k+1} and u_{k+2} are not pendent vertices, the first inequality is strict. It follows that $H(G) > H(T_n^*(i,+))$.

Assume that $G = U_4^1(p_1, p_2, r; a_1, a_2, \ldots, a_k)$. Let $T = T_n(r; a_1, a_2, \ldots, a_k, p_2, p_1 + 1)$ be the tree with center u and pseu-centers $u_1, u_2, \ldots, u_k, u_{k+1}, u_{k+2}$. It is clear that $G = T + u_{k+1}v$ where $v \in P(u_{k+2})$. Lemma 3 indicates that

$$H(G) \geq H(T) + \frac{1}{2} \geq H(T_n^*) + \frac{1}{2} = H(T_n^*(i,+)).$$

Since u_{k+1} is not a pendent vertex, the first inequality is strict. It follows that $H(G) > H(T_n^*(i,+))$.

Similarly, if G has the form of U_5^1, we also have $H(G) > H(T_n^*(i,+))$. This completes the result. □

Lemma 10. *If $G \in \mathcal{U}_n^4$ has the form of U_4^2, then $H(G) > H(T_n^*(i,+))$.*

Proof. Assume that $G = U_4^2(p_1, p_2, p_3, p_4)$ with $n = p_1 + p_2 + p_3 + p_4 + 4$. Without loss of generality, assume that $p_1 \geq p_4$. It is clear that the graph $G' = U_3^2(p_3, p_2, p_4; p_1)$ can be obtained from G by deleting the edge u_1u_2 and adding the edge u_2u_4 (see Fig. 4). By immediate calculation, we have

$$\begin{cases} H(G) = n + \dfrac{1}{2}\left(\binom{p_1}{2} + \binom{p_2}{2} + \binom{p_3}{2} + \binom{p_4}{2} + 2p_1 + 2p_2 + 2p_3 + 2p_4 + 2\right) \\ \qquad + \dfrac{1}{3}(p_1p_2 + p_2p_3 + p_3p_4 + p_4p_1 + p_1 + p_2 + p_3 + p_4) + \dfrac{1}{4}(p_1p_3 + p_2p_4), \\ H(G') = n + \dfrac{1}{2}\left(\binom{p_1}{2} + \binom{p_2}{2} + \binom{p_3}{2} + \binom{p_4}{2} + p_1 + 2p_2 + 2p_3 + 3p_4 + 2\right) \\ \qquad + \dfrac{1}{3}(p_1p_4 + 2p_1 + p_4p_2 + p_4p_3 + p_3p_2 + p_3 + p_2) + \dfrac{1}{4}(p_1p_3 + p_1p_2). \end{cases}$$

It leads to that $H(G) - H(G') = \frac{(p_2+2)(p_1-p_4)}{12} \geq 0$, and thus $H(G) \geq H(G')$. Note that $H(G') > H(T_n^*(i,+))$ in view of Lemma 9. We have $H(G) > H(T_n^*(i,+))$. It completes the proof. □

Table 1
The table used in Lemma 11.

	G	G'	$H(G)-H(G')$
$p_5 \geq 2,\ p_1, p_3 \geq 1$	$U_5^2(p_1, p_2, p_3, p_4, p_5)$	$U_5^1(p_2-1, p_4-1, 0; p_1, p_3, p_5-1)$	$\frac{p_1p_2+p_2p_3+p_3p_4+p_4p_5+p_5p_1+p_1+p_3+4p_5-13}{12} \geq 0$
$p_5 \geq 2,\ p_1 = 0,\ p_3 \neq 0$	$U_5^2(0, p_2, p_3, p_4, p_5)$	$U_5^1(p_2-1, p_4-1, 1; p_3, p_5-1)$	$\frac{p_2p_3+p_3p_4+p_4p_5+p_3+4p_5-13}{12} \geq 0$
$p_5 = 1,\ p_1, p_3 \geq 1$	$U_5^2(p_1, p_2, p_3, p_4, 1)$	$U_5^1(p_2-1, p_4-1, 1; p_1, p_3)$	$\frac{p_1p_2+p_2p_3+p_3p_4+2p_1+p_3+p_4-9}{12} \geq 0$
$p_5 = 1,\ p_1 = 0,\ p_3 \neq 0$	$U_5^2(0, p_2, p_3, p_4, 1)$	$U_5^1(p_2-1, p_4-1, 2; p_3)$	$\frac{p_2p_3+p_3p_4+p_3+p_4-9}{12} \geq 0$
$p_5 = 0,\ p_1, p_3 \geq 1$	$U_5^2(p_1, p_2, p_3, p_4, 0)$	$U_5^1(p_2-1, p_4-1, 0; p_1, p_3)$	$\frac{p_1p_2+p_2p_3+p_3p_4+2p_1+p_2+2p_3+p_4-5}{12} \geq 0$
$p_5 = 0,\ p_1 = 0,\ p_3 \neq 0$	$U_5^2(0, p_2, p_3, p_4, 0)$	$U_5^1(p_2-1, p_4-1, 1; p_3)$	$\frac{p_2p_3+p_3p_4+p_2+2p_3+p_4-5}{12} \geq 0$
$p_5 = 0,\ p_1 \neq 0,\ p_3 = 0$	$U_5^2(p_1, p_2, 0, p_4, 0)$	$U_5^1(p_2-1, p_4-1, 1; p_1)$	$\frac{p_1p_2+2p_1+p_2+p_4-5}{12} \geq 0$

Lemma 11. *If $G \in \mathcal{U}_n^4$ has the form of U_5^2, then $H(G) > H(T_n^*(i,+))$.*

Proof. Assume that $G = U_5^2(p_1, p_2, p_3, p_4, p_5)$ where $n = \sum_{i=1}^5 (p_i + 1)$. By calculations, one can verify that

$$
\begin{aligned}
H(G) = n &+ \frac{1}{2}\left(\binom{p_1}{2} + \binom{p_2}{2} + \binom{p_3}{2} + \binom{p_4}{2} + \binom{p_5}{2} + 2p_1 + 2p_2 + 2p_3 + 2p_4 + 2p_5 + 5\right) \\
&+ \frac{1}{3}(p_1p_2 + p_2p_3 + p_3p_4 + p_4p_5 + p_5p_1 + 2p_1 + 2p_2 + 2p_3 + 2p_4 + 2p_5) \\
&+ \frac{1}{4}(p_1p_3 + p_2p_4 + p_3p_5 + p_4p_1 + p_5p_2).
\end{aligned}
$$

Without loss of generality, assume that $p_2p_4 \neq 0$. We divide different cases to discuss according to the values of p_1, p_3 and p_5. For each case, we consider the corresponding graph G' listed in Table 1. It is easy to verify that $|V(G')| = |V(G)| = n$ for all cases. By calculations, we have $H(G) > H(G')$ for all cases (see Table 1). Note that $H(G') > H(T_n^*(i,+))$ for all cases in view of Lemma 9. We have $H(G) > H(T_n^*(i,+))$. It completes the proof. □

Remark 1. Because of the symmetry of p_2 and p_4, we only need to consider the cases in Table 1. For example, the case of $p_5 \geq 1$ and $p_1 = p_3 = 0$ is the same as $p_5 = 0$, $p_1 \geq 1$ and $p_3 = 0$ by exchanging the label of p_2 and p_4 and changing the other labels correspondingly.

Lemma 12. *If $G \in \mathcal{U}_n^4$ has the form of U_7, then $H(G) > H(T_n^*(i,+))$.*

Proof. Assume that $G = U_7(p_1, p_2, p_3)$ with $n = p_1 + p_2 + p_3 + 7$. We divide the following cases to discuss.

Case 1. $p_2 \geq 1$.

In this case we consider the graph $G' = U_5^1(p_1, p_3, 0; p_2 + 1)$ (see Fig. 5). Clearly, the order of G' is $p_1 + p_3 + p_2 + 1 + 1 + 5 = n$. By calculations, we have

$$
\begin{cases}
H(G) = n + \frac{1}{2}\left(\sum_{i=1}^{3}\left(\binom{p_i}{2} + 2p_i\right) + 7\right) + \frac{1}{3}\left(p_1p_2 + p_2p_3 + 2\sum_{i=1}^{3} p_i + 7\right) \\
\qquad + \frac{1}{4}\left(p_1p_3 + 2\sum_{i=1}^{3} p_i\right), \\
H(G') = n + \frac{1}{2}\left(\binom{p_1}{2} + \binom{p_2+1}{2} + \binom{p_3}{2} + 2p_1 + (p_2+1) + 2p_3 + 7\right) + \frac{1}{3}(2(p_2+1) + p_1 + 1 \\
\qquad + p_3 + 1 + 2p_3 + 2p_1) + \frac{1}{4}((p_1+1)(p_2+1) + (p_3+1)(p_2+1) + p_1p_3).
\end{cases}
$$

It leads to that $H(G) - H(G') = \dfrac{(p_2-1)(p_1+p_3)}{12} \geq 0$, and thus $H(G) \geq H(G')$. Note that $H(G') > H(T_n^*(i,+))$ in view of Lemma 9. We have $H(G) > H(T_n^*(i,+))$.

Case 2. $p_2 = 0$.

In this case, without loss of generality, assume that $p_1 \geq p_3$. We consider the graph $G'' = U_7(p_1 - 1, 1, p_3)$ (see Fig. 5). Therefore, we have

$$H(G) - H(G'') = \frac{p_1 - 1}{6} - \frac{p_3}{12} = \frac{(p_1 - p_3) + (p_1 - 2)}{12} \geq 0.$$

It means that $H(G) \geq H(G'')$. Since Case 1 implies that $H(G'') > H(T_n^*(i,+))$, we have $H(G) > H(T_n^*(i,+))$.

This completes the proof. □

Lemma 13. *If $G \in \mathcal{U}_n^4$ has the form of U_6^1, then $H(G) > H(T_n^*(i,+))$.*

Proof. Assume that $G = U_6^1(p_1, p_2, p_3)$ with $n = p_1 + p_2 + p_3 + 6$. Without loss of generality, assume that $p_1 \geq p_3$. If $p_1 \geq 1$ then we consider the graph $G' = U_7(p_1 - 1, p_2, p_3)$ (see Fig. 6). By calculations, one can obtain that

$$H(G) - H(G') = \frac{3p_1 + p_2 - 2}{12} > 0.$$

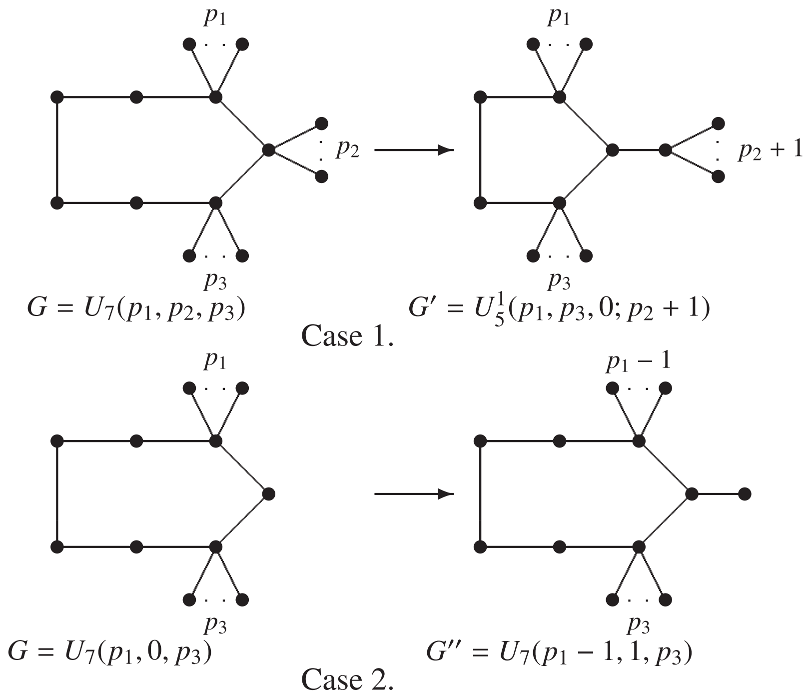

Fig. 5. The graphs used in Lemma 12.

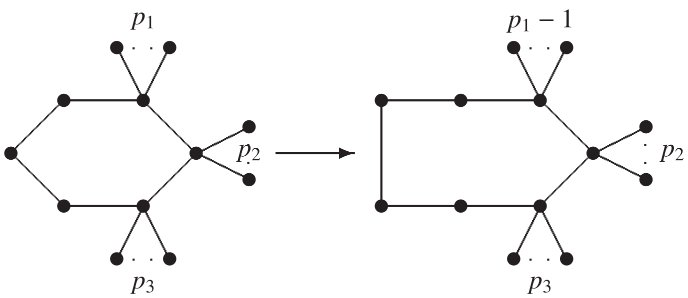

Fig. 6. The graphs used in Lemma 13.

Therefore, $H(G) > H(G')$. Note that $H(G') > H(T_n^*(i,+))$ in view of Lemma 11. We have $H(G) > H(T_n^*(i,+))$. If $p_1 = 0$ then $p_2 \geq 1$. We consider the graph $G'' = U_7(0, p_2 - 1, p_3)$. Similarly, we also have $H(G) > H(G'') > H(T_n^*(i,+))$. $\square$

Lemma 14. *If $G \in \mathcal{U}_n^4$ has the form of U_6^2, then $H(G) > H(T_n^*(i,+))$.*

Proof. Assume that $G = U_6^2(p_1, p_2, p_3)$ with $n = p_1 + p_2 + p_3 + 6$ and $p_1 \geq p_2 \geq p_3$. Let $G_0 = U_6^2(a_1, a_2, a_3)$ with $a_1 \geq a_2 \geq a_3$, $a_1 + a_2 + a_3 = n - 6$ be the unicyclic graph having form of U_6^2 with minimum Harary index. We first prove that $a_1 - a_3 \leq 1$. Suppose to the contrary that $a_1 - a_3 \geq 2$. We consider the graph $G' = U_6^2(a_1 - 1, a_2, a_3 + 1)$. By calculations, we have

$$H(G_0) - H(G') = \frac{a_1 - a_3 - 1}{4} > 0.$$

It means that $H(G_0) > H(G')$, a contradiction.

By calculations, we have

$$H(G_0) = \begin{cases} \dfrac{n^2}{6} + \dfrac{2n}{3}, & \text{if } n \equiv 0 \pmod 3 \\ \dfrac{n^2}{6} + \dfrac{2n}{3} + \dfrac{1}{12}, & \text{otherwise.} \end{cases}$$

We divide three cases to discuss according to the value of n. If $n \equiv 1 \pmod 3$ then we consider the graph $G'' = U_3^1(0, 0; \underbrace{2, \ldots, 2}_{(n-4)/3})$. Since G'' is obtained from $T(0; 2, 2, \ldots, 2)$ by adding an edge connecting two pendent vertices with the

Table 2
The table used in Lemma 14.

	G_0	G''	$H(G_0) - H(G'')$
$n \equiv 0 \pmod 3$	$U_6^2(a_1, a_2, a_3)$	$U_3^1(1, 0; 3, 2, \ldots, 2)$	$\frac{17n^2+73n}{108} + \frac{5}{27} \geq 0$
$n \equiv 1 \pmod 3$	$U_6^2(a_1, a_2, a_3)$	$U_3^1(0, 0; 2, \ldots, 2)$	$\frac{17n^2+77n}{108} - \frac{10}{27} \geq 0$
$n \equiv 2 \pmod 3$	$U_6^2(a_1, a_2, a_3)$	$U_3^1(1, 0; 2, \ldots, 2)$	$\frac{17n^2+69n}{108} + \frac{3}{4} \geq 0$

same neighbor, Lemma 3 implies that

$$H(G'') = H(T(0; 2, \ldots, 2)) + 1/2 = \frac{17n^2 + 77n}{108} - \frac{10}{27}.$$

Therefore, $H(G) \geq H(G_0) > H(G'') \geq H(T_n^*(i, +))$. If $n \equiv 0$ or $2 \pmod 3$, we consider the graph $G'' = U_3^1(1, 0; 3, \underbrace{2, \ldots, 2}_{(n-9)/3})$ and $G'' = U_3^1(1, 0; \underbrace{2, \ldots, 2}_{(n-5)/3})$, respectively. One can similarly verify that $H(G) \geq H(G_0) > H(G'') \geq H(T_n^*(i, +))$ (see Table 2). It completes the proof. □

Now we are in the position to prove our main result.

Proof of Theorem 3.. Combining Lemmas 8–14, the result follows. □

From Theorems 2 and 3, we see that the graphs minimizing the Harary index among unicyclic graphs with diameter 3 and 4 do not have a similar form. It compels us to discuss all the forms of unicyclic graphs one by one. Since the unicyclic graphs with diameter 5 have many distinct forms, it will be very fussy to discuss all of the forms like what we do in this paper. Therefore, we look forward a more general and effective method to determine the lower bound of the Harary index.

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