Research Article

The Harary Index of All Unicyclic Graphs with Given Diameter

Bao-Hua Xing,1 Gui-Dong Yu1,2 Li-Xiang Wang,1 and Jinde Cao1,3

1School of Mathematics and Computation Sciences, Anqing Normal University, Anqing 246133, China
2Basic Department, Hefei Preschool Education College, Hefei 230013, China
3School of Mathematics, Southeast University, Nanjing 210096, China

Correspondence should be addressed to Jinde Cao; jdcao@seu.edu.cn

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The Harary index of a graph is the sum of reciprocals of distances between any two vertices in the graph. In this paper, we obtain the graphs with the maximum and second-maximum Harary indices among n-vertex unicyclic graphs with diameter d.

1. Introduction

In this paper, all graphs are simple, undirected, and connected. Denote by $E(G_1)$, $V(G_1)$ the edge set and vertex set of $G_1$, and $|E(G_1)|$, $|V(G_1)|$ the number of edges and vertices in $G_1$, respectively. Then $E(G_1) = |V(G_1)|$, the graph $G_1$ is called a unicyclic graph. Let $d(x)$ (or $d_G(x)$), $N_G(x)$ be the degree and the neighborhood of a vertex $x$ in $G_1$, respectively. When $d(x) = 1$, we call $x$ a pendant vertex. The distance between $x_1$ and $x_1$ ($x_1, x_2 \in V(G_1)$) is denoted by $d_{G_1}(x_1, x_2)$. The diameter $d$ of $G_1$ is $d = \max\{d_{G_1}(x_1, x_2) \mid x_1, x_2 \in V(G_1)\}$. The graph $G_1$ is $k$-partite if and only if $d_{G_1}(x_1, x_2) \geq k$. Let $P_k$ be a path of length $k$.

The Harary index of $G_1$ has been introduced independently in [2, 3]. Its calculation is as follows:

$$H(G_1) = \sum_{x_1, x_2 \in V(G_1)} \frac{1}{d_{G_1}(x_1, x_2)},$$

(1)

where $d_{G_1}(x_1, x_2)$ is defined above and the sum goes over all the pairs of vertices in $G_1$.

The set of $n$-vertex unicyclic graphs with diameter $d$ is denoted by $U_{n,d}$. The graph $\delta_{n,d}^1$ (see Figure 1) on $n$ vertices arisen from $P_d = v_1v_2 \cdots v_d$ by attaching $n - d - 2$ pendant edges to $v_{d/2}$ and adding a new vertex $v_{d+1}$ to be adjacent to $v_{d/2}$ and $v_{d/2+1}$.

The graph $\delta_{n,d}^2$ (see Figure 1) arisen from $P_d = v_1v_2 \cdots v_d$ by attaching $n - d - 2$ pendant edges to $v_{d/2}$ and adding a new vertex $v_{d+1}$ to be adjacent to $v_{d/2}$ and $v_{d/2+1}$.

The $n$-vertex graph arisen from $P_d = v_1v_2 \cdots v_d$ by attaching $n - d - 2$ pendant edges to $v_{d/2}$ and adding two new adjacent vertices $v_{d+1}$ and $v_{d+2}$ to be adjacent to $v_{d/2}$ and $v_{d/2+1}$, denoted by $\delta_{n,d}^{2a}$ (see Figure 2). So, if $d = 2$, the graph $\delta_{n,2}^{2a}$ arisen from $C_3$ by attaching $n - 3$ pendant edges to one vertex of $C_3$.

Note that $n$-vertex graph $\delta_{n,d}^1$ arisen from $P_d = v_1v_2 \cdots v_d$ by attaching $n - d - 3$ pendant edges to $v_{d/2}$ and one pendant edge to $v_{d/2+1}$ and adding a new vertex $v_{d+1}$ to be adjacent to $v_{d/2}$ and $v_{d/2+1}$. $\delta_{n,d}^{2a}$ arisen from $P_d = v_1v_2 \cdots v_d$ by attaching $n - d - 2$ pendant edges to $v_{d/2}$ and adding a new vertex $v_{d+1}$ to be adjacent to $v_{d/2}$ and $v_{d/2+1}$.

Let $P_d = v_0v_1 \cdots v_d$, $U_d(v_j)$ be the graph with $d + 2$ vertices arisen from $P_d$ by adding a new vertex $u_j$ to be adjacent to one vertex $v_i$ ($v_i \in V(P_d)$, $1 \leq i \leq d - 1$). $P_d(C_3; v_i)$ arisen from $P_d = v_1v_2 \cdots v_d$ by attaching $n - d - 3$ pendant vertices to $v_i$ ($1 \leq i \leq d - 1$) and identifying $v_i$ with one vertex of $C_3$, denote $U_d^{n,i} = \{P_d(C_3; v_i) \mid 1 \leq i \leq d - 1\}$. Let $U_{d+1}^* = \{u_i \mid 1 \leq i \leq d - 2\}$, $U_{d+2}^* = \{u_i \mid 1 \leq i \leq d - 2\}$. Let $U_{d+1}^*$ be a $(d + 2)$-vertex unicyclic graph arisen from $P_d = v_1v_2 \cdots v_d$ by adding a new vertex $v_{d+1}$ to be adjacent to $v_k$ and $v_{k+1}$ (see Figure 2), $U_{d+2}^*(n - d - 2; v_j)$ arisen from $U_{d+2}$ by attaching $n - d - 2$
Lemma 2 (see [9]). Let \( G_1 \) be an \( n \)-vertex unicyclic graph and \( \nabla_{n,2} \) be the graph defined as above. Then
\[
H(G_1) \leq H(\nabla_{n,2}),
\]
if and only if \( G_1 \cong \nabla_{n,2} \), and the equality holds. When \( d = 1 \), then \( G_1 \cong C_3 \), and when \( d = 2, n \leq 5 \), then \( G_1 \cong C_4 \).

2. Lemmas

Lemma 1 (see [14]). Let \( A, H_1, \) and \( H_2 \) be three connected, pairwise disjoint graphs; note that \( u_1, u_2 \in V(A), v_1 \in V(H_1), \) \( w_1 \in V(H_2) \). The graph \( G \) is obtained by identifying the vertices \( u_1, v_1 \) and \( u_2, w_1 \) between \( A, H_1, H_2 \), respectively. \( G' \) is obtained by identifying the vertices \( u_1, v_1, w_1 \) from \( A, H_1, H_2 \) and \( G'' \) is obtained by identifying the vertices \( u_2, v_1, w_1 \) from \( A, H_1, H_2 \); then we can get
\[
H(G) < H(G') \quad \text{or} \quad H(G) < H(G'').
\]

Lemma 3. Let \( U_0(v_j) \) be the graph defined as above; then
\[
H(U_0(v_{(d/2)})) \geq H(U_0(v_j));
\]
if and only if \( i = \lfloor d/2 \rfloor \), the equality holds.

Proof. By the calculation of Harary index, we can get the following.
(1) If \( 1 \leq i < \lfloor d/2 \rfloor \),
\[
H(U_0(v_{i+1})) - H(U_0(v_i)) = \left( \frac{1}{i+2} - \frac{1}{d-i+1} \right) > 0.
\]
(2) If \( \lfloor d/2 \rfloor \leq i \leq d-1 \),
\[
H(U_0(v_{i-1})) - H(U_0(v_i)) = \left( \frac{1}{d-i+2} - \frac{1}{i+1} \right) > 0.
\]

When \( d \) is odd, we can get \( H(U_0(v_{(d/2)})) = H(U_0(v_{(d/2)+1})) \).
Thus the result holds.

Lemma 4. Let \( U_{n,d}^{2} = \{U_{d+2}(n - d - 2; v) \mid 1 \leq j \leq d - 1, \text{ or } j = d + 1 \} \) and \( \Delta_{n,d}^{1} \) and \( \Delta_{n,d}^{2} \) be the set and two graphs defined as above, respectively. \( G_1 \in U_{n,d}^{2} \); then
\[
H(G_1) \leq H(\Delta_{n,d}^{1});
\]
if and only if \( G_1 \cong \Delta_{n,d}^{1} \), the equality holds.
Proof. Choose a graph \( G_1 \in U_{n,d}^2 \) (3 ≤ \( d \leq n-2 \)), such that \( H(G_1) \) is the maximum. The following claims play a crucial role.

Claim 1. \( j \in \{ k, k + 1, \lfloor d/2 \rfloor, \lceil d/2 \rceil + 1 \} \).

Proof. First, we prove \( j \neq d + 1 \). Otherwise, \( j = d + 1 \); denote \( u_i \in N_{G_j}(v_{d+1}) \setminus \{ v_k, v_{k+1} \} \), \( 1 \leq i \leq n-d-2 \); let

\[
G_1^* = G_1 - \sum_{j=i}^{n-d-2} v_{d+1} u_i + \sum_{j=i}^{n-d-2} v_k u_i \quad \text{or} \quad G_1^* = G_1 - \sum_{j=i}^{n-d-2} v_{d+1} u_i + \sum_{j=i}^{n-d-2} v_{k+1} u_i.
\]

(8)

using Lemma 1, we get \( H(G_1) < H(G_1^*) \), a contraction. So, 1 ≤ \( j \leq d-1 \), we let \( u_i \in N_{G_j}(v_j) \setminus \{ v_j-1, v_{j+1} \} \), \( 1 \leq i \leq n-d-2 \), \( N_{G_j}(v_j') = \{ v_{j-1}, v_{j+1} \} \).

(1) If 1 ≤ \( j < k \leq \lfloor d/2 \rfloor \), let

\[
G_1^* = G_1 - \sum_{i=1}^{n-d-2} v_j w_i + \sum_{i=1}^{n-d-2} v_k w_i.
\]

(9)

if \([d/2] \leq k < k + 1 < j \leq d-1 \), let

\[
G_1^* = G_1 - \sum_{i=1}^{n-d-2} v_j w_i + \sum_{i=1}^{n-d-2} v_{k+1} w_i.
\]

(10)

(2) If 1 ≤ \( k+1 < j \leq [d/2] \) or \([d/2] \leq j < k+1 \leq d-1 \), let

\[
G_1^* = G_1 - \sum_{i=1}^{n-d-2} v_j w_i - v_{d+1} v_k + v_{d+1} v_j - v_{d+1} v_{j+1}.
\]

(11)

(3) If 1 ≤ \( j < \lfloor d/2 \rfloor \leq k + 1 \leq d-1 \), let

\[
G_1^* = G_1 - \sum_{i=1}^{n-d-2} v_j w_i - v_{d+1} v_k - v_{d+1} v_{k+1} + \sum_{i=1}^{n-d-2} v_{d+1} v_{j+1}.
\]

(12)

i.e., \( G_1^* = \Delta_{n,d}^1 \); if 1 ≤ \( k < k + 1 < \lfloor d/2 \rfloor + 1 < j \leq d-1 \), let

\[
G_1^* = G_1 - \sum_{i=1}^{n-d-2} v_j w_i - v_{d+1} v_k - v_{d+1} v_{k+1} + \sum_{i=1}^{n-d-2} v_{d+1} v_{j+1}.
\]

(13)

i.e., \( G_1^* = \Delta_{n,d}^2 \).

From Lemma 3 and the calculation of \( H(G_1) \), we can calculate that \( H(G_1) < H(G_1^*) \), a contraction.

Claim 2. \( k = \lfloor d/2 \rfloor \).

Proof. Otherwise, if \( k = j < \lfloor d/2 \rfloor \), let \( G_1^* = G_1 - v_{d+1} v_d + v_0 v_d \); if \( k = j > \lfloor d/2 \rfloor \), let \( G_1^* = G_1 - v_0 v_j + v_0 v_d \). From Lemma 3, we can get \( H(G_1) < H(G_1^*) \), a contraction.

By Claims 1-2, we have the graph \( G_1 \equiv \Delta_{n,d}^1 \) or \( G_1 \equiv \Delta_{n,d}^2 \).

Claim 3. \( H(\Delta_{n,d}^1) \leq H(\Delta_{n,d}^2) \).

Proof. If \( d = 2t \) is even, we have

\[
H(\Delta_{n,d}^1) - H(\Delta_{n,d}^2) = H(\Delta_{2t}^2) - H(\Delta_{n-2t}^1) = (n - 2t - 2) \left( \frac{1}{t+1} - \frac{1}{t+2} \right) + 2 \sum_{i=1}^{t+1} \frac{1}{i}.
\]

(14)

< 0.

If \( d = 2t + 1 \) is odd, \( \Delta_{n,2t+1}^1 \equiv \Delta_{n,2t+1}^2 \), \( H(\Delta_{n,2t+1}^1) - H(\Delta_{n,2t+1}^2) = 0 \).

By Claims 1-3, we have \( G_1 \equiv \Delta_{n,d}^1 \). Thus the result follows.

\( \square \)

3. Main Results

In this section, we will list our main results.

Theorem 5. Let \( U_{n,d} \) and \( \Delta_{n,d}^1 \) be defined in Section I, the \( n \)-vertex graph \( G_1 \in U_{n,d} \) (3 ≤ \( d \leq n-2 \)); then

\[
H(\Delta_{n,d}^1) \geq H(\Delta_{n,d}^1);
\]

(15)

if and only if \( G_1 \equiv \Delta_{n,d}^1 \), the equality holds.

Proof. Let \( G_1 \in U_{n,d} \); using Lemma 2, the result holds for \( d = 1, 2 \). If \( d = n-1 \), then \( G_1 \equiv \mathcal{C}_n \). So, we discuss that \( 3 \leq d \leq n-2 \).

Choose a graph \( G_1 \in U_{n,d} \) with \( H(G_1) \) being the maximum. Note that \( \mathcal{C}_n \) is the only cycle and \( P_d = v_0 v_1 \cdots v_d \) is the induced path in \( G_1 \); assume that \( d(v_0) = 1 \); we consider the following claims.

Claim 1. \( |V(C_d)| \cap |V(P_d)| > 0 \).

Proof. Otherwise, suppose that there exists a path \( P_k = v_0 v_{g+1} \cdots v_g v_{k-1} v_k \) connecting the cycle \( C_d \) and the path \( P_d \) with \( v_k \in V(P_d), v_1 \in V(C_d) \); denote \( u_i \in N_{G_i}(v_j) \setminus \{ v_{g+1} \} \), \( 1 \leq s \leq d(v_0) - 1 \) and \( w_j \in N_{G_i}(v_k) \setminus \{ v_{g+1} \} \), \( 1 \leq j \leq d(v_1) - 1 \). Let

\[
G_1^* = G_1 - \sum_{i=1}^{d(v_0)-1} v_i w_i + \sum_{i=1}^{d(v_0)-1} v_i u_i \quad \text{or} \quad G_1^* = G_1 - \sum_{j=1}^{d(v_1)-1} v_j w_j + \sum_{j=1}^{d(v_1)-1} v_j u_j.
\]

(16)

Then, applying Lemma 1, \( H(G_1) < H(G_1^*) \), a contraction.
Using Claim 1, we note that $V(C_q) \cap V(P_d) = \{v_1, v_{t+1}, \ldots, v_{t+k}\}, V(C_q) \setminus V(P_d) = \{v_{d+1}, v_{d+2}, \ldots, v_t\}$.

Claim 2. For any $v \in V(G_1) \setminus (V(P_d) \cup V(C_q)), d(v) = 1$.

Proof. Otherwise, assume that there exists a vertex $u \in V(G_1) \setminus (V(P_d) \cup V(C_q))$ with $uv_i, (1 \leq b \leq d(u) - 1), uv_j \in E(G_1)$, $v_i \in V(G_1) \setminus (V(P_d) \cup V(C_q)), v_j \in V(P_d) \cup V(C_q)$. Suppose that $u' \in N_{G_1}(v_j) \setminus \{u\}, 1 \leq s \leq d(v_j) - 1$. Let

$$
G_1' = G_1 - \sum_{i=1}^{d(v_j) - 1} v_i u_i + \sum_{i=1}^{d(v_j) - 1} uu_i' \text{ or }
G_1' = G_1 - \sum_{b=1}^{d(u) - 1} v_b u + \sum_{b=1}^{d(u) - 1} v_b v_j.
$$

Then, using Lemma 1, $H(G_1) < H(G_1')$, a contraction.

By Claim 2, we have any vertex $v \in V(G_1) \setminus (V(P_d) \cup V(C_q))$ is pendant vertex.

Claim 3. $|V(C_q) \cap V(P_d)| \leq 2$.

Proof. Otherwise, suppose that $V(C_q) \cap V(P_d) = \{v_1, v_{t+1}, \ldots, v_{t+k}\}, k \geq 2$.

(1) If $t \leq \lfloor d/2 \rfloor - 1$, denote $u_i \in N_{G_1}(v_i) \setminus \{v_1, v_{t+1}, v_{t+2}\}, 1 \leq i \leq d(v_i) - 3$ (if exists), $N_{P_2}(v_i) = \{v_{t+1}, v_{t+2}\}$. Let

$$
G_1^* = G_1 - v_1 v_t + v_{t+1} v_{t+2} - \sum_{i=1}^{d(v_i) - 3} v_i u_i + \sum_{i=1}^{d(v_i) - 3} v_i v_{i+1} u_i.
$$

(2) If $t + k \geq \lfloor d/2 \rfloor + 2$, denote $u_i \in N_{G_1}(v_{t+k}) \setminus \{v_{t+1}, v_{t+k-1}, v_{t+k+1}\}, 1 \leq s \leq d(v_{t+k}) - 3$ (if exists), $N_{P_2}(v_{t+k}) = \{v_{t+k-1}, v_{t+k+1}\}$. Let

$$
G_1^* = G_1 - v_{d+1} v_{t+k} + v_{d+1} v_{t+k-1} - \sum_{i=1}^{d(v_{t+k}) - 3} v_{t+k} u_i + \sum_{i=1}^{d(v_{t+k}) - 3} v_{t+k} v_{i+1} u_i.
$$

Then, applying Lemma 3 and the calculation of $H(G_1)$, $H(G_1) < H(G_1')$, a contraction.

Claim 4. (1) if $|V(C_q) \cap V(P_d)| = 2, s = d + 1$; (2) if $|V(C_q) \cap V(P_d)| = 1, s = d + 2$.

Proof. (1) Otherwise, we assume that $s \geq d + 2$. The graph $G_1^*$ arisen by deleting all edges in $E(C_q)$ of $G_1$ and incidence with $C_q$ except the edges $v_i v_{t+k}, v_i v_{t+k+1}$ of $G_1$, adding the edge $v_i v_{t+1}$, connecting all isolated vertices to the vertex $v_i$ (if $t \geq \lfloor d/2 \rfloor$) or to the vertex $v_{t+1}$ (if $t + 1 \leq \lfloor d/2 \rfloor$) of $G_1$. Together with the definition of the Harary index and Lemma 3, $H(G_1) < H(G_1^*)$, a contraction.

(2) Otherwise, we assume that $s \geq d + 3$. The graph $G_1^*$ is obtained from $G_1$ by deleting all edges in $E(C_q)$ and incidence with $C_q$ except the edges $v_i v_{t+1}, v_i v_{t+d+1}$, adding the edge $v_i v_{d+1}, v_i v_{d+2}$, connecting all isolated vertices to the vertex $v_i$. We can calculate that $H(G_1) < H(G_1^*)$, a contraction.

By Claim 4 and Lemmas 1 and 3, we get $G_1 \in U_{nd}^1 \cup U_{nd}^2$. If $G_1 \in U_{nd}^1$, applying Lemma 3, $G_1 \cong \nabla_{nd}$ (see Figure 2); if $G_1 \in U_{nd}^2$, applying Lemma 4, $G_1 \cong \Delta_{nd}^1$.

Claim 5. $H(\Delta_{nd}^1) > H(\nabla_{nd})$.

Proof. If $d = 2t$ is even, we have

$$
H(\Delta_{nd}^1) - H(\nabla_{nd}) = H(\Delta_{nd}^1) - H(\nabla_{nt+1})
$$

$$
= \left\{ \left( \frac{1}{t+1} + \frac{1}{t+1} \right) - \left( \frac{2}{t+1} + \frac{1}{t+1} \right) \right\}
$$

$$
= 1 - \frac{1}{t+1} > 0.
$$

If $d = 2t + 1$ is odd, we have

$$
H(\Delta_{nd}^1) - H(\nabla_{nd}) = H(\Delta_{nd}^1) - H(\nabla_{nt+1})
$$

$$
= \left\{ \left( \frac{1}{t+1} + \frac{1}{t+1} \right) - \left( \frac{2}{t+1} + \frac{1}{t+1} \right) \right\}
$$

$$
= 1 - \frac{1}{t+1} > 0.
$$

By Claims 1-5, we have $G_1 \cong \Delta_{nd}^1$. Thus the result follows.
In fact, 
\[
H (\Delta^3_{n,d}) - H (\Delta^2_{n,d}) = (n - d - 3) \left(1 - \frac{1}{2} \right) + \left( \frac{3}{t+1} - \frac{1}{t+2} \right) < 0, \\
H (\nabla_{n,d}) - H (\Delta^4_{n,d}) = (n - d - 3) \left(1 - \frac{1}{2} \right) + \left( \frac{3}{t+1} - \frac{1}{t+2} \right) < 0,
\]

(26)

Thus the result follows. \(\square\)

**Data Availability**

The data used to support the findings of this study are included within the article.

**Conflicts of Interest**

The authors declare that they have no conflicts of interest.

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