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Minimal Harary Index of Graphs with Small Parameters[1]

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Abstract

Let G be a simple connected graph with vertex set $V(G)$. The Harary index 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 u and v. In this paper, we study the minimal Harary index of graphs with small graph parameters such as diameter, matching number and independence number. In many cases, we also determine the extremal graphs.

1 Introduction

Throughout this paper, we consider only undirected graphs without loops and multiple edges. Let $G = (V(G), E(G))$ be a simple connected undirected graph with $|V(G)| = n$, $|E(G)| = \varepsilon(G)$. For any two distinct vertices u and v in G, the distance between u and v, denoted by $d_G(u,v)$, is the number of edges in a shortest path joining u and v. The diameter $diam(G)$ of G is the maximum distance between any two vertices of G.

The so called topological indices have been found to be useful in chemical documentation, structure-activity (SAR) relationships and pharmaceutical drug design in organic

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chemistry [31]. Many researchers were devoted to study various topological indices such as the Wiener polarity index [27, 28], Randić index [23, 32], Balaban index [4], graph energy [14], matching energy [2, 3], indices involving eccentricities [16, 40, 41] and the HOMO-LUMO index [22]. As one of the most popular topological indices [11, 13, 30, 34], the *Wiener index* of a graph G, denoted by $W(G)$, is defined as

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

Independently introduced in [29] and [17] in 1993, the *Harary index* was considered as the "reciprocal analogue" of the Wiener index. Explicitly, the *Harary index* $H(G)$ of a graph G is defined as

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

In later years this invariant is found can be rewritten as the half-sum of the elements in the reciprocal distance matrix (also called the Harary matrix [20]), and was reported to have a number of interesting chemical physics properties [19]. The Harary index and its related molecular descriptors as well as various modifications have shown somewhat success in structure property correlations [8–10, 18, 25, 26].

Up to now, rather extensive results were obtained concerning the Harary index of a graph. Gutman [13] shown that the path and the star are the trees with minimal and maximal Harary index. In [7, 12, 36, 42] the authors presented some upper and lower bounds for the Harary index of connected graphs, triangle-free, quadrangle-free graphs, graphs with given diameter, matching number. Ilić, Yu and Feng [15] 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 [21], trees with given degree sequence [33], unicyclic graphs [35], bicyclic graphs [35,39], the ordering [38]. Other results related to distance and its invariants, one can see [24, 37].

While plenty of results were obtained for the sharp upper bounds of Harary index of various graph classes, few were found for the sharp lower bounds. In general, the graphs with minimal Harary indices are quite different from those of the Wiener index. Some experimental outcomes reveal that to find the exact lower bounds for some graphs classes seems to be much more difficult. In [6], the following problem was proposed:

Problem: Characterize the extremal tree with minimal Harary index among trees of order n and independence number α.

The focus of this paper is an attempt to find the lower bounds for the Harary index of some simple graph classes with small parameters such as diameter, matching number, independence number. We also try to find the extremal graphs.

We recall some terminologies in graph theory. We use $deg_G(v)$ to denote the degree of v in the graph G. The *independence number* of G, denoted by $\alpha(G)$, is the cardinality of the maximal independent sets of G, where an independent set is the subset of $V(G)$ such that every pair vertices of this set are not adjacent. The *matching number* of a graph G is the maximum size of all matching of graphs, and denoted by $\beta(G)$ or β. Let S_n and P_n be a star and a path on n vertices, respectively. $G-v$, $G-uv$ denote the graph obtained from G by deleting vertex $v \in V(G)$, deleting edge $uv \in E(G)$, respectively. Similarly, $G+uv$ is obtained from G by adding an edge $uv(\notin E(G))$. Other notations in graph theory can be found in [1].

The following two lemmas will be used in the sequel.

Lemma 1. *Let G be a connected graph with v_i, v_j as its two nonadjacent vertices and $e \in E(G)$. Then $H(G+v_iv_j) > H(G)$; $H(G-e) < H(G)$.*

Lemma 2. *[38, 39] Let $w_1w_2 \in E(G)$ be a cut edge in G, and $G - w_1w_2 = G_1 \cup G_2$ with $n_i = |V(G_i)| \geq 2$ for $i = 1, 2$. Suppose that $w_i \in V(G_i)$ for $i = 1, 2$. Assume that G' is a graph obtained from G by identifying vertex w_1 and w_2 (the new vertex is labeled as w) and attaching at w a pendent vertex w_0. Then $H(G) < H(G')$.*

2 Trees with small diameter

Let $\mathbb{T}_{n,d}$ be the set of trees of order n and diameter d. There is only one tree in $\mathbb{T}_{n,2}$, which is the star.

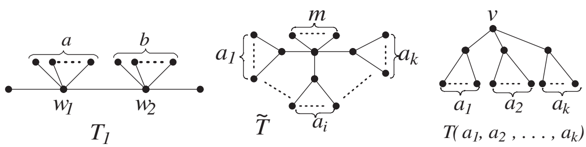

Figure 1: Three trees.

The trees in $\mathbb{T}_{n,3}$ must be a double star T_1 (as depicted in Figure 1), where $a+b = n-4$.

Theorem 3. *For $T \in \mathbb{T}_{n,3}$, we have*

$$H(T) \geq \begin{cases} \frac{5}{24}n^2 + \frac{5}{12}n - \frac{2}{3} & \text{if } n \text{ is even;} \\ \frac{5}{24}n^2 + \frac{5}{12}n - \frac{5}{8} & \text{if } n \text{ is odd.} \end{cases}$$

The equality holds if and only if $T \cong T_1$ with $|a-b| \leq 1$.

Proof. Let t_i denote the number of pairs of vertices $\{u, v\} \subseteq V(G)$ such that $d(u, v) = i$. It is easy to check that $t_1 = n-1$, $t_2 = \binom{a+1}{2} + \binom{b+1}{2} + a + b + 2$ and $t_3 = a + b + 1 + ab$. Therefore, bearing in mind that $a + b = n - 4$, we have

$$\begin{aligned} H(T) &= n - 1 + \frac{t_2}{2} + \frac{t_3}{3} \\ &= \frac{a^2}{6} - \frac{(n-4)a}{6} + \frac{n^2}{4} + \frac{n}{12}. \end{aligned}$$

It follows that

$$H(T) = \frac{1}{6}\left(a - \frac{n-4}{2}\right)^2 + \frac{n^2}{4} + \frac{n}{12} - \frac{(n-4)^2}{24}.$$

If n is even, then this is minimized for $a = \frac{n-4}{2}$ to get

$$H(T) \geq \frac{5}{24}n^2 + \frac{5}{12}n - \frac{2}{3}.$$

If n is odd, then this is minimized for $a = \frac{n-3}{2}$ or $a = \frac{n-5}{2}$ to get

$$H(T) \geq \frac{5}{24}n^2 + \frac{5}{12}n - \frac{5}{8},$$

as desired. ■

From above, one may find that when the diameter is 2 or 3, the extremal trees with minimal Harary index and maximal Wiener index coincide [34].

Next, we consider the trees with diameter 4.

The trees in $\mathbb{T}_{n,4}$ must be of the form like $\widetilde{T} = T(m; a_1, a_2, \ldots, a_k)$ with $m \geq 0$, as shown in Figure 1, where $\sum_{i=1}^{k} a_i + m + k + 1 = n$. This tree is obtained from a path $P_5 = v_1v_2v_3v_4v_5$ by attaching some pendent edges at v_2, v_4, and/or attaching some pendent edges at v_3, and/or identifying v_3 with a pendent vertex of a star. We call v_3 the center of $\widetilde{T}$.

For $2 \leq k \leq n-3$, if $m = 0$ and $deg(v_3) = k$, we write $T(a_1, a_2, \ldots, a_k)$ instead of $\widetilde{T}$.

For $1 \leq i < j \leq k$, we denote the tree $T(a_1, a_2, \ldots, a_k)$ by $T^*(n, k)$ if $|a_i - a_j| \leq 1$.

Lemma 4. *For any tree of order $n \geq 16$ of the form $\widetilde{T} = T(m; a_1, a_2, \ldots, a_k) \in \mathbb{T}_{n,4}$, where $k \geq 2, m \geq 1$, there exists a tree of order $n \geq 16$ of the form $T = T(b_1, b_2, \ldots, b_t)$ such that $H(\widetilde{T}) > H(T)$.*

Proof. We first consider the case $k \geq 3, m \geq 1$. Without loss of generality, we assume $a_1 \leq a_2 \leq \ldots \leq a_k$. Let $T' = T(m-1; a_1+1, a_2, \ldots, a_k)$. Directly, we have

$$\begin{aligned} H(\widetilde{T}) &= n-1+\frac{1}{2}\left(\sum_{i=1}^{k}\binom{a_i}{2}+\sum_{i=1}^{k}a_i+\binom{k+m}{2}\right) \\ &\quad +\frac{1}{3}(k+m-1)\sum_{i=1}^{k}a_i+\frac{1}{4}\left(a_1(a_2+\ldots+a_k)+\cdots+a_{k-1}a_k\right), \end{aligned}$$

$$\begin{aligned} H(T') &= n-1+\frac{1}{2}\left(\binom{a_1+1}{2}+\sum_{i=2}^{k}\binom{a_i}{2}+\sum_{i=1}^{k}a_i+1+\binom{k+m-1}{2}\right) \\ &\quad +\frac{1}{3}(k+m-2)\left(\sum_{i=1}^{k}a_i+1\right)+\frac{1}{4}\left((a_1+1)(a_2+\ldots+a_k)+\cdots+a_{k-1}a_k\right). \end{aligned}$$

It follows that

$$\begin{aligned} H(\widetilde{T})-H(T') &= \frac{1}{2}\left(\binom{a_1}{2}-\binom{a_1+1}{2}-1+\binom{k+m}{2}-\binom{k+m-1}{2}\right) \\ &\quad +\frac{1}{3}\left(\sum_{i=1}^{k}a_i+2-k-m\right)-\frac{1}{4}\sum_{i=2}^{k}a_i \\ &= \frac{1}{6}(k+m-a_1-2)+\frac{1}{12}\sum_{i=2}^{k}a_i \\ &= \frac{1}{6}(k+m-a_1-2)+\frac{1}{12}(n-k-m-1-a_1) \\ &= \frac{1}{12}(n+k+m-5-3a_1)>0, \end{aligned}$$

the last inequality holds as $n \geq ka_1+m+k+1$. This implies the result.

If $k=2, m \geq 2$, in this case, by Lemma 2, the tree $T(a_1, a_2, m-1)$ has smaller Harary index.

If $k=2, m=1$, for $T(1; a_1, a_2) := T_1$, we consider $T_2 = T(a_1, a_2-1, 1)$. Similarly,

$$\begin{aligned} &H(T_1)-H(T_2) \\ &= n-1+\frac{1}{2}\left(\binom{a_1}{2}+\binom{a_2}{2}+3+a_1+a_2\right)+\frac{2}{3}(a_1+a_2)+\frac{1}{4}a_1a_2 \end{aligned}$$

$$
\begin{aligned}
& - \left(n-1+\frac{1}{2}\left(\binom{a_1}{2}+\binom{a_2-1}{2}+3+a_1+a_2\right)+\frac{2}{3}\left(a_1+a_2\right)+\frac{1}{4}(a_1a_2+a_2-1)\right) \\
& = \frac{1}{4}(a_2-1)>0.
\end{aligned}
$$

So we get the result. ∎

Remark. From Lemma 4, one can see that the extremal tree must be of the form like $T(a_1,a_2,\ldots,a_k)$, and thus we must have $n-1-k\geq k$, i.e., $k\leq\frac{n-1}{2}$.

Lemma 5. *Let $T=T(a_1,a_2,\ldots,a_k)$ be the tree of order n with diameter 4 as depicted in Figure 1. Then we have*

$$H(T)=\frac{1}{24}\left(3n^2+16n-19+2kn+k^2-6k\right)+\frac{1}{8}\sum_{i=1}^{k}a_i^2. \tag{1}$$

And $H(T)$ is minimized when a_i's are almost equal.

Proof. We assume $a_1\leq a_2\leq\ldots\leq a_k$. Let t_i be the number of pairs of $\{u,v\}\subseteq V(T)$ such that $d(u,v)=i$. Apparently, $t_1=n-1$. By a direct calculation, we get

$$
\begin{aligned}
t_2 &= n-k-1+\binom{k}{2}+\sum_{i=1}^{k}\binom{a_i}{2}, \\
t_3 &= (k-1)\sum_{i=1}^{k}a_i, \\
t_4 &= \binom{n-k-1}{2}-\sum_{i=1}^{k}\binom{a_i}{2}.
\end{aligned}
$$

Thus we have

$$
\begin{aligned}
H(T) &= (n-1)+\frac{1}{2}\left(n-k-1+\binom{k}{2}+\sum_{i=1}^{k}\binom{a_i}{2}\right)+\frac{1}{3}(k-1)\sum_{i=1}^{k}a_i \\
&\quad +\frac{1}{4}\left(\binom{n-k-1}{2}-\sum_{i=1}^{k}\binom{a_i}{2}\right) \\
&= n-1+\frac{(n-k-1)^2}{8}+\frac{1}{8}\sum_{i=1}^{k}a_i^2+\frac{4k-1}{12}(n-k-1)+\frac{k(k-1)}{4} \\
&= \frac{1}{24}\left(3n^2+16n-19+2kn+k^2-6k\right)+\frac{1}{8}\sum_{i=1}^{k}a_i^2.
\end{aligned}
$$

This implies the result.

If $a_k-a_1\geq 2$, then we may consider $T=T(a_1+1,a_2,\ldots,a_k-1)$, the rest can be obtained directly. ∎

We give an analysis for the right-hand side of expression (1). We first regard k as a real.

Obviously, (1) is minimized for $a_i = \frac{n-k-1}{k}$, $i = 1, 2, \ldots, k$. Thus the minimal value of (1) should be

$$f(k) = \frac{1}{24}\left(3n^2 + 16n - 19 + 2kn + k^2 - 6k\right) + \frac{1}{8}\frac{(n-k-1)^2}{k}.$$

Now we take derivative with respect to k,

$$\frac{df(k)}{dk} = \frac{1}{24}\left(2(n+k-3) - \frac{3}{k^2}\left(2k(n-k-1) + (n-k-1)^2\right)\right),$$

and it is easy to check $\frac{d^2f(k)}{dk^2} > 0$, so $f(k)$ has only one minimum value, which is attained at the point k_0 satisfying

$$2(n+k-3) - \frac{3}{k^2}\left(2k(n-k-1) + (n-k-1)^2\right) = 0,$$

or equivalently,

$$2k^3 + k^2(2n-3) - 3(n-1)^2 = 0.$$

Thus, k_0, as a real, must lie in the interval $\left[\sqrt{\frac{4n}{3}}, \sqrt{\frac{3n}{2}}\,\right]$.

But all k we considered here should be integers, and the minimum value may be taken at two consecutive integers, thus we have, k_0, as an integer, lies in the interval $\left[\sqrt{\frac{4n}{3}} - 1, \sqrt{\frac{3n}{2}} + 1\right]$.

From Lemmas 4, 5 and the above discussion, we immediately have

Theorem 6. *Let $T \in \mathbb{T}_{n,4}$. Then*

$$H(T) \geq \min\{H(T^*(n,k)), k_0 - 1 \leq k \leq k_0 + 1\},$$

where k_0 is the largest root of the cubic equation $2k^3 + k^2(2n-3) - 3(n-1)^2 = 0$, and $k_0 \in \left[\sqrt{\frac{4n}{3}}, \sqrt{\frac{3n}{2}}\,\right]$.

Using Matlab, we can obtain the tree(s) $T^*(n,k)$, $2 \leq k \leq \frac{n-1}{2}$, with the minimum value of Harary index for small n and k, part of them are shown in Table 1, where "EG" denotes the words "Extremal Graph", and the ordered pair (a,b) denotes $T^*(a,b)$.

n	5	6	7	8	9	10
EG	$(5,2)$	$(6,2)$	$(7,3)$	$(8,3)$	$(9,3)$	$(10,3)$
n	11	12	13	14	15	16
EG	$(11,4)$	$(12,4)$	$(13,4)$	$(14,4)$	$(15,4)$	$(16,4)$
n	17	18	19	20	21	22
EG	$(17,4)$	$(18,4)=(18,5)$	$(19,5)$	$(20,5)$	$(21,5)$	$(22,5)$
n	23	24	25	26	27	28
EG	$(23,5)$	$(24,5)$	$(25,6)$	$(26,5)=(26,6)$	$(27,6)$	$(28,6)$
n	34	35	45	46	57	58
EG	(34,6)=(34,7)	$(35,7)$	$(45,7)=(45,8)$	$(46,8)$	$(57,8)$	$(58,9)$

Table 1: Some trees of small order with diameter 4 and minimal Harary index.

3 Trees with small matching number

Let $\mathbb{A}_{n,\beta}$ be the set of trees on n vertices with fixed matching number β. The tree with $\beta = 1$ is exactly the star.

Let $\mathbb{A}_1$ be the set of trees of order n of the form T_1 (see Figure 1) with $a + b = n - 4$. Let $\mathbb{A}_2$ be the set of trees of order n of the form T_2 (see Figure 2) with $a + b = n - 5$. It is easy to find $\mathbb{A}_1 \cup \mathbb{A}_2$ contains all trees with matching number 2.

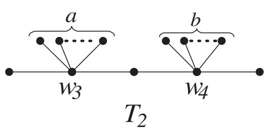

Figure 2: The tree T_2 with $\beta = 2$.

Theorem 7. *If $T \in \mathbb{A}_{n,2}$, then*

$$H(T) \geq \begin{cases} \frac{3}{16}n^2 + \frac{11}{24}n - \frac{1}{2} & \text{if } n \text{ is even;} \\ \frac{3}{16}n^2 + \frac{11}{24}n - \frac{9}{16} & \text{if } n \text{ is odd.} \end{cases}$$

The equality holds if and only if $T \cong T_2$ with $|a - b| \leq 1$.

Proof. If $T \in \mathbb{A}_{n,2}$, then $T \in \mathbb{A}_1$ or $T \in \mathbb{A}_2$. By Lemma 2, for any $T \in \mathbb{A}_1$, there exists $T^* \in \mathbb{A}_2$ such that $H(T) > H(T^*)$. Thus we need only consider $T \in \mathbb{A}_2$. Let t_i denote the number of pairs of vertices $\{u, v\} \subseteq V(T)$ with $d(u, v) = i$. Then $t_1 = n - 1$. By direct calculation we obtain

$$t_2 = \binom{a+2}{2} + \binom{b+2}{2} + 1,$$

$$t_3 = a+b+2,$$
$$t_4 = a+b+1+ab.$$

Therefore, bearing in mind that $a+b=n-5$, we have

$$\begin{aligned} H(T) &= t_1+\frac{t_2}{2}+\frac{t_3}{3}+\frac{t_4}{4} \\ &= \frac{n^2}{4}-\frac{n}{6}+1-\frac{ab}{4} \\ &= \frac{a^2}{4}-\frac{(n-5)a}{4}+\frac{n^2}{4}-\frac{n}{6}+1 \\ &= \frac{1}{4}\left(a-\frac{n-5}{2}\right)^2+\frac{n^2}{4}-\frac{n}{6}+1-\frac{(n-5)^2}{16}. \end{aligned}$$

If n is even, then the above expression is minimized for $a=\frac{n-4}{2}$ or $a=\frac{n-6}{2}$, and

$$H(T) \geq \frac{3}{16}n^2+\frac{11}{24}n-\frac{1}{2}.$$

If n is odd, then the above expression is minimized for $a=\frac{n-5}{2}$, and

$$H(T) \geq \frac{3}{16}n^2+\frac{11}{24}n-\frac{9}{16},$$

as desired. ■

For $T=T(a_1,a_2,a_3)$ defined as in Figure 1 of Section 1, we obviously have $T \in \mathbb{A}_{n,3}$.

Lemma 8. *For $T=T(a_1,a_2,a_3)$, we have $H(T) \geq H(T^*(n,3))$ with equality holding if and only if $T \cong T^*(n,3)$ and*

$$H(T^*(n,3)) = \begin{cases} \frac{1}{6}n^2+\frac{7}{12}n-\frac{1}{2} & if n-4 \equiv 0 \text{ (mod 3)}; \\ \frac{1}{6}n^2+\frac{7}{12}n-\frac{5}{12} & if n-4 \equiv 1 \text{ (mod 3)}; \\ \frac{1}{6}n^2+\frac{7}{12}n-\frac{5}{12} & if n-4 \equiv 2 \text{ (mod 3)}. \end{cases}$$

Proof. From Lemma 5, we immediately get the result. ■

Let $\mathbb{M}_i \subseteq \mathbb{A}_{n,3}$ be the set of all the trees of diameter i, where $i=4,5,6$. Obviously $\mathbb{M}_4$ contains the trees of the form $T(a_1,a_2,a_3)$ as in Lemma 8 (we denote this set of trees by $\mathbb{M}_4'$) and the trees of the form T_3' in Figure 3 (we denote this set of trees by $\mathbb{M}_4''$).
$\mathbb{M}_5$ contains the trees of the form T_3'' in Figure 3.
$\mathbb{M}_6$ is the set of trees of the form T_3 (see Figure 3), where $a+b+c=n-7$.

Theorem 9. *Let $T \in \mathbb{A}_{n,3}$ and $\frac{5n-48}{20}=t$. Then*

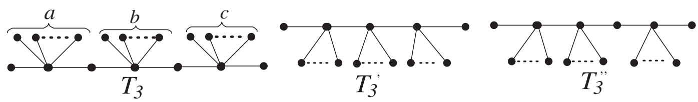

Figure 3: The trees with $\beta = 3$.

(1) If $0 \le t - \lfloor t \rfloor \le \frac{1}{2}$ *and* $n \not\equiv \lfloor t \rfloor$ *(mod 2), then*

$$H(T) \ge \frac{1}{6}\lfloor t \rfloor^2 - \frac{1}{3}t\lfloor t \rfloor + \frac{1}{6}n^2 + \frac{11}{30}n + \frac{5}{12},$$

with equality holding if and only if $T \cong T_3$ *with* $a = c = \frac{n-7-\lfloor t \rfloor}{2}, b = \lfloor t \rfloor$.

(2) If $0 \le t - \lfloor t \rfloor \le \frac{1}{2}$ *and* $n \equiv \lfloor t \rfloor$ *(mod 2), then*

$$H(T) \ge \min\left\{\frac{1}{6}\lceil t \rceil^2 - \frac{1}{3}t\lceil t \rceil + \frac{1}{6}n^2 + \frac{11}{30}n + \frac{5}{12}, \frac{1}{6}\lfloor t \rfloor^2 - \frac{1}{3}t\lfloor t \rfloor + \frac{1}{6}n^2 + \frac{11}{30}n + \frac{1}{2}\right\}.$$

(3) If $0 \le \lceil t \rceil - t \le \frac{1}{2}$ *and* $n \not\equiv \lceil t \rceil$ *(mod 2), then*

$$H(T) \ge \frac{1}{6}\lceil t \rceil^2 - \frac{1}{3}t\lceil t \rceil + \frac{1}{6}n^2 + \frac{11}{30}n + \frac{5}{12},$$

with equality holding if and only if $T \cong T_3$ *with* $a = c = \frac{n-7-\lceil t \rceil}{2}, b = \lceil t \rceil$.

(4) If $0 \le \lceil t \rceil - t \le \frac{1}{2}$ *and* $n \equiv \lceil t \rceil$ *(mod 2), then*

$$H(T) \ge \min\left\{\frac{1}{6}\lfloor t \rfloor^2 - \frac{1}{3}t\lfloor t \rfloor + \frac{1}{6}n^2 + \frac{11}{30}n + \frac{5}{12}, \frac{1}{6}\lceil t \rceil^2 - \frac{1}{3}t\lceil t \rceil + \frac{1}{6}n^2 + \frac{11}{30}n + \frac{1}{2}\right\}.$$

Proof. For any tree $T \in \mathbb{A}_{n,3}$ with diameter $diam(T)$, we have $diam(T) \in \{4, 5, 6\}$.

If $diam(T) = 4$, by Lemma 2, for any tree $T = T(a_1, a_2, a_3) \in \mathbb{M}_4'$, there exists one tree $T^{\#} \in \mathbb{M}_4''$ of the form T_3' such that $H(T^{\#}) > H(T)$, and also there exists another tree $T''' \in \mathbb{M}_6$ of the form T_3 such that $H(T^{\#}) > H(T''')$.

For any tree $T \in \mathbb{M}_5$, then it is of the form T_3'' in Figure 3, there exists one tree $T' \in \mathbb{M}_6$ such that $H(T) > H(T')$.

Therefore the tree(s) with minimal Harary index must belong to $\mathbb{M}_6$ or $\mathbb{M}_4'$.

Now we first consider the case when $T \in \mathbb{M}_6$. Suppose the longest path of T is $P = v_0v_1v_2v_3v_4v_5v_6$. We denote $deg(v_i) - 2 = a_i \ge 0$ for $i = 1, 3, 5$, respectively.

If $a_1 - a_5 \ge 2$, then we construct a tree T' from T by removing one pendent vertex of v_1 to v_5. Then we obtain

$$H(T) - H(T') = 1 + \frac{1}{2}a_1 + \frac{1}{5} + \frac{1}{6}(a_5 + 1) - \left(1 + \frac{1}{2}(a_5 + 1) + \frac{1}{5} + \frac{1}{6}a_1\right)$$

$$= \frac{1}{3}(a_1 - a_5 - 1) > 0.$$

Therefore, we conclude the tree in $\mathbb{M}_6$ with minimal Harary index must satisfy $a_1 - a_5 \leq 1$.

If $a_1 - a_5 = 0$, as $a_1 + a_3 + a_5 = n - 7$, $a_1 = \frac{n-7-a_3}{2}$. From definition, we have

$$\begin{aligned} H(T) &= n - 1 + \frac{1}{2}\left(\binom{a_1+2}{2} + \binom{a_3+2}{2} + \binom{a_5+2}{2} + 2\right) + \frac{1}{3}(n - 3 + a_3) \\ &\quad + \frac{1}{4}(n - 4 + a_3 + a_1a_3 + a_3a_5) + \frac{1}{5}(a_1 + a_5 + 2) + \frac{1}{6}(a_1 + a_5 + 1 + a_1a_5) \\ &= \frac{a_3^2}{4} - \frac{15n-118}{60}a_3 + \frac{n^2}{4} - \frac{4}{5}n + \frac{9}{2} - \frac{a_1a_5}{3} \\ &= \frac{1}{6}a_3^2 - \frac{5n-48}{60}a_3 + \frac{1}{6}n^2 + \frac{11}{30}n + \frac{5}{12} := g(a_3). \end{aligned}$$

If $a_1 - a_5 = 1$, as $a_1 + a_3 + a_5 = n - 7$, we have $a_5 = \frac{n-8-a_3}{2}$. Then, similarly

$$H(T) = \frac{1}{6}a_3^2 - \frac{5n-48}{60}a_3 + \frac{1}{6}n^2 + \frac{11}{30}n + \frac{1}{2} := f(a_3).$$

A simple calculation shows that $f(a_3)$ and $g(a_3)$ are minimized when $a_3 = \lfloor t \rfloor$ or $a_3 = \lceil t \rceil$, where $t = \frac{5n-48}{20}$.

Note that

$$f(t+1) \geq \max\left\{f\left(\lceil t \rceil\right), f\left(\lfloor t \rfloor\right), g\left(\lceil t \rceil\right), g\left(\lfloor t \rfloor\right)\right\}.$$

By Lemma 8, for any tree $T \in \mathbb{M}_4'$, we have $H(T) \geq H(T^*(n,3)) \geq \frac{1}{6}n^2 + \frac{7}{12}n - \frac{1}{2}$. But

$$\left(\frac{1}{6}n^2 + \frac{7}{12}n - \frac{1}{2}\right) - f(t+1) = \frac{1}{6}\left(\frac{5n-48}{20}\right)^2 + \frac{13}{60}n - \frac{7}{6} > 0.$$

Hence, we conclude that $H(T^*(n,3)) > f(t+1)$. Therefore the extremal tree from $\mathbb{A}_{n,3}$ must lie in $\mathbb{M}_6$. Clearly, the function $f(a_3)$ requires $n \equiv a_3 \pmod 2$ according to $a_1 = a_5 + 1$ and $a_1 + a_3 + a_5 = n - 7$. Analogously the function $g(a_3)$ requires that $n \not\equiv a_3 \pmod 2$, according to $a_1 = a_5$ and $a_1 + a_3 + a_5 = n - 7$. In the following statements, we distinguish four cases.

Case 1. If $0 \leq t - \lfloor t \rfloor \leq \frac{1}{2}$ and $n \not\equiv \lfloor t \rfloor \pmod 2$, then $f(a_3)$ is minimized at $a_3 = \lceil t \rceil$ and $g(a_3)$ is minimized at $a_3 = \lfloor t \rfloor$. Since

$$f\left(\lceil t \rceil\right) \geq f\left(\lfloor t \rfloor\right) \quad \text{and} \quad f\left(\lfloor t \rfloor\right) - g\left(\lfloor t \rfloor\right) = \frac{1}{12},$$

we obtain

$$\min\{H(T)|T \in \mathbb{A}_{n,3}\} = \min\{g\left(\lfloor t \rfloor\right), f\left(\lceil t \rceil\right)\} = g\left(\lfloor t \rfloor\right).$$

Case 2. If $0 \leq t - \lfloor t \rfloor \leq \frac{1}{2}$ and $n \equiv \lfloor t \rfloor \pmod 2$, then $f(a_3)$ is minimized at $a_3 = \lfloor t \rfloor$ and $g(a_3)$ is minimized at $a_3 = \lceil t \rceil$. Thus

$$\min\{H(T)|T \in \mathbb{A}_{n,3}\} = \min\{g\left(\lceil t \rceil\right), f\left(\lfloor t \rfloor\right)\}.$$

Case 3. If $0 \leq \lceil t \rceil - t \leq \frac{1}{2}$ and $n \not\equiv \lceil t \rceil \pmod 2$, then $f(a_3)$ is minimized at $a_3 = \lfloor t \rfloor$ and $g(a_3)$ is minimized at $a_3 = \lceil t \rceil$. Since

$$f\left(\lfloor t \rfloor\right) \geq f\left(\lceil t \rceil\right) \quad \text{and} \quad f\left(\lceil t \rceil\right) - g\left(\lceil t \rceil\right) = \frac{1}{12},$$

we obtain

$$\min\{H(T)|T \in \mathbb{A}_{n,3}\} = \min\{g\left(\lceil t \rceil\right), f\left(\lfloor t \rfloor\right)\} = g\left(\lceil t \rceil\right).$$

Case 4. If $0 \leq \lceil t \rceil - t \leq \frac{1}{2}$ and $n \equiv \lceil t \rceil \pmod 2$, then $g(a_3)$ is minimized at $a_3 = \lfloor t \rfloor$ and $f(a_3)$ is minimized at $a_3 = \lceil t \rceil$. Thus

$$\min\{H(T)|T \in \mathbb{A}_{n,3}\} = \min\{f\left(\lceil t \rceil\right), g\left(\lfloor t \rfloor\right)\},$$

as desired. ■

Remark. The *dumbbell* $B_{n,a,b}$ is the graph obtained from a path P_{n-a-b} by attaching a and b pendent vertices to two end vertices of P_{n-a-b}, respectively. $B_{n,a,b}$ is called *balanced* if $|a - b| \leq 1$. Dankelmann [5] obtained that the balanced dumbbell has the maximal Wiener index among graphs with given matching number. However, it is not the one with the minimal Harary index. We give a example to illustrate. The trees G_i, $i = 0, 1, 2, 3$, depicted in Figure 4, are of order 16 and matching number 3. Direct calculation yields

$$\begin{aligned} H(G_0) &= H(G_1) + \frac{1}{4} + \frac{1}{5} > H(G_1), \\ H(G_2) &= H(G_1) + \frac{1}{4} - \frac{1}{5} > H(G_1), \\ H(G_3) &= H(G_2) + \frac{5}{12} - \frac{1}{5} > H(G_2). \end{aligned}$$

4 Graphs with small independence number

It is well known that $\alpha + \beta = n$ for trees of order n, thus the results in Section 3 also can be rewritten as the minimal Harary index of trees with given independence number $n-1, n-2, n-3$. In this section, we consider more general graphs.

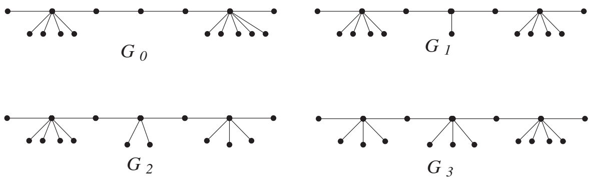

Figure 4: Four trees with $n = 16$ and $\beta = 3$.

Let $\mathbb{G}_{n,\alpha}$ be the set of all connected graphs of order n with independence number α. If $\alpha = 1$, then $G = K_n$. We assume $\alpha \geq 2$ in the following.

For $n_1 + n_2 = n, |n_1 - n_2| \leq 1$, let $P_{n,2}$ be the graph obtained by adding one edge between two complete graphs K_{n_1} and K_{n_2}.

Theorem 10. *If $G \in \mathbb{G}_{n,2}$, $n \geq 3$, then we have $H(G) \geq H(P_{n,2})$ with equality holding if and only if $G \cong P_{n,2}$ and*

$$H(P_{n,2}) = \begin{cases} \frac{1}{3}n^2 - \frac{1}{3}n + \frac{1}{3} & \text{if } n \text{ is even;} \\ \frac{1}{3}n^2 - \frac{1}{3}n + \frac{1}{2} & \text{if } n \text{ is odd.} \end{cases}$$

Proof. Let $G \in \mathbb{G}_{n,2}$ be the graph with minimum Harary index. Obviously, the diameter of G equals 2 or 3; otherwise, $\alpha(G) \neq 2$.

Case 1. $diam(G) = 2$. A Turán-type theorem for connected graphs states (see [1, Page 277, Theorem 5]) that

$$\varepsilon(G) \geq \varepsilon(P_{n,2}),$$

with equality if and only if $G \cong P_{n,2}$. Since $diam(G) \neq diam(P_{n,2})$ we have $G \neq P_{n,2}$ and thus

$$\begin{aligned} H(G) &= \sum_{d_G(u,v)=1} \frac{1}{d_G(u,v)} + \sum_{d_G(u,v)=2} \frac{1}{d_G(u,v)} \\ &= \frac{1}{4}n(n-1) + \frac{1}{2}\varepsilon(G) \\ &> \frac{1}{4}n(n-1) + \frac{1}{2}\varepsilon(P_{n,2}) \\ &\geq H(P_{n,2}), \end{aligned}$$

a contradiction to the minimality of $H(G)$.

Case 2. $diam(G) = 3$. There are two vertices $u, v \in V(G)$ with $d_G(u,v) = 3$. It is easily seen that G consists of two cliques induced by $N[u]$ and $N[v]$, respectively, where

$N[u] = N(u) \cup \{u\}$, and there is exactly one edge between these two cliques. Assume $|N[u]| = n_1$, then $|N[v]| = n - n_1$. From the definition of Harary index, we have

$$\begin{aligned} H(G) &= H(K_{n_1}) + H(K_{n-n_1}) + 1 + \frac{1}{2}(n - n_1 - 1) + (n_1 - 1)\left(\frac{1}{2} + \frac{1}{3}(n - n_1 - 1)\right) \\ &= \frac{2}{3}n_1^2 - \frac{2n}{3}n_1 + \frac{n^2}{2} - \frac{n}{3} + \frac{1}{3}. \end{aligned}$$

If n is even, the above expression is minimized at $n_1 = \frac{n}{2}$ and thus $H(G) \geq \frac{1}{3}n^2 - \frac{1}{3}n + \frac{1}{3}$.

If n is odd, the above expression is minimized at $n_1 = \frac{n-1}{2}$, thus $H(G) \geq \frac{1}{3}n^2 - \frac{1}{3}n + \frac{1}{2}$, as desired. ■

Let $\mathbb{G}_i \subseteq \mathbb{G}_{n,3}$ be the set of graphs of diameter i, where $i = 2, 3, 4, 5$, the candidates are as depicted in Figure 5, where the cycles represent complete graphs. Thus $\mathbb{G}_5$ contains the candidates of the form G_5 as depicted in Figure 5.

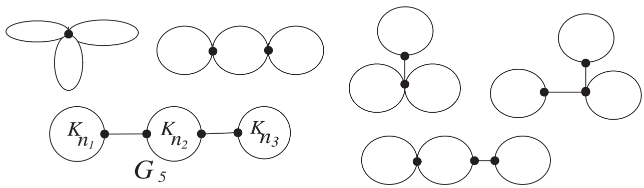

Figure 5: The graphs with $\alpha = 3$.

Theorem 11. *Let $G \in \mathbb{G}_{n,3}$ and $s = \frac{16n-7}{56}$. Then we have*

(1) If $0 \leq s - \lfloor s \rfloor \leq \frac{1}{2}$ and $n \equiv \lfloor s \rfloor$ (mod 2), then

$$H(G) \geq \frac{7}{15}\lfloor s \rfloor^2 - \frac{14}{15}s\lfloor s \rfloor + \frac{3}{10}n^2 + \frac{17}{60}n + \frac{7}{10},$$

with equality holding if and only if $G \cong G_5$ with $n_1 = n_3 = \frac{n - \lfloor s \rfloor}{2}, n_2 = \lfloor s \rfloor$.

(2) If $0 \leq s - \lfloor s \rfloor \leq \frac{1}{2}$ and $n \not\equiv \lfloor s \rfloor$ (mod 2), then

$$\begin{aligned} H(G) \geq \min\Big\{ &\frac{7}{15}\lfloor s \rfloor^2 - \frac{14}{15}s\lfloor s \rfloor + \frac{3}{10}n^2 + \frac{17}{60}n + \frac{9}{10}, \\ &\frac{7}{15}\lceil s \rceil^2 - \frac{14}{15}s\lceil s \rceil + \frac{3}{10}n^2 + \frac{17}{60}n + \frac{7}{10}\Big\}. \end{aligned}$$

(3) If $0 \leq \lceil s \rceil - s \leq \frac{1}{2}$ and $n \equiv \lceil s \rceil$ (mod 2), then

$$H(G) \geq \frac{7}{15}\lceil s \rceil^2 - \frac{14}{15}s\lceil s \rceil + \frac{3}{10}n^2 + \frac{17}{60}n + \frac{7}{10},$$

with equality holding if and only if $G \cong G_5$ with $n_1 = n_3 = \frac{n - \lceil s \rceil}{2}, n_2 = \lceil s \rceil$.

(4) If $0 \le \lceil s \rceil - s \le \frac{1}{2}$ *and* $n \not\equiv \lceil s \rceil$ *(mod 2), then*

$$\begin{aligned} H(G) &\ge \min\Big\{\frac{7}{15}\lfloor s \rfloor^2 - \frac{14}{15}s\lfloor s \rfloor + \frac{3}{10}n^2 + \frac{17}{60}n + \frac{7}{10}, \\ &\qquad \frac{7}{15}\lceil s \rceil^2 - \frac{14}{15}s\lceil s \rceil + \frac{3}{10}n^2 + \frac{17}{60}n + \frac{9}{10}\Big\}. \end{aligned}$$

Proof. Let $G \in \mathbb{G}_{n,3}$ be the candidate with minimum Harary index. Then $diam(G) \in \{2,3,4,5\}$. By Lemmas 1, 2 and simple calculation, for any graph $G_0 \in \mathbb{G}_2 \cup \mathbb{G}_3 \cup \mathbb{G}_4$, there exists one graph $G_0' \in \mathbb{G}_5$ such that $H(G_0) > H(G_0')$. Therefore G is the graph of the form G_5 (see Figure 5), where $n_1 + n_2 + n_3 = n$.

If $n_1 - n_3 \ge 2$, then we let $G' \in \mathbb{G}_5$ be the graph obtained by deleting one vertex of K_{n_1} and adding one vertex of K_{n_3}. We obtain

$$\begin{aligned} & H(G) - H(G') \\ = \;& \frac{n_1(n_1-1)}{2} + \frac{n_1(n_3-1)}{2} + \frac{1}{3} + \frac{1}{4}(n_1 - 1 + n_3 - 1) + \frac{1}{5}(n_1-1)(n_3-1) \\ & - \left(\frac{(n_1-1)(n_1-2)}{2} + \frac{(n_3+1)n_3}{2} + \frac{1}{3} + \frac{1}{4}(n_1 - 2 + n_3) + \frac{1}{5}n_3(n_1-2)\right) \\ = \;& n_1 - 1 - n_3 + \frac{1}{5}(n_3 - n_1 + 1) \\ = \;& \frac{4}{5}((n_1 - n_3) - 1) > 0. \end{aligned}$$

Therefore, the graph G with minimal Harary index must satisfy $n_1 - n_3 \le 1$.

We first consider the case $n_1 - n_3 = 0$. Since $n_1 + n_2 + n_3 = n$, $n_1 = \frac{n-n_2}{2}$. From definition, we have

$$\begin{aligned} H(G) &= H(K_{n_1}) + H(K_{n_2}) + H(K_{n_3}) + 1 + \frac{1}{2}(n_2 - 1) + (n_1 - 1)\left(\frac{1}{2} + \frac{1}{3}(n_2 - 1)\right) \\ & \quad + \frac{1}{3} + \frac{1}{4}(n_3 - 1) + (n_1 - 1)\left(\frac{1}{4} + \frac{1}{5}(n_3 - 1)\right) + 1 \\ & \quad + \frac{1}{2}(n_3 - 1) + (n_2 - 1)\left(\frac{1}{2} + \frac{1}{3}(n_3 - 1)\right) \\ &= \frac{2}{3}n_2^2 + \left(\frac{7}{60} - \frac{2}{3}n + \frac{4}{5}n_1\right)n_2 + \frac{n^2}{2} - \frac{17}{60}n + \frac{7}{10} - \frac{4}{5}nn_1 + \frac{4}{5}n_1^2 \\ &= \frac{7}{15}n_2^2 - \left(\frac{4}{15}n - \frac{7}{60}\right)n_2 + \frac{3}{10}n^2 - \frac{17}{60}n + \frac{7}{10} := g_0(n_2). \end{aligned}$$

Next we consider the the case $n_1 - n_3 = 1$. Since $n_1 + n_2 + n_3 = n$, $n_3 = \frac{n-n_2-1}{2}$. As above, we similarly have

$$H(G)=\frac{7}{15}n_2^2-\left(\frac{4}{15}n-\frac{7}{60}\right)n_2+\frac{3}{10}n^2-\frac{17}{60}n+\frac{9}{10}:=f_0(n_2).$$

A simple calculation shows that the above expression is minimized at $n_2=\lfloor s\rfloor$ or $n_2=\lceil s\rceil$, where $s=\frac{16n-7}{56}$. Clearly, the function $g_0(n_2)$ requires that the parity of n and n_2 are the same and n_2 is an integer, according to $n_1=n_3$ and $n_1+n_2+n_3=n$. Similarly, the function $f_0(n_2)$ requires that the parity of n and n_2 are the opposite and n_2 is an integer, according to $n_1=n_3+1$ and $n_1+n_2+n_3=n$. In the following argument, we distinguish four cases.

Case 1. If $0\le s-\lfloor s\rfloor\le\frac{1}{2}$ and $n\equiv\lfloor s\rfloor \pmod 2$, then $f_0(n_2)$ is minimized at $n_2=\lceil s\rceil$ and $g_0(n_2)$ is minimized at $n_2=\lfloor s\rfloor$. Since

$$f_0\left(\lceil s\rceil\right)\ge f_0\left(\lfloor s\rfloor\right)\quad\text{and}\quad f_0\left(\lfloor s\rfloor\right)-g_0\left(\lfloor s\rfloor\right)=\frac{1}{5},$$

we obtain

$$\min\{H(G)|G\in\mathbb{G}_{n,3}\}=\min\{g_0\left(\lfloor s\rfloor\right),f_0\left(\lceil s\rceil\right)\}=g_0\left(\lfloor s\rfloor\right).$$

Case 2. If $0\le s-\lfloor s\rfloor\le\frac{1}{2}$ and $n\not\equiv\lfloor s\rfloor \pmod 2$, then $f_0(n_2)$ is minimized at $n_2=\lfloor s\rfloor$ and $g_0(n_2)$ is minimized at $n_2=\lceil s\rceil$. Thus

$$\min\{H(G)|G\in\mathbb{G}_{n,3}\}=\min\{g_0\left(\lceil s\rceil\right),f_0\left(\lfloor s\rfloor\right)\}.$$

Case 3. If $0\le\lceil s\rceil-s\le\frac{1}{2}$ and $n\equiv\lceil s\rceil \pmod 2$, then $f_0(n_2)$ is minimized at $n_2=\lfloor s\rfloor$ and $g_0(n_2)$ is minimized at $n_2=\lceil s\rceil$. Since

$$f_0\left(\lfloor s\rfloor\right)\ge f_0\left(\lceil s\rceil\right)\quad\text{and}\quad f_0\left(\lceil s\rceil\right)-g_0\left(\lceil t\rceil\right)=\frac{1}{5},$$

we obtain

$$\min\{H(G)|G\in\mathbb{G}_{n,3}\}=\min\{g_0\left(\lceil s\rceil\right),f_0\left(\lfloor s\rfloor\right)\}=g_0\left(\lceil s\rceil\right).$$

Case 4. If $0\le\lceil s\rceil-s\le\frac{1}{2}$ and $n\not\equiv\lceil s\rceil \pmod 2$, then $g_0(n_2)$ is minimized at $n_2=\lfloor s\rfloor$ and $f_0(n_2)$ is minimized at $n_2=\lceil s\rceil$. Thus

$$\min\{H(G)|G\in\mathbb{G}_{n,3}\}=\min\{f_0\left(\lceil s\rceil\right),g_0\left(\lfloor s\rfloor\right)\},$$

as desired. ■

5 Concluding Remarks

In this paper, motivated by an open problem in [6], we consider the minimal Harary index of graphs with small diameter, matching number and independence number carefully. Many examples show that this is difficult to tackle and the structure of the extremal graphs is different from that of Wiener index as well as many other topological indices. Up to now, we can not find a unified approach for general graphs, even for trees with any given parameter, things are not that easy. We leave these questions for further research.

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