MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **90** (2023) 649–671
ISSN: 0340–6253
doi: 10.46793/match.90-3.649H

On the Harary Index of Graphs with Given Dissociation Number*

Jing Huang[a], **Minjie Zhang**[b†]

[a] *School of Mathematics and Information Science, Guangzhou University, Guangzhou, 510006, China*

[b] *School of Mathematics and Statistics, Hubei University of Arts and Science, Xiangyang 441053, China*

jhuangmath@foxmail.com, zhangmj1982@qq.com

(Received December 17, 2022)

Abstract

For a graph $G = (V_G, E_G)$, a subset $S \subseteq V_G$ is called a maximum dissociation set if the induced subgraph $G[S]$ does not contain P_3 as its subgraph, and the subset has maximum cardinality. The dissociation number of G is the number of vertices in a maximum dissociation set of G. This paper mainly studies the problem of determining the maximum or minimum values of the Harary indices among all trees, bipartite graphs and general connected graphs with fixed order and dissociation number. To be specific, we determine the sharp upper bound of the Harary index among all connected graphs (resp. bipartite graphs, trees) with given order and dissociation number. The extremal graphs meeting these upper bounds are fully characterized. Furthermore, the graphs having the minimum Harary indices with fixed order n and dissociation number $\varphi \in \{2, \lceil \frac{2}{3}n \rceil, n-2, n-1\}$ are also showed.

*J. Huang was partially supported by the National Natural Science Foundation of China (Grant No. 12001202). M. Zhang was partially supported by the National Natural Science Foundation of China (Grant No. 11901179), the Research ability cultivation fund of HUAS, China (Grant No. 2020kypytd006) and Excellent young and middle-aged science and Technology Innovation team project of the Education Department of Hubei Province (T2022029)

†Corresponding author.

1 Introduction

We start with introducing some background information that leads to our main results. Our main results will also be given in this section.

1.1 Background and definitions

All graphs considered in this paper are undirected, simple and connected. Let $G = (V_G, E_G)$ be a graph with vertex set V_G and edge set E_G. We call $|V_G|$ the *order* of G. As usual, let P_n, S_n and K_n be a path, a star and a complete graph with n vertices, respectively. The vertex with degree $n-1$ is called the *center* of S_n. The *distance* between vertices u and v, denoted by $d_G(u, v)$, is the length of a shortest path connecting them. The *diameter* of G, written as $diam(G)$, is the maximum distance between any two vertices of G. We follow the notation and terminology in [6] except otherwise stated.

Let $N_G(v)$ be the set of neighbors of a vertex $v \in V_G$, and $N_G[v] := N_G(v) \cup \{v\}$ be the closed neighborhood of $v \in V_G$. We call $d_G(v) := |N_G(v)|$ the *degree* of v. The subscripts will be omitted without ambiguity. A vertex of a graph G is called a *pendent vertex* (or a *leaf*) if it is a vertex with degree one in G, whereas a vertex of G is called a *quasi-pendent vertex* if it is adjacent to a pendent vertex in G. For the sake of simplicity, we use $G - v, G - uv$ to denote the graph obtained from G by deleting vertex $v \in V_G$, or edge $uv \in E_G$, respectively. For two graphs G_1 and G_2, denote by $G_1 \cup G_2$ and $G_1 \vee G_2$ the disjoint union and join of G_1 and G_2, respectively. For simplicity, we use kG to denote the disjoint union of k copies of G.

A subset is called an *independent set* if any two vertices of it are not adjacent. The *independence number* of a graph G is the maximum cardinality among all independent sets of G. A subset $S \subseteq V_G$ is called a *dissociation set* if the induced subgraph $G[S]$ does not contain P_3 as its subgraph. A *maximum dissociation set* of G is a dissociation set with the maximum cardinality. The *dissociation number* of G, written as $\varphi(G)$, is the cardinality of a maximum dissociation set in G. The problem of computing $\varphi(G)$ was originally raised by Yannakakis [39] in 1981, and in the same paper, he showed this problem is NP-complete for bipartite graphs.

A single number that can be used to describe some properties of a graph is called a *topological index*, or *graph invariant*. Topological index is a graph theoretic property that is preserved by isomorphism. For quite a long time, researchers have been interested in the computation of topological indices, which is mainly related to the applications of these topological indices in nonempirical quantitative structure property relationships and quantitative structure activity relationships. Hundreds of topological indices have been introduced and studied, one may refer to [18, 22, 24, 41–43] for some recent results.

In 1947, Wiener [25] introduced a well-known distance-based graph invariant, namely the *Wiener index* of a graph G, which is defined as

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

Wiener index is probably the best known one among hundreds of topological indices, and it enjoys a prominent place in chemical graph theory for its significant theoretical importance and practical applications in modeling the physical properties of alkanes. Mathematical properties and applications of Wiener index are extensively studied in the literature, one may be referred to [13, 35] and the references therein.

Comparing with the Wiener index, Plavšić et al. [23] and Ivanciuc et al. [20] independently proposed another distance-based graph constant, namely the *Harary index*, which is defined as

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

In the following years, this invariant is rewritten as the half-sum of the elements of the so-called *reciprocal distance matrix* (also known as the *Harary matrix* [21]), and it has been verified to have many interesting chemical and physical properties [19]. It is worth mentioning that the Harary index and its related molecular descriptors, as well as various modifications have shown great advantages in structure performance correlations [10–12].

Up to now, a number of results were obtained on the Harary index of a graph. Gutman [16] showed that P_n and S_n are, respectively, the unique tree having the minimum and maximum Harary index among all trees with n vertices. Upper or lower bounds of the Harary index for some special classes of graphs were also presented, such as unicyclic graphs [15, 28], bicyclic graphs [28, 40], bipartite graphs [9], splitting graphs [5], Eulerian graphs [4], one may refer to [7, 27, 29–35, 37, 38] for more related results.

In recent years, the problem of finding the upper or lower bounds of the Harry index and their corresponding extremal graphs among graphs with given order and independence number has attracted more and more researchers' attention. Das et al. [8] determined the sharp upper bound and the corresponding extremal tree on Harary index among all trees with given order and independence number. Feng et al. [14] characterized all the extremal trees with order n and independence number $\alpha \in \{n-3, n-2, n-1\}$ having the minimum Harary indices. Very recently, Borovićanin et al. [1] showed that these trees also have the minimum Harary indices among all connected graphs with the same constraints. In the same paper, they also determined all the extremal graphs with order n and independence number $n-4$ having the minimum Harary indices.

Note that the dissociation number is a natural generalization of the independence number. Hence it is natural and interesting to consider the same problem for the graphs with fixed order and dissociation number. In this paper, we focus on the problem of determining the maximum or minimum value of the Harary indices and characterizing the corresponding extremal graphs for connected graphs (resp. bipartite graphs, trees) with fixed order and dissociation number.

1.2 Main results

In this subsection, we give some basic notation and then describe our main results. Let $\mathscr{G}_{n,\varphi}$ (resp. $\mathscr{B}_{n,\varphi}$, $\mathscr{T}_{n,\varphi}$) denote the set of connected graphs (resp. bipartite graphs, trees) with fixed order n and dissociation number φ.

Note that adding an edge to a connected graph will strictly increase its Harary index. Then our first main result about the maximum value of the Harary index and the corresponding extremal graph over all graphs in $\mathscr{G}_{n,\varphi}$ is obvious.

Theorem 1.1. *Let $G \in \mathscr{G}_{n,\varphi}$. Then*

$$H(G) \leq \begin{cases} \frac{n(n-1)}{2} - \frac{\varphi(\varphi-2)}{4}, & \text{if } \varphi \text{ is even;} \\ \frac{n(n-1)}{2} - \frac{(\varphi-1)^2}{4}, & \text{if } \varphi \text{ is odd.} \end{cases}$$

with equality if and only if

$$G \cong \begin{cases} K_{n-\varphi} \vee \left(\frac{\varphi}{2} K_2\right), & \text{if } \varphi \text{ is even;} \\ K_{n-\varphi} \vee \left(\frac{\varphi-1}{2} K_2 \cup K_1\right), & \text{if } \varphi \text{ is odd.} \end{cases}$$

Our second result establishes a sharp upper bound on the Harary indices of bipartite graphs with fixed order and dissociation number. The corresponding extremal graph is also characterized.

Theorem 1.2. *Let $G \in \mathscr{B}_{n,\varphi}$ $(n \geq 3)$. Then $H(G) \leq \frac{n^2+(2\varphi-1)n-2\varphi^2}{4}$ with equality if and only if $G \cong K_{\varphi,n-\varphi}$.*

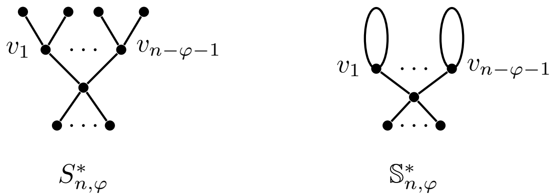


Figure 1. Trees $S^*_{n,\varphi}$ and $\mathbb{S}^*_{n,\varphi}$.

Denote by $S^*_{n,\varphi}$ the tree on n vertices obtained from the star $S_{n-\varphi}$ by attaching exactly two pendent edges to each leaves of $S_{n-\varphi}$ and attaching $3\varphi - 2n + 2$ pendent edges to the center of $S_{n-\varphi}$. Let $\mathbb{S}^*_{n,\varphi}$ be a set of n-vertex trees obtained from $S_{n-\varphi}$ by attaching exactly two pendent edges or one pendent path of length two to each leaf of $S_{n-\varphi}$ and then attaching $3\varphi - 2n + 2$ pendent edges to the center of $S_{n-\varphi}$. Obviously, $S^*_{n,\varphi} \in \mathbb{S}^*_{n,\varphi}$. Figure 1 gives an example for $S^*_{n,\varphi}$ and $\mathbb{S}^*_{n,\varphi}$, where each ellipse implies two pendent edges or one pendent path of length two is attached at vertices $v_1, v_2, \ldots, v_{n-\varphi+1}$.

The next result characterizes all the tree $T \in \mathscr{T}_{n,\varphi}$ having the maximum Harary index.

Theorem 1.3. *Let $T \in \mathscr{T}_{n,\varphi}$ $(n \geq 3)$. Then $H(T) \leq \frac{1}{12}n^2 + \frac{17}{12}n + \frac{1}{6}\varphi^2 - \frac{5}{6}\varphi - \frac{3}{2}$ with equality if and only if $T \cong S^*_{n,\varphi}$.*

Let $S(\ell_1, \ell_2)$ be the tree obtained by attaching ℓ_1 pendent edges and ℓ_2 pendent paths of length two to an isolated vertex, respectively. Denote by $T_1(s_1, t_1)$ the tree obtained from P_4 by attaching one pendent edge and s_1 pendent paths of length two to one leaf of P_4, and then attaching t_1 pendent paths of length two to another leaf of P_4. Let $T_2(s_2, t_2)$ be the tree obtained from P_4 by attaching s_2 and t_2 pendent paths of length two to the two leaves of P_4, respectively. Figure 2 gives an example for $S(\ell_1, \ell_2), T_1(s_1, t_1)$ and $T_2(s_2, t_2)$. Obviously, the orders of $S(\ell_1, \ell_2), T_1(s_1, t_1)$ and $T_2(s_2, t_2)$ are $\ell_1 + 2\ell_2 + 1, 2s_1 + 2t_1 + 5$ and $2s_2 + 2t_2 + 4$, respectively.

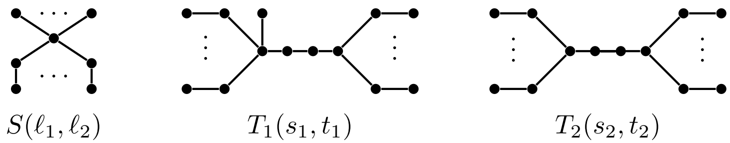


Figure 2. Graphs $S(\ell_1, \ell_2), T_1(s_1, t_1)$ and $T_2(s_2, t_2)$

Our last result characterizes all the graphs with order n and dissociation number $\varphi \in \{2, \lceil \frac{2}{3}n \rceil, n-2, n-1\}$ having the minimum Harary indices.

Theorem 1.4. *Let G be a graph in $\mathscr{G}_{n,\varphi}$, where $\varphi \in \{2, \lceil \frac{2}{3}n \rceil, n-2, n-1\}$.*

(i) *If $\varphi = \lceil \frac{2}{3}n \rceil$, then $H(G) \geq n \sum_{k=1}^{n-1} \frac{1}{k} - n + 1$ with equality if and only if $G \cong P_n$.*

(ii) *If $\varphi = 2$, then*

$$H(G) \geq \begin{cases} \frac{n(2n-3)}{4}, & \text{if } n \text{ is even;} \\ \frac{(n-1)(2n-1)}{4}, & \text{if } n \text{ is odd} \end{cases}$$

with equality if and only if $G \cong K_n - M(K_n)$, where $M(K_n)$ is a maximum matching of K_n.

(iii) *If* $n \geq 3$ *and* $\varphi = n-1$, *then*

$$H(G) \geq \begin{cases} \frac{17n^2+58n-88}{96}, & \text{if } n \text{ is even;} \\ \frac{(n-1)(17n+69)}{96}, & \text{if } n \text{ is odd} \end{cases}$$

with equality if and only if

$$G \cong \begin{cases} S\left(1, \frac{n-2}{2}\right), & \text{if } n \text{ is even;} \\ S\left(0, \frac{n-1}{2}\right), & \text{if } n \text{ is odd} \end{cases}$$

(iv) *If* $n \geq 6$ *and* $\varphi = n-2$, *then*

$$H(G) \geq \begin{cases} \frac{85n^2+198n-72}{480} - \frac{311}{420}\left\lfloor\frac{n-4}{4}\right\rfloor\left\lceil\frac{n-4}{4}\right\rceil, & \text{if } n \text{ is even;} \\ \frac{85n^2+116n+375}{480} + \left\lfloor\frac{n-4}{4}\right\rfloor\left(\frac{7}{15} - \frac{311}{420}\left\lceil\frac{n-4}{4}\right\rceil\right), & \text{if } n \text{ is odd;} \end{cases}$$

with equality if and only if

$$G \cong \begin{cases} T_2\left(\left\lfloor\frac{n-4}{4}\right\rfloor, \left\lceil\frac{n-4}{4}\right\rceil\right), & \text{if } n \text{ is even;} \\ T_1\left(\left\lfloor\frac{n-5}{4}\right\rfloor, \left\lceil\frac{n-5}{4}\right\rceil\right), & \text{if } n \text{ is odd.} \end{cases}$$

The remainder of this paper is organized as follows: In Section 2, we review some definitions and preliminary results. In Section 3, we give a proof for Theorem 1.2. In Section 4, we present a proof for Theorem 1.3, while in Section 5, we give a proof for Theorem 1.4. In the last section, we give some brief comments on our findings and proposed some problems for future studies.

2 Preliminary results

In this section, we give some preliminary results, which will be used to prove our main results. The following result immediately follows from the definition of dissociation number.

Lemma 2.1. *Let* G *be a simple graph. Then* $\varphi(G) - 1 \leq \varphi(G-v) \leq \varphi(G)$ *for any* $v \in V_G$.

Brešar et al. [2] gave a beautiful lower bound on the number of dissociation number of a tree, as showed below.

Lemma 2.2 ([2]). *Let T be a tree with n vertices. Then $\varphi(T) \geq \frac{2n}{3}$.*

For a graph G, denote by $\mathcal{P}(G)$ (resp. $\mathcal{Q}(G)$) the set of all pendent vertices (resp. quasi-pendent vertices) of G. In particular, let $\mathcal{Q}_2(G)$ be the set of all quasi-pendent vertices of degree 2 in G. The following result says that there exists a maximum dissociation set of G such that it contains all vertices of $\mathcal{P}(G) \cup \mathcal{Q}_2(G)$, which will play a crucial role in the proof of Theorem 1.3.

Lemma 2.3. *Let G be a graph with order $n \geq 5$. Then there exists a maximum dissociation set $S(G)$ such that $\mathcal{P}(G) \cup \mathcal{Q}_2(G) \subseteq S(G)$.*

Proof. First we show that there exist some maximum dissociation sets containing all pendent vertices of G. Let $\hat{S}(G)$ be a maximum dissociation set such that $|\hat{S}(G) \cap \mathcal{P}(G)|$ is as large as possible. Suppose that there is a vertex $v \in \mathcal{P}(G) \setminus \hat{S}(G)$. Let u be the neighbor of v. Then $u \in \hat{S}(G) \setminus \mathcal{P}(G)$. Let $\hat{S}'(G) = (\hat{S}(G) \setminus \{u\}) \cup \{v\}$. Then $\hat{S}'(G)$ is a maximum dissociation set of G such that $|\hat{S}'(G) \cap \mathcal{P}(G)| > |\hat{S}(G) \cap \mathcal{P}(G)|$, a contradiction. Therefore, $\mathcal{P}(G) \subseteq \hat{S}(G)$.

Denote by $\mathscr{D}(G)$ the set of all maximum dissociation sets that contain all pendent vertices of G. Similarly, let $S(G)$ be a set in $\mathscr{D}(G)$ such that $|S(G) \cap \mathcal{Q}_2(G)|$ is as large as possible. Suppose that there is a vertex $u \in \mathcal{Q}_2(G) \setminus S(G)$. Assume $N(u) = \{w, v\}$ with $d(v) = 1$. Then $\{v, w\} \subseteq S(G)$ and $w \notin \mathcal{Q}_2(G) \cup \mathcal{P}(G)$ since $n \geq 5$. Let $S'(G) = (S(G) \setminus \{w\}) \cup \{u\}$. Then $S'(G) \in \mathscr{D}(G)$ and $|S'(G) \cap \mathcal{Q}_2(G)| > |S(G) \cap \mathcal{Q}_2(G)|$, a contradiction. Consequently, $\mathcal{P}(G) \cup \mathcal{Q}_2(G) \subseteq S(G)$.

This completes the proof. ■

The next three conclusions involve the change of the Harary index after some graph transformations.

Lemma 2.4. *Let G be a simple connected graph. Then $H(G+uv) > H(G)$ for any $uv \notin E_G$.*

Lemma 2.5 ([36]). *Let G_1 and G_2 be two vertex-disjoint connected graphs with $v_i \in V_{G_i}$ and $|V_{G_i}| \geq 2$. Denote by G the graph obtained from $G_1 \cup G_2$ by joining an edge between v_1 and v_2, and G' the graph obtained from $G_1 \cup G_2$ by identifying vertices v_1 and v_2 (the new vertex is labeled by v) and attaching a pendent edge at v. Then $H(G) < H(G')$.*

The following result immediately follows from Lemma 2.5.

Corollary 2.6. *Let G be a connected graph with $|V_G| \geq 4$. Assume $v \in \mathcal{Q}_2(G)$ with $N(v) = \{w, u\}$ and $w \in \mathcal{P}(G)$. Then $H(G) < H(G - vw + uw)$.*

3 Proof of Theorems 1.2

In this section, we give the proof for Theorem 1.2, by which we characterize all the connected bipartite graphs with fixed order and dissociation number having the maximum Harary index.

Proof of Theorem 1.2. Assume $G^\star = (X, Y)$ is a connected bipartite graph having the maximum Harary index in $\mathscr{B}_{n,\varphi}$. Without loss of generality, assume that $|X| \geq |Y|$. Let S be a maximum dissociation set of $G^\star$. Then $\varphi = |S| \geq |X|$.

If $\varphi = |X|$, then $G^\star \cong K_{\varphi, n-\varphi}$ by Lemma 2.4. In the following, assume that $\varphi > |X|$. Then S can be partitioned as $S = X_1 \cup Y_2$ with $X_1 \subseteq X$ and $Y_2 \subseteq Y$. Let $X_2 = X \setminus X_1$ and $Y_1 = Y \setminus Y_2$, and let $|X_1| = a, |Y_1| = b, |X_2| = c$ and $|Y_2| = d$. Note that $|X_1 \cup Y_2| > |X| \geq |Y|$. Then $a > b$ and $c < d$. Recall that $G^\star$ is the bipartite graph with the maximum Harary index. Lemma 2.4 tells us that each vertex in X_1 is adjacent to each vertex in Y_1, each vertex in X_2 is adjacent to each vertex in Y, and there are as many matching edges as possible between X_1 and Y_2. If $d \geq a$, then there exists a set $Y_{21} \subseteq Y_2$ with $|Y_{21}| = d$ such that

$G^\star[X_1 \cup Y_{21}]$ is a perfect matching. By some direct calculations, we get

$$\begin{aligned} H(G^\star) =&(ac+bc+cd+a)+\frac{1}{2}\left[\binom{a}{2}+\binom{b}{2}+\binom{c}{2}+\binom{d}{2}+ac+bd\right] \\ &+\frac{1}{3}\left[a(a-1)+a(d-a)\right] \\ =&\frac{1}{4}(a^2+b^2+c^2+d^2)+\frac{1}{6}\left(6ab+3ac+2ad+6bc+3bd+6cd\right) \\ &+\frac{1}{12}(5a-3b-3c-3d). \end{aligned}$$

On the other hand, it is routine to check that

$$\begin{aligned} H(K_{a+d,b+c}) =&(a+d)(b+c)+\frac{1}{2}\left[\binom{a+d}{2}+\binom{b+c}{2}\right] \\ =&\frac{1}{4}(a^2+b^2+c^2+d^2)+\frac{1}{2}\left(2ab+2ac+ad+bc\right. \\ &\left.+2bd+2cd\right)-\frac{1}{4}(a+b+c+d). \end{aligned}$$

Therefore,

$$H(K_{a+d,b+c})-H(G^\star)=\frac{1}{6}(3c+d-4)a+\frac{1}{2}(d-c)b. \tag{1}$$

Note that $n \geq 3$ and $G^\star$ is connected. Then $\max\{b,c\} \geq 1$. If $c=0$, then $b \geq 1$ and thus $d \geq a \geq 2$. In view of (1), we get

$$H(K_{a+d,b+c})-H(G^\star) \geq \frac{1}{6}(a+3b-4)a > 0$$

If $c \geq 1$, then $d \geq 2$ and thus $H(K_{a+d,b+c})-H(G^\star) > 0$ immediately follows from (1). All the possible cases yield that $H(G^\star) < H(K_{a+d,b+c})$, contradicting to the choice of $G^\star$ since $\varphi(K_{a+d,b+c}) = a+d = \varphi(G^\star)$. In a similar way, there is also a contradiction when $d < a$. Therefore, $G^\star \cong K_{\varphi,n-\varphi}$. By a short calculation, we have $H(K_{\varphi,n-\varphi}) = \frac{n^2+(2\varphi-1)n-2\varphi^2}{4}$ and we are done. ■

4 Proof of Theorem 1.3

In this section, we give a proof for Theorem 1.3, by which we establish a sharp upper bound on the Harary index of a tree with given order and dissociation number. The extremal tree meeting the upper bound is also characterized. In order to achieve this goal, we need some crucial results.

Lemma 4.1 ([16,26])**.** *Let $T \in \mathscr{T}_n$. Then*

$$n\sum_{k=1}^{n-1}\frac{1}{k} - n + 1 \leq H(T) \leq \frac{(n-1)(n+2)}{4}.$$

The left equality holds if and only if $T \cong P_n$, whereas the right equality holds if and only if $T \cong S_n$.

Lemma 4.2. *Let $T \in \mathscr{T}_{n,\varphi}$ $(n \geq 3)$ and $\Delta(T)$ be the maximum degree of T. Then $\Delta(T) \leq 2\varphi - n + 1$ with equality if and only if $T \in \mathbb{S}^*_{n,\varphi}$.*

Proof. If $1 \leq n \leq 9$, then it is straightforward to check that $\Delta(T) \leq 2\varphi - n + 1$ with equality if and only if $T \in \mathbb{S}^*_{n,\varphi}$. Next, we assume that the result is true for each tree with order less than n.

Now, let T be a tree with order $n\,(\geq 10)$ and dissociation number φ. Choose a diameter path $P_\ell = v_1v_2v_3v_4\cdots v_\ell$ of T such that $d_T(v_2)$ is as large as possible. Then $N_T(v_2) \setminus \{v_3\} \subseteq \mathcal{P}(T)$ and $N_T(v_3) \setminus \{v_4\} \subseteq \mathcal{P}(T) \cup \mathcal{Q}(T)$.

If $d_T(v_2) \geq 4$, then it follows from Lemma 2.3 that $T - v_1 \in \mathscr{T}_{n-1,\varphi-1}$. Hence, by the induction hypothesis, one has

$$\Delta(T) \leq \Delta(T - v_1) + 1 \leq 2(\varphi - 1) - (n-1) + 1 + 1 = 2\varphi - n + 1. \quad (2)$$

The equality in (2) holds if and only if v_2 is the unique vertex with maximum degree $2\varphi - n + 1$ in T and $T - v_1 \in \mathbb{S}^*_{n-1,\varphi-1}$. This together with $d_{T-v_1}(v_2) = \Delta(T - v_1) = 2\varphi - n > 3$ gives the inequality in (2) with equality if and only if $T \in \mathbb{S}^*_{n,\varphi}$.

If $d_T(v_2) = 3$, then by Lemma 2.3, we have $T - v_1 - v_2 - w \in \mathscr{T}_{n-3,\varphi-2}$, where w is the unique vertex in $N_T(v_2) \setminus \{v_1, v_3\}$. Applying the induction hypothesis to $T - v_1 - v_2 - w$ yields

$$\begin{aligned} \Delta(T) &\leq \Delta(T - v_1 - v_2 - w) + 1 \\ &\leq 2(\varphi - 2) - (n - 3) + 1 + 1 \\ &= 2\varphi - n + 1. \end{aligned} \tag{3}$$

The equality in (3) holds if and only if v_3 is the unique vertex with maximum degree $2\varphi - n + 1$ in T and $T - v_1 - v_2 - w \in \mathbb{S}^*_{n-3,\varphi-2}$. Note that $d_{T-v_1-v_2-w}(v_3) = \Delta(T - v_1 - v_2 - w) = 2\varphi - n > 3$. Therefore, the equality in (3) holds if and only if $T \in \mathbb{S}^*_{n,\varphi}$.

If $d_T(v_2) = 2$ and $d_T(v_3) = 2$, then again by Lemma 2.3 and the induction hypothesis, one has

$$\begin{aligned} \Delta(T) &\leq \Delta(T - v_1 - v_2 - v_3) + 1 \\ &\leq 2(\varphi - 2) - (n - 3) + 1 + 1 \\ &= 2\varphi - n + 1. \end{aligned} \tag{4}$$

The equality in (4) holds if and only if v_4 is the unique vertex with maximum degree $2\varphi - n + 1$ in T and $T - v_1 - v_2 - v_3 \in \mathbb{S}^*_{n-3,\varphi-2}$. In a similar way as above, the equality in (4) holds if and only if $T \in \mathbb{S}^*_{n,\varphi}$.

If $d_T(v_2) = 2$ and $d_T(v_3) \geq 3$, then $d_T(z) \leq 2$ for every $z \in N_T(v_3) \setminus \{v_4\}$ and thus $T - v_1 \in \mathscr{T}_{n-1,\varphi-1}$ by Lemma 2.3. This leads to

$$\Delta(T) = \Delta(T - v_1) \leq 2(\varphi - 1) - (n - 1) + 1 < 2\varphi - n + 1.$$

This completes the proof. ■

Now we are ready to give the proof for Theorem 1.3, by which we determine the sharp upper bound and the corresponding extremal tree of the Harary index in $\mathscr{T}_{n,\varphi}$.

Proof of Theorem 1.3. We proceed by induction on n. If $\varphi = n - 1$, then Lemma 4.1 gives $H(T) \leq \frac{(n-1)(n+2)}{4}$ with equality if and only if $T \cong S_n \cong S^*_{n,n-1}$. If $3 \leq n \leq 9$, then it is straightforward to check that $H(T) \leq \frac{1}{12}n^2 + \frac{17}{12}n + \frac{1}{6}\varphi^2 - \frac{5}{6}\varphi - \frac{3}{2}$ and the equality holds if and only if

$T \cong S^*_{n,\varphi}$, as desired. In the following, we assume that the result holds for each tree with order less than n and dissociation number $\varphi \le n-2$.

Now, choose $T \in \mathscr{T}_{n,\varphi}$ $(n \ge 10, \varphi \le n-2)$ such that $H(T)$ is as large as possible. Let $P_k = v_1v_2v_3v_4\cdots v_k$ be a diametral path of T. Then it follows from Lemma 2.1 that $\varphi(T-v_1) \in \{\varphi, \varphi-1\}$. We proceed by distinguishing the following two cases to complete the proof.

Case 1. $\varphi(T-v_1) = \varphi-1$. It follows from Lemma 4.2 that $\Delta(T-v_1) \le 2\varphi - n$. Then

$$\begin{aligned}\sum_{v\in V_{T-v_1}} \frac{1}{d_{T-v_1}(v,v_2)+1} \le & 1 + \frac{1}{2}d_{T-v_1}(v_2) + \frac{1}{3}(n - d_{T-v_1}(v_2) - 2)\\ =&\frac{1}{6}d_{T-v_1}(v_2) + \frac{1}{3}n + \frac{1}{3}\\ \le&\frac{1}{6}n + \frac{1}{3}\varphi + \frac{1}{3}. \end{aligned} \tag{5}$$

The equality in (5) holds if and only if $d_{T-v_1}(v_2) = \Delta(T-v_1) = 2\varphi - n$ and $d_{T-v_1}(v,v_2) = 2$ for any $v \notin N_{T-v_1}[v_2]$. Again by Lemma 4.2, we have (5) holds with equality if and only if $T - v_1 \cong S^*_{n-1,\varphi-1}$ with $d_{T-v_1}(v_2) = 2\varphi - n$.

The induction hypothesis together with (5) yields

$$\begin{aligned} H(T) =& H(T-v_1) + \sum_{v\in V_{T-v_1}} \frac{1}{d_T(v,v_1)}\\ =&H(T-v_1) + \sum_{v\in V_{T-v_1}} \frac{1}{d_{T-v_1}(v,v_2)+1}\\ \le&\frac{1}{12}(n-1)^2 + \frac{17}{12}(n-1) + \frac{1}{6}(\varphi-1)^2 - \frac{5}{6}(\varphi-1)\\ &-\frac{3}{2} + \frac{1}{6}n + \frac{1}{3}\varphi + \frac{1}{3}\\ =&\frac{1}{12}n^2 + \frac{17}{12}n + \frac{1}{6}\varphi^2 - \frac{5}{6}\varphi - \frac{3}{2}. \end{aligned} \tag{6}$$

The equality in (6) holds if and only if $T-v_1 \cong S^*_{n-1,\varphi-1}$ with $d_{T-v_1}(v_2) = \Delta(T-v_1) = 2\varphi-n$. Note that $\varphi \ge \frac{2}{3}n$ by Lemma 2.2. Then $2\varphi-n \ge \frac{n}{3} > 3$, implying (6) holds with equality if and only if $T \cong S^*_{n,\varphi}$.

If $\varphi \le n-3$, then there exist at least two pendent vertices such that the distance between them is 4, contradicting to the fact that v_1 lies on a diameter path of T. Therefore, $T \ncong S^*_{n,\varphi}$ and then $H(T) < \frac{1}{12}n^2 + \frac{17}{12}n + \frac{1}{6}\varphi^2 - \frac{5}{6}\varphi - \frac{3}{2} = H(S^*_{n,\varphi})$, which contradicts to the choice of T. Consequently, $\varphi = n-2$ and $H(T) \le \frac{1}{4}n^2 - \frac{1}{12}n + \frac{5}{6}$ with equality if and only if $T \cong S^*_{n,n-2}$.

Case 2. $\varphi(T - v_1) = \varphi$. Then there exists a maximum dissociation set, say $S(T)$, such that $v_1 \notin S(T)$. Combining with Lemma 2.3, we get $d(v_2) \le 3$ and thus $d(v_2) = 3$ by Corollary 2.6. Assume that w is the unique vertex in $N(v_2) \setminus \{v_1, v_3\}$. Put $T' := T - v_1 - v_2 - w$. Then $T' \in \mathscr{T}_{n-3,\varphi-2}$ again by Lemma 2.3. In a similar way as in Case 1, we get

$$\begin{aligned}\sum_{v\in V_{T'}} \frac{1}{d_{T'}(v,v_3)+2} &\le \frac{1}{6}n + \frac{1}{6}\varphi - \frac{1}{2},\\ \sum_{v\in V_{T'}} \frac{1}{d_{T'}(v,v_3)+1} &\le \frac{1}{6}n + \frac{1}{3}\varphi - \frac{1}{3}.\end{aligned} \tag{7}$$

Each equality in (7) holds if and only if $T' \cong S^*_{n-3,\varphi-2}$ with $d_{T'}(v_3) = \Delta(T') = 2\varphi - n$ and $d_{T'}(v, v_3) = 2$ for any $v \notin N_{T'}[v_3]$. The induction hypothesis together with (7) yields

$$\begin{aligned}H(T) =& H(T') + 2\sum_{v\in V_{T'}} \frac{1}{d_T(v,v_1)} + \sum_{v\in V_{T'}} \frac{1}{d_T(v,v_2)} + \frac{5}{2}\\ =& H(T') + 2\sum_{v\in V_{T'}} \frac{1}{d_{T'}(v,v_3)+2} + \sum_{v\in V_{T'}} \frac{1}{d_{T'}(v,v_3)+1} + \frac{5}{2}\\ \le& \frac{(n-3)^2}{12} + \frac{17(n-3)}{12} + \frac{(\varphi-2)^2}{6} - \frac{5(\varphi-2)}{6} - \frac{3}{2}\\ &+ 2\left(\frac{n}{6} + \frac{\varphi}{6} - \frac{1}{2}\right) + \left(\frac{n}{6} + \frac{\varphi}{3} - \frac{1}{3}\right) + \frac{5}{2}\\ =& \frac{1}{12}n^2 + \frac{17}{12}n + \frac{1}{6}\varphi^2 - \frac{5}{6}\varphi - \frac{3}{2}.\end{aligned} \tag{8}$$

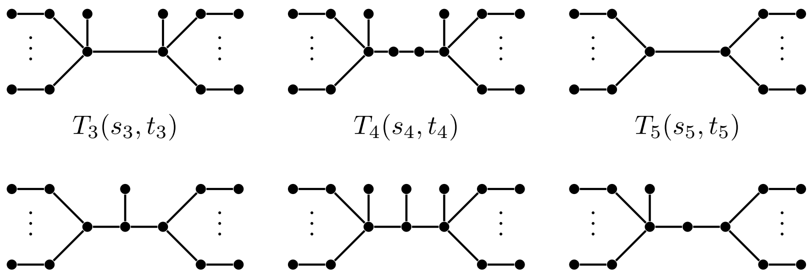
The equality in (8) holds if and only if $T' \cong S^*_{n-3,\varphi-2}$ with $d_{T'}(v_3) = \Delta(T') = 2\varphi - n > 3$, which means (8) holds with equality if and only if $T \cong S^*_{n,\varphi}$.

This completes the proof. ∎

5 Proof of Theorem 1.4

In this section, we give the proof for Theorem 1.4, by which we characterize all the graphs with order n and dissociation number $\varphi \in \{2, \lceil \frac{2}{3}n \rceil, n-2, n-1\}$ having the minimum Harary indices.

Let $T_3(s_3, t_3)$ (resp. $T_4(s_4, t_4)$) be the tree obtained from P_4 (resp. P_6) by attaching s_3 (resp. s_4) and t_3 (resp. t_4) pendent paths of length two to the two quasi-pendent vertices of P_4 (resp. P_6), respectively. Let $T_5(s_5, t_5)$ (resp. $T_6(s_6, t_6)$) be the tree obtained from K_2 (resp. S_4) by attaching s_5 (resp. s_6) and t_5 (resp. t_6) pendent paths of length two to two leaves of K_2 (resp. S_4), respectively. Let $T_7(s_7, t_7)$ be the tree obtained from $S(1, 2)$ by attaching s_7 and t_7 pendent paths of length two to the two quasi-pendent vertices with degree 2 of $S(1, 2)$, respectively. Let $T_8(s_8, t_8)$ be the tree obtained from P_3 by attaching one pendent edge and s_8 pendent paths of length two to one leaf of P_3, and then attaching t_8 pendent paths of length two to another leaf of P_3. Figure 3 gives an example for $T_i(s_i, t_i)$ $(3 \le i \le 8)$. Obviously, $|V_{T_i(s_i,t_i)}| = 2s_i + 2t_i + 4$ for $i \in \{3, 6, 8\}$, $|V_{T_j(s_j,t_j)}| = 2s_j + 2t_j + 6$ for $j \in \{4, 7\}$ and $|V_{T_5(s_5,t_5)}| = 2s_5 + 2t_5 + 2$.



$T_3(s_3, t_3)$ $T_4(s_4, t_4)$ $T_5(s_5, t_5)$

$T_6(s_6, t_6)$ $T_7(s_7, t_7)$ $T_8(s_8, t_8)$

Figure 3. Tree $T_i(s_i, t_i)$ $(3 \le i \le 8)$.

In order to show Theorem 1.4, we need some preliminaries. The following result is well known.

Lemma 5.1 ([28,40]). *Let G be a connected graph with n vertices. Then*

$$H(G) \geq n\sum_{k=1}^{n-1}\frac{1}{k} - n + 1$$

with equality if and only if $G \cong P_n$.

Lemma 5.2. *If $s_2 \geq t_2 \geq 1$, then $H(T_2(s_2, t_2)) < H(T_2(s_2+1, t_2-1))$.*

Proof. Note that $T_2(s_2, t_2)$ can be obtained from $T_2(s_2, t_2-1)$ by attaching a pendent path of length two to the vertex of degree t_2, whereas $T_2(s_2+1, t_2-1)$ can be obtained from $T_2(s_2, t_2-1)$ by attaching a pendent path of length two to the vertex of degree s_2+1. Then

$$\begin{aligned}
&H(T_2(s_2+1, t_2-1)) - H(T_2(s_2, t_2))\\
=&\left[\left(1+\frac{s_2+1}{2}+\frac{s_2+1}{3}+\frac{1}{4}+\frac{t_2-1}{5}+\frac{t_2-1}{6}\right)+\left(\frac{1}{2}+\frac{s_2+1}{3}+\frac{s_2+1}{4}\right.\right.\\
&\left.\left.+\frac{1}{5}+\frac{t_2-1}{6}+\frac{t_2-1}{7}\right)\right]-\left[\left(1+\frac{t_2}{2}+\frac{t_2}{3}+\frac{1}{4}+\frac{s_2}{5}+\frac{s_2}{6}\right)\right.\\
&\left.+\left(\frac{1}{2}+\frac{t_2}{3}+\frac{t_2}{4}+\frac{1}{5}+\frac{s_2}{6}+\frac{s_2}{7}\right)\right]\\
=&\frac{311}{420}(s_2-t_2+1) > 0.
\end{aligned}$$

This completes the proof. ∎

Lemma 5.3. *If $(s_4, t_4) \neq (0, 0)$, then*

$$H(T_4(s_4, t_4)) > \min\left\{H(T_2(s_4, t_4+1)), H(T_2(s_4+1, t_4))\right\}.$$

Proof. Assume, without loss of generality, that $s_4 \geq t_4$. Then $s_4 \geq 1$. A short calculation yields

$$\begin{aligned}&H(T_4(s_4,t_4))-H(T_2(s_4,t_4+1))\\=&\left[1+\frac{1}{2}(s_4+1)+\frac{1}{3}(s_4+1)+\frac{1}{4}+\frac{1}{5}(t_4+1)+\frac{1}{6}t_4\right]\\&-\left[1+\frac{1}{2}+\frac{1}{3}(t_4+1)+\frac{1}{4}(t_4+1)+\frac{1}{5}+\frac{1}{6}s_4+\frac{1}{7}\right]\\=&\frac{11}{21}s_4-\frac{13}{60}t_4>0.\end{aligned}$$

This completes the proof. ∎

Now we are ready to give the proof for Theorem 1.4, by which we concentrate on graphs having the minimum Harary indices with given order n and dissociation number $\varphi \in \{2, \lceil \frac{2}{3}n \rceil, n-2, n-1\}$.

Proof of Theorem 1.4. (i) It immediately follows from Lemma 5.1 and $\varphi(P_n) = \lceil \frac{2}{3}n \rceil$.

(ii) Let $G \in \mathscr{G}_{n,2}$ be the graph having the minimum Harary index. Then G does not contain $3K_1$ or $K_2 \cup K_1$ as its induced subgraph, which implies $d_{\bar{G}}(v) \le 1$ for every $v \in V_G$, where $\bar{G}$ is the complement graph of G. That is to say, $E_{\bar{G}}$ is a matching of K_n. Combining with Lemma 2.4, we get $G \cong K_n - M(K_n)$, where $M(K_n)$ is a maximum matching of K_n. Some direct calculations yield that $H(K_n - M(K_n)) = \frac{n(2n-3)}{4}$ if n is even and $H(K_n - M(K_n)) = \frac{(n-1)(2n-1)}{4}$ otherwise.

(iii) Let $G \in \mathscr{G}_{n,n-1}$ ($n \ge 3$) be the graph having the minimum Harary index and let $S = S_1 \cup S_2$ be a maximum dissociation set of G such that $G[S_1]$ is a perfect matching and S_2 is an independent set. Assume that $V_G = \{v_1, v_2, \ldots, v_n\}$ and $S = V_G \setminus \{v_1\}$. Then $S_2 \subseteq N(v_1) \cap \mathcal{P}(G)$.

If there exist two vertices, say v_{n-1} and v_n, such that $\{v_{n-1}, v_n\} \subseteq S_2$, then put $G' = G - v_1v_{n-1} + v_nv_{n-1}$ and thus $G' \in \mathscr{G}_{n,n-1}$ by Lemma 2.3. In view of Corollary 2.6, we have $H(G') < H(G)$, contradicting to the choice of G. Therefore, $|S_2| \le 1$. This implies $G \cong S\left(1, \frac{n-2}{2}\right)$ if n is even and $G \cong S\left(0, \frac{n-1}{2}\right)$ if n is odd, where $S(\ell_1, \ell_2)$ is the graph as shown in

Figure 2. Some simple calculations give $H(S\left(1, \frac{n-2}{2}\right)) = \frac{17n^2+58n-88}{96}$ and $H(S\left(0, \frac{n-1}{2}\right)) = \frac{(n-1)(17n+69)}{96}$.

(iv) Let $G \in \mathscr{G}_{n,n-2}$ $(n \geq 6)$ be the graph having the minimum Harary index and let $S = S_1 \cup S_2$ be a maximum dissociation set of G such that $G[S_1]$ is a perfect matching and S_2 is an independent set. Assume that $V_G = \{v_1, v_2, \ldots, v_n\}$ and $S = V_G \setminus \{v_1, v_2\}$. Note that $\varphi(G) = n - 2$. Then $\min\{|N(v_1) \setminus \{v_2\}|, |N(v_2) \setminus \{v_1\}|\} \geq 1$. Since $|N(v_1) \cap N(v_2)| \leq 1$ by Lemma 2.4, there are at least $|S_2| - 1$ leaves in S_2. In a similar way as in (iii), we get $|S_2| \leq 3$. If n is even, then $|S_2| \in \{0, 2\}$. We proceed by distinguishing the following two cases to complete the proof.

Case 1. $N(v_1) \cap N(v_2) = \emptyset$. If $|S_2| = 2$ and $v_1 \in N(v_2)$, then $G \cong T_3(s_3, t_3)$ for $\min\{s_3, t_3\} \geq 1$ and $s_3 + t_3 = \frac{n-4}{2}$. By Lemma 2.5, we have $H(T_2(s_3, t_3)) < H(T_3(s_3, t_3))$. Note that $T_2(s_3, t_3) \in \mathscr{G}_{n,n-2}$, a contradiction.

If $|S_2| = 2$ and $v_1 \notin N(v_2)$, then $G \cong T_4(s_4, t_4)$ for $s_4 + t_4 = \frac{n-6}{2}$. Furthermore, if $(s_4, t_4) = (0, 0)$, then $G \cong T_2(1, 0)$. If $(s_4, t_4) \neq (0, 0)$, then by Lemma 5.3, $\min\{H(T_2(s_4, t_4 + 1)), H(T_2(s_4 + 1, t_4))\} < H(G)$, which leads to a contradiction since $\{T_2(s_4, t_4 + 1), T_2(s_4 + 1, t_4)\} \subseteq \mathscr{G}_{n,n-2}$.

If $|S_2| = 0$ and $v_1 \in N(v_2)$, then $G \cong T_5(s_5, t_5)$ with $\min\{s_5, t_5\} \geq 1$ and $s_5 + t_5 = \frac{n-2}{2}$. In addition, if $s_5 = t_5 = 1$, then $G \cong T_2(1, 0)$. If $(s_5, t_5) \neq (1, 1)$, then it is obvious $H(G) > \begin{cases} H(T_2(s_5 - 1, t_5)), & \text{if } s_5 \geq 2; \\ H(T_2(s_5, t_5 - 1)), & \text{if } t_5 \geq 2, \end{cases}$ which is impossible since $\{T_2(s_5 - 1, t_5), T_2(s_5, t_5 - 1)\} \subseteq \mathscr{G}_{n,n-2}$.

If $|S_2| = 0$ and $v_1 \notin N(v_2)$, then $G \cong T_2(s_2, t_2)$ with $s_2 + t_2 = \frac{n-4}{2}$.

Case 2. $|N(v_1) \cap N(v_2)| = 1$. In this case, one has $v_1 \notin N(v_2)$ by Lemma 2.4. If $|S_2| = 0$, then $G \cong T_6(s_6, t_6)$ with $(s_6, t_6) \neq (0, 0)$ and $s_6 + t_6 = \frac{n-4}{2}$, leading to a contradiction since $H(T_2(s_6, t_6)) < H(G)$ by Lemma 2.5 and $T_2(s_6, t_6) \in \mathscr{G}_{n,n-2}$.

If $|S_2| = 2$ and $N(v_1) \cap N(v_2) \subseteq S_1$, then $G \cong T_7(s_7, t_7)$ with $(s_7, t_7) \neq (0, 0)$ and $s_7 + t_7 = \frac{n-6}{2}$. Again by Lemma 2.5, $H(T_4(s_7, t_7)) < H(G)$. Note that $T_4(s_7, t_7) \in \mathscr{G}_{n,n-2}$, a contradiction.

If $|S_2| = 2$ and $N(v_1) \cap N(v_2) \subseteq S_2$, then $G \cong T_8(s_8, t_8)$ with $t_8 \geq 1$ and $s_8 + t_8 = \frac{n-4}{2}$. Similarly, $G \cong T_2(0, t_8)$ for $s_8 = 0$ and $H(T_2(s_8, t_8)) < H(G)$

for $s_8 \geq 1$, a contradiction.

All the possible cases lead to $G \cong T_2(s_2, t_2)$ for some $s_2 + t_2 = \frac{n-4}{2}$ and then

$$\begin{aligned}
H(T_2(s_2,t_2)) =& n-1+\frac{1}{2}\left[\binom{s_2+1}{2}+\binom{t_2+1}{2}+s_2+t_2+2\right]+\frac{1}{3}\left[2\binom{s_2}{2}\right. \\
&\left.+2\binom{t_2}{2}+2s_2+2t_2+1\right]+\frac{1}{4}\left[\binom{s_2}{2}+\binom{t_2}{2}+2s_2+2t_2\right] \\
&+\frac{1}{5}(s_2+t_2+s_2t_2)+\frac{1}{6}\cdot 2s_2t_2+\frac{1}{7}s_2t_2 \\
=&\frac{17}{96}n^2+\frac{33}{80}n-\frac{3}{20}-\frac{311}{420}s_2t_2. \qquad (9)
\end{aligned}$$

Therefore, $G \cong T_2\left(\left\lfloor\frac{n-4}{4}\right\rfloor, \left\lceil\frac{n-4}{4}\right\rceil\right)$ by Lemma 5.2 and then

$$H(G) = \frac{85n^2+198n-72}{480} - \frac{311}{420}\left\lfloor\frac{n-4}{4}\right\rfloor\left\lceil\frac{n-4}{4}\right\rceil$$

by (9).

In a similar way, we obtain $G \cong T_1\left(\left\lfloor\frac{n-5}{4}\right\rfloor, \left\lceil\frac{n-5}{4}\right\rceil\right)$ and

$$H(G) = \frac{85n^2+116n+375}{480} + \left\lfloor\frac{n-4}{4}\right\rfloor\left(\frac{7}{15}-\frac{311}{420}\left\lceil\frac{n-4}{4}\right\rceil\right)$$

when n is odd.

This completes the proof. ■

6 Concluding remarks

In 1986, Brualdi and Solheid [3] put forward the following well-known problem, which has became to be one of the classical problems in spectral graph theory.

Problem 1. *For a set* $\mathbb{G}$ *of graphs satisfying some certain conditions, determine* $\min\{\rho(G) \mid G \in \mathbb{G}\}$ *and* $\max\{\rho(G) \mid G \in \mathbb{G}\}$*, and characterize the extreme graphs which achieve the minimum or maximum value, where* $\rho(G)$ *denotes the spectral radius of* G*.*

Inspired by Problem 1, it's natural to consider the following interesting problem:

Problem 2. *For a set* $\mathbb{G}$ *of graphs satisfying some certain conditions, determine* $\min\{H(G)\,|\,G\in\mathbb{G}\}$ *and* $\max\{H(G)\,|\,G\in\mathbb{G}\}$*, and characterize the extreme graphs which achieve the minimum or maximum value.*

In this paper we focus on Problem 2 for $\mathbb{G}\in\{\mathscr{G}_{n,\varphi},\mathscr{B}_{n,\varphi},\mathscr{T}_{n,\varphi}\}$. Theorem 1.1 (resp. Theorem 1.2, Theorem 1.3) characterizes all the connected graphs (resp. bipartite graphs, trees) having the maximum Harary indices among all connected graphs (resp. bipartite graphs, trees) with given order and dissociation number. Theorem 1.4 determines the graphs with fixed order n and dissociation number $\varphi\in\{2,\left\lceil\frac{2}{3}n\right\rceil,n-2,n-1\}$ having the minimum Harary indices.

It is nature to extend this study through examining the following extreme graphs:

- trees with fixed order n and dissociation number φ_1 having the minimum Harary indices, where $\left\lceil\frac{2}{3}n\right\rceil<\varphi_1<n-2$;
- connected bipartite graphs with fixed order n and dissociation number φ_2 having the minimum Harary indices, where $\left\lceil\frac{n}{2}\right\rceil<\varphi_2<n-2$;
- graphs with fixed order n and dissociation number φ_3 having the minimum Harary indices, where $2<\varphi_3<n-2$.

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