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On Harary index of graphs[☆]

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ABSTRACT

The Harary index is defined as the sum of reciprocals of distances between all pairs of vertices of a connected graph. For a connected graph $G = (V, E)$ and two nonadjacent vertices v_i and v_j in $V(G)$ of G, recall that $G+v_iv_j$ is the supergraph formed from G by adding an edge between vertices v_i and v_j. Denote the Harary index of G and $G + v_iv_j$ by $H(G)$ and $H(G + v_iv_j)$, respectively. We obtain lower and upper bounds on $H(G + v_iv_j) - H(G)$, and characterize the equality cases in those bounds. Finally, in this paper, we present some lower and upper bounds on the Harary index of graphs with different parameters, such as clique number and chromatic number, and characterize the extremal graphs at which the lower or upper bounds on the Harary index are attained.

1. Introduction

The Harary index of a graph G, denoted by $H(G)$, has been introduced independently by Plavšić et al. [24] and by Ivanciuc et al. [19] in 1993. It has been named in honor of Professor Frank Harary on the occasion of his 70th birthday. The Harary index is defined as follows:

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

where the summation goes over all unordered pairs of vertices of G and $d_G(u, v)$ denotes the distance of the two vertices u and v in the graph G (i.e., the number of edges in a shortest path connecting u and v). Mathematical properties and applications of H are reported in [4,8,9,23,29–31,33].

Another two related distance-based topological indices of the graph G are the Wiener index $W(G)$ and the hyper-Wiener index $WW(G)$. As an oldest topological index, the Wiener index of a (molecular) graph G, first introduced by Wiener [28] in 1947, was defined as

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

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with the summation going over all unordered pairs of vertices of G. The hyper-Wiener index of G, first introduced by Randić [25] in 1993, is nowadays defined as [22]:

$$WW(G) = \frac{1}{2}\sum_{u,v\in V(G)} d_G(u,v) + \frac{1}{2}\sum_{u,v\in V(G)} d_G(u,v)^2.$$

Mathematical properties and applications of Wiener index and hyper-Wiener index are extensively reported in the literature [6,7,9–16,28].

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

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

The maximum value of k for which $\gamma(G,k)$ is non-zero, is the diameter of the graph G, and will be denoted by d.

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

$$H(G) = \sum_{i=1}^{k} H(G_i) \quad \text{where } G_1, G_2, \ldots, G_k \text{ are the components of } G.$$

A molecular graph is a connected graph of maximum degree at most 4. It models the skeleton of a molecule [27]. The bounds of a descriptor are important information of a (molecular) graph in the sense that they establish the approximate range of the descriptor in terms of molecular structural parameters. Since determining the exact value of the Harary index of a (molecular) graph, though this formula (1) is efficient, is generally difficult, providing some (upper or lower) bounds for the Harary index of some (molecular) graphs is very useful. Its applications in this aspect includes the characterization of molecular graphs, measuring landscape connectivity [20,26], etc. (see [5,21,33] and the references therein).

All graphs considered in this paper are finite and simple. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The *degree* of $v_i \in V(G)$, denoted by $d_G(v_i)$ or $d(v_i)$ for short, is the number of vertices in G adjacent to v_i. For a subset W of $V(G)$, let $G - W$ be the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, for a subset E' of $E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. If $W = \{v_i\}$ and $E' = \{v_jv_k\}$, the subgraphs $G - W$ and $G - E'$ will be written as $G - v_i$ and $G - v_jv_k$ for short, respectively. For any two nonadjacent vertices v_i and v_j in graph G, we use $G + v_iv_j$ to denote the graph obtained by adding a new edge v_iv_j to graph G. The *chromatic number* of a graph G, denoted by $\chi(G)$, is the minimum number of colors such that G can be colored with these colors such that no two adjacent vertices have the same color. A *clique* of graph G is a subset V_0 of $V(G)$ such that in $G[V_0]$, the subgraph of G induced by V_0, any two vertices are adjacent. The *clique number* of G, denoted by $\omega(G)$, is the number of vertices in the largest clique of G. We denote by K_n, P_n and C_n the complete graph, the path and the cycle on n vertices throughout this paper. For other undefined notations and terminology from graph theory, the readers are referred to [1].

Let $\mathcal{W}_{n,k}$ and $\mathcal{X}_{n,k}$ be the set of connected n-vertex graphs with clique number k and the set of connected graphs of order n with chromatic number k, respectively. Assume that $n_1+n_2+\cdots+n_k = n$. We denote by $K_{n_1,n_2,\ldots,n_k}$ the complete k-partite graph of order n whose partition sets are of size $n_1, n_2, \ldots, n_k$, respectively. Recall that, as a special k-partite graph of order n, the Turán graph $T_n(k)$ is a complete k-partite graph whose partition sets differ in size by at most 1. Denote by $K_{n,k}$ the graph obtained by identifying one vertex of K_k with a pendent vertex of path P_{n-k+1}. Note that $K_{n,k}$ is just a *kite graph*.

The paper is organized as follows. In Section 2, we give a list of lemmas and preliminaries. In Section 3, we obtain lower and upper bounds on $H(G + v_iv_j) - H(G)$, and characterize the equality cases in those bounds, where v_i and v_j are two nonadjacent vertices of G. Finally, in Section 4, we present some lower and upper bounds on the Harary index of graphs with different parameters, such as clique number and chromatic number, and characterize the extremal graphs at which the lower or upper bounds on the Harary index are attained, in particular, the extremal graphs in $\mathcal{W}_{n,k}$ and $\mathcal{X}_{n,k}$ are completely characterized, respectively.

2. Preliminaries

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

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

Since the following two lemmas are from an unpublished paper [29] (which is under review in some journal), we give the proofs below for them.

Lemma 2.1 ([29]). *Let G be a graph of order n and v_i be a pendent vertex of G with $v_iv_j \in E(G)$. Then we have $H(G) = H(G - v_i) + n - 1 - Q_{G-v_i}(v_j)$.*

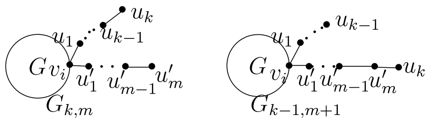

Fig. 1. The graphs $G_{k,m}$ and $G_{k-1,m+1}$.

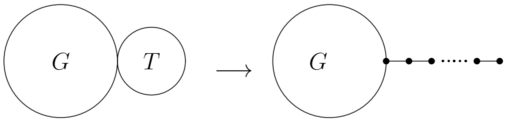

Fig. 2. The graphs in Corollary 2.1.

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

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

completing the proof of the lemma. □

Let G be a graph with $v_i \in V(G)$. As shown in Fig. 1, for two integers $m \geq k \geq 1$, let $G_{k,m}$ be the graph obtained from G by attaching at v_i two new paths $P : v_iu_1u_2\cdots u_k$ and $Q : v_iu'_1u'_2\cdots u'_m$ of lengths k and m, where $u_1, u_2, \ldots, u_k$ and $u'_1, u'_2, \ldots, u'_m$ are distinct new vertices. Suppose that $G_{k-1,m+1} = G_{k,m} - u_{k-1}u_k + u'_mu_k$. A related graph transformation is given in the following lemma.

Lemma 2.2 ([29]). *Let $G \neq K_1$ be a connected graph of order n and $v_i \in V(G)$. If $m \geq k \geq 1$, then $H(G_{k,m}) > H(G_{k-1,m+1})$.*

Proof. By Lemma 2.1, we have

$$\begin{aligned}
&H(G_{k,m}) = H(G_{k-1,m}) + n + k + m - 1 - Q_{G_{k-1,m}}(u_{k-1}),\\
&H(G_{k-1,m+1}) = H(G_{k-1,m}) + n + k + m - 1 - Q_{G_{k-1,m}}(u'_m), \text{ and}\\
&H(G_{k,m}) - H(G_{k-1,m+1}) = Q_{G_{k-1,m}}(u'_m) - Q_{G_{k-1,m}}(u_{k-1})\\
&\qquad = Q_{G-v_i}(u'_m) - Q_{G-v_i}(u_{k-1})\\
&\qquad \text{(because of the symmetry of } u'_m \text{ and } u_{k-1} \text{ in the path } P = u_{k-1}u_{k-2}\cdots u_1v_iu'_1\cdots u'_m)\\
&\qquad > 0.
\end{aligned}$$

Note that the last inequality holds because of the fact that $d_{G-v_i}(v_j, u'_m) > d_{G-v_i}(v_j, u_{k-1})$ for any vertex v_j in $G - v_i$. □

By repeating Lemma 2.2, the following remark is easily obtained.

Corollary 2.1. *If a tree T of size t attached to a graph G is replaced by a path P_{t+1} as shown in Fig. 2, the Harary index decreases.*

Lemma 2.3. *Let G be a connected graph of order $n > 2$ and v_i, v_j be its distinct vertices with $Q_G(v_i) = Q_G(v_j)$. Suppose that $G^*_{s,t}$ is a graph obtained from G by attaching at v_i one path $P_s(v_i) : v_iu_1u_2\ldots u_s$ and at v_j the other path $P_t(v_j) : yu'_1u'_2\ldots u'_t$, and $G^*_{s+1,t-1} = G^*_{s,t} - u'_{t-1}u'_t + u_su'_t$. If $s \geq t \geq 1$, then $H(G^*_{s,t}) > H(G^*_{s+1,t-1})$.*

Proof. Applying Lemma 2.1 to u'_t's of $G^*_{s,t}$ and $G^*_{s+1,t-1}$, respectively, we have

$$\begin{aligned}
&H(G^*_{s,t}) = H(G^*_{s,t-1}) + n + s + t - 1 - Q_{G^*_{s,t-1}}(u'_{t-1}),\\
&H(G^*_{s+1,t-1}) = H(G^*_{s,t-1}) + n + s + t - 1 - Q_{G^*_{s,t-1}}(u_s).
\end{aligned}$$

Therefore, we obtain

$$\begin{aligned}
H(G^*_{s,t}) - H(G^*_{s+1,t-1}) &= Q_{G^*_{s,t-1}}(u_s) - Q_{G^*_{s,t-1}}(u'_{t-1})\\
&> 0.
\end{aligned}$$

Note that the last inequality holds in view of the facts that $Q_G(v_i) = Q_G(v_j)$ and $s > t - 1$. Thus we complete the proof of this lemma. □

Based on Lemma 2.3, we obtain the next corollary immediately.

Corollary 2.2. *Let G be a connected graph of order $n > 2$ and v_i, v_j be its distinct vertices with $Q_G(v_i) = Q_G(v_j)$. Suppose that $G^*_{s,t}$ is a graph obtained from G by attaching at v_i one path of length s and at v_j the other path of length t, G^*_{s+t} is a graph obtained from G by attaching at v_i (or v_j) a path of length $s + t$. Then $H(G^*_{s,t}) > H(G^*_{s+t})$.*

3. Bounds on $H(G + v_iv_j) - H(G)$

For a connected graph G and two nonadjacent vertices v_i and v_j in $V(G)$ of G, recall that $G + v_iv_j$ is the supergraph formed from G by adding an edge between vertices v_i and v_j. In this section, we consider the relationship between $H(G + v_iv_j)$ and $H(G)$. Here we give upper and lower bounds on $H(G + v_iv_j) - H(G)$ and characterize the extremal graphs.

Theorem 3.1. *Let G be a connected graph with $n \geq 2$ vertices, m edges and diameter d. If there exist two nonadjacent vertices v_i and v_j in G, then*

$$\frac{1}{2} \leq H(G + v_iv_j) - H(G) \leq \left(1 - \frac{1}{d}\right) + \frac{n(n-1) - 2m - 2}{2}\left(\frac{1}{2} - \frac{1}{d}\right) \tag{2}$$

with equality on the left hand side if and only if $d_G(v_i) = d_G(v_j) = 1$ and $d_G(v_i, v_j) = 2$ in G, and equality on the right hand side if and only if G is isomorphic to a graph of diameter 2.

Proof. Denote by $d^*_G(v_r, v_s)$ the distance of two vertices v_r and v_s in $G + v_iv_j$. We have

$$\begin{aligned} H(G + v_iv_j) - H(G) &= \sum_{1 \leq r < s \leq n} \left(\frac{1}{d^*_G(v_r, v_s)} - \frac{1}{d_G(v_r, v_s)}\right) \\ &= \left(\frac{1}{d^*_G(v_i, v_j)} - \frac{1}{d_G(v_i, v_j)}\right) + \sum_{1 \leq r < s \leq n, (r,s) \neq (i,j)} \left(\frac{1}{d^*_G(v_r, v_s)} - \frac{1}{d_G(v_r, v_s)}\right). \end{aligned} \tag{3}$$

Since

$$\frac{1}{d^*_G(v_i, v_j)} - \frac{1}{d_G(v_i, v_j)} \geq \frac{1}{2} \quad \text{and} \quad d^*_G(v_r, v_s) \leq d_G(v_r, v_s) \text{ for } (r, s) \neq (i, j),$$

from (3), we get the lower bound in (2).

Now suppose that the left hand side equality holds in (2). Then

$$\frac{1}{d^*_G(v_i, v_j)} - \frac{1}{d_G(v_i, v_j)} = \frac{1}{2} \quad \text{and} \quad d^*_G(v_r, v_s) = d_G(v_r, v_s) \text{ for } (r, s) \neq (i, j).$$

Thus we have $d_G(v_i, v_j) = 2$ and $d^*_G(v_r, v_s) = d_G(v_r, v_s)$ for $(r, s) \neq (i, j)$. By contradiction we show that $d_G(v_i) = 1$. For this we assume that $d_G(v_i) \neq 1$. Let v_iv_c, $v_jv_c \in E(G)$ and v_p be another vertex adjacent to vertex v_i. Now we have $d_G(v_p, v_j) = 3 > 2 = d^*_G(v_p, v_j)$, a contradiction. Thus we have $d_G(v_i) = 1$. Similarly, we have $d_G(v_j) = 1$. Hence the left hand side equality holds in (2) if and only if $d_G(v_i) = d_G(v_j) = 1$ and $d_G(v_i, v_j) = 2$ in G.

Again since

$$\frac{1}{d^*_G(v_i, v_j)} - \frac{1}{d_G(v_i, v_j)} \leq 1 - \frac{1}{d},$$

and

$$\frac{1}{d^*_G(v_r, v_s)} - \frac{1}{d_G(v_r, v_s)} \leq \frac{1}{2} - \frac{1}{d} \quad \text{for } (r, s) \neq (i, j) \text{ and } d_G(v_r, v_s) \geq 2,$$

from (3), we get the upper bound in (2).

Now suppose that the right hand side equality holds in (2). Then

$$\frac{1}{d^*_G(v_i, v_j)} - \frac{1}{d_G(v_i, v_j)} = 1 - \frac{1}{d} \quad \text{and} \quad \frac{1}{d^*_G(v_r, v_s)} - \frac{1}{d_G(v_r, v_s)} = \frac{1}{2} - \frac{1}{d} \quad \text{for } (r, s) \neq (i, j)$$

and $d_G(v_r, v_s) \geq 2$, that is, $d_G(v_i, v_j) = d$. By contradiction we show that G is isomorphic to a graph of diameter 2. For this we assume that G is a graph of diameter 3 or more. Then there exists a vertex v_t adjacent to the vertex v_j such that $d_G(v_i, v_t) = d - 1$. Then

$$\frac{1}{d_G^*(v_i, v_t)} - \frac{1}{d_G(v_i, v_t)} = \frac{1}{2} - \frac{1}{d-1} < \frac{1}{2} - \frac{1}{d},$$

a contradiction. Hence G is isomorphic to a graph of diameter 2.

Conversely, one can see easily that the left hand side equality holds in (2) for $d_G(v_i) = d_G(v_j) = 1$ and $d_G(v_i, v_j) = 2$ in G, and the right hand side equality holds in (2) for graph of diameter 2. □

Corollary 3.1. *Let G be a graph with v_i, v_j as its two nonadjacent vertices and $e \in E(G)$. Then*

(1) [30] $H(G + v_i v_j) > H(G)$;
(2) $H(G - e) < H(G)$.

From Lemma 2.1 and Corollary 3.1(2), the following corollary is obvious.

Corollary 3.2. *Let G be a graph of order n and $v_i v_j \in E(G)$. Then*

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

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

The term $\sum_{i=1}^{n} d_i^2$ is known as the first Zagreb index of G, denoted by $M_1(G)$ [3,17]. The following result is a lower and an upper bound on $H(G + v_i v_j) - H(G)$ for triangle- and quadrangle-free connected graphs.

Theorem 3.2. *Let G be a triangle- and quadrangle-free connected graph with $n \geq 2$ vertices, m edges and diameter d. Let v_i and v_j be nonadjacent vertices in G, then*

$$\frac{1}{2} \leq H(G + v_i v_j) - H(G) \leq \left(1 - \frac{1}{d}\right) + \frac{n(n-1) - M_1(G) - 2}{2}\left(\frac{1}{2} - \frac{1}{d}\right) \tag{4}$$

with equality in left hand side if and only if $d_G(v_i) = d_G(v_j) = 1$ and $d_G(v_i, v_j) = 2$ in G, and equality in right hand side if and only if G is isomorphic to a graph of diameter 2.

Proof. The proof of left hand side of (4) is same as Theorem 3.1.

Since there are $\binom{n}{2}$ vertex pairs (at distance at least 1) in G, the number of vertex pairs at distance 1 is m and the number of vertex pairs at distance 2 is $\frac{1}{2} M_1(G) - m$ as G is triangle- and quadrangle-free. From (3), we get the right hand side of (4). Moreover, the equality holds in right hand side if and only if G is isomorphic to a graph of diameter 2. □

Recall that the reciprocal complementary Wiener number of the graph G is defined as [2,18,32]

$$\mathrm{RCW}(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{1}{d + 1 - d_G(v_i, v_j)} = \sum_{i<j} \frac{1}{d + 1 - d_G(v_i, v_j)},$$

where d is the diameter of graph G.

We now obtain the relation between Wiener, reciprocal complementary Wiener and the Harary index in the following theorem.

Theorem 3.3. *Let G be connected graph of n vertices, m edges and diameter d. Then*

$$\text{(i)}\ (W(G) - m - d)\left(H(G) - m - \frac{1}{d}\right) \geq \left(\frac{n(n-1)}{2} - m - 1\right)^2 \tag{5}$$

and

$$\text{(ii)}\ \left(\frac{n(n-1)(d+1)}{2} - md - 1 - W(G)\right)\left(\mathrm{RCW}(G) - \frac{m}{d} - 1\right) \geq \left(\frac{n(n-1)}{2} - m - 1\right)^2, \tag{6}$$

where $W(G)$ is the Wiener index, $H(G)$ is the Harary index and $\mathrm{RCW}(G)$ is the reciprocal complementary Wiener index. Moreover, the equality holds in (5) (or (6)) if and only if G has diameter at most 2.

Proof. (i) If diameter of G is equal to 1, then the equality holds in (5). Otherwise, the diameter of G is greater than or equal to 2. Using Arithmetic mean greater than or equal to Harmonic mean on $d_G(v_i, v_j) 1 \le i < j \le n$, $d_G(v_i, v_j) > 1$ (there exists one pair (v_i, v_j) such that $d_G(v_i, v_j) = d$ is not considered here), we have

$$\frac{\sum\limits_{1\le i<j\le n, d_G(v_i,v_j)>1} d_G(v_i, v_j)}{\frac{n(n-1)}{2} - m - 1} \ge \frac{\frac{n(n-1)}{2} - m - 1}{\sum\limits_{1\le i<j\le n, d_G(v_i,v_j)>1} \frac{1}{d_G(v_i,v_j)}}, \tag{7}$$

which gives the required result (5).

The equality holds in (7) if and only if $d_G(v_i, v_j) = d_G(v_\ell, v_k) > 1$ for any two pairs (v_i, v_j) and (v_ℓ, v_k). Hence the equality holds in (5) if and only if G has diameter at most 2.

(ii) In this case, we replace $d_G(v_i, v_j)$ by $d + 1 - d_G(v_i, v_j)$ in (7) and we get the required result (6). Moreover, the equality holds in (6) if and only if G has diameter at most 2. □

4. Bounds on $H(G)$ including clique number and chromatic number

In this section, we consider lower and upper bounds on the Harary index including clique number and chromatic number and determine the corresponding extremal graphs. If $k = 1$, the set $\mathcal{X}_{n,k}$ contains a single graph with n isolated vertices. When $k = n$, the only graph in $\mathcal{X}_{n,k}$ is K_n. Therefore, in the following, we always assume that $1 < k < n$. The following lemma presents the value of the Harary index of complete k-partite graph.

Lemma 4.1. *If $K_{n_1,n_2,\ldots,n_k}$ is a complete k-partite graph of order n, then*

$$H(K_{n_1,n_2,\ldots,n_k}) = \frac{n^2}{2} - \frac{n}{4} - \frac{1}{4}\sum_{i=1}^{k} n_i^2.$$

Proof. Note that, in $K_{n_1,n_2,\ldots,n_k}$, any two vertices in a same partition set are at the distance 2, while any two vertices from different partition sets are adjacent, that is, they are at the distance 1. From Eq. (1), we have

$$\begin{aligned}
H(K_{n_1,n_2,\ldots,n_k}) &= \sum_{1\le i<j\le k} n_i n_j + \sum_{i=1}^{k} \frac{1}{2}\binom{n_i}{2} \\
&= \frac{1}{2}\sum_{i=1}^{k} n_i(n-n_i) + \frac{1}{4}\sum_{i=1}^{k} n_i(n_i-1) \\
&= \frac{1}{2} n \sum_{i=1}^{k} n_i - \frac{1}{4}\sum_{i=1}^{k} n_i^2 - \frac{1}{4}\sum_{i=1}^{k} n_i \\
&= \frac{n^2}{2} - \frac{n}{4} - \frac{1}{4}\sum_{i=1}^{k} n_i^2, \quad \square
\end{aligned}$$

completing the proof of this lemma. □

Here we define a function

$$f(x_1, x_2, \ldots, x_k) = x_1^2 + x_2^2 + \cdots + x_k^2$$

where $x_1, x_2, \ldots, x_k$ are positive integers.

Lemma 4.2. *Suppose that $f(x_1, x_2, \ldots, x_k)$ is a function defined as above and let $\sum_{i=1}^{k} x_i = n$ be a fixed positive integer. If $x_i - x_j \ge 2$, $1 \le i, j \le k$ and $i \ne j$, then*

$$f(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_k) > f(x_1, \ldots, x_i - 1, \ldots, x_j + 1, \ldots, x_k).$$

Proof. By the definition of the function $f(x_1, x_2, \ldots, x_k)$, we have

$$\begin{aligned}
f(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_k) - f(x_1, \ldots, x_i - 1, \ldots, x_j + 1, \ldots, x_k) &= x_i^2 + x_j^2 - (x_i-1)^2 - (x_j+1)^2 \\
&= 2(x_i - x_j) - 2 > 0,
\end{aligned}$$

which finishes the proof of this lemma. □

Repeating Lemma 4.2, the following corollary can be easily obtained.

Corollary 4.1. *Suppose that $f(x_1, x_2, \ldots, x_k)$ is a function defined as above and $\sum_{i=1}^{k} x_i = n, x_1 \geq x_2 \geq \cdots \geq x_k$. Then $f(x_1, x_2, \ldots, x_k)$ reaches its minimum value when the values of $x_1, x_2, x_3, \ldots, x_k$ differ by at most 1.*

Assume that $n = kq + r$ where $0 \leq r < k$, i.e., $q = \lfloor \frac{n}{k} \rfloor$. Now, by the following theorem, we characterize the graph from $\mathcal{X}_{n,k}$ with the maximal Harary index.

Theorem 4.1. *Let $G \in \mathcal{X}_{n,k}$. Then we have*

$$H(G) \leq H(T_n(k)) = \frac{n^2}{2} - \frac{n}{4} - \frac{1}{4}\left[(k-r)\left\lfloor \frac{n}{k} \right\rfloor^2 + r\left\lceil \frac{n}{k} \right\rceil^2\right]$$

with the equality holding if and only if $G \cong T_n(k)$.

Proof. From the definition of chromatic number, any graph G from $\mathcal{X}_{n,k}$ has k color classes each of which is an independent set. Suppose that the k classes have order $n_1, n_2, \ldots, n_k$, respectively. Assume that $G_1 \in \mathcal{X}_{n,k}$ has the Harary index as large as possible. By Corollary 3.1(1), we find that $G_1 \cong K_{n_1,n_2,\ldots,n_k}$.

From Lemma 4.1 and Corollary 4.1, we claim that $G_1 \cong T_n(k)$. Thanks to Lemma 4.1, again, we have $H(T_n(k)) = \frac{n^2}{2} - \frac{n}{4} - \frac{1}{4}\left[(k-r)\lfloor \frac{n}{k} \rfloor^2 + r\lceil \frac{n}{k} \rceil^2\right]$, ending the proof of this theorem. □

The following well-known lemma can be found in [1].

Lemma 4.3 (*Turán's Theorem*)**.** *Let G be a connected graph of order n and $m(G)$ edges. If G contains no K_{k+1}, then $m(G) \leq m(T_n(k))$, with equality holding if and only if $G \cong T_n(k)$.*

Theorem 4.2. *Let $G \in \mathcal{W}_{n,k}$. Then we have*

$$H(G) \leq \frac{n^2}{2} - \frac{n}{4} - \frac{1}{4}\left[(k-r)\left\lfloor \frac{n}{k} \right\rfloor^2 + r\left\lceil \frac{n}{k} \right\rceil^2\right]$$

with the equality holding if and only if $G \cong T_n(k)$.

Proof. Suppose that G from $\mathcal{W}_{n,k}$ has the largest Harary index. From formula (1) and Lemma 4.3, we have

$$\begin{aligned} H(G) &\leq m(G) + \frac{1}{2}\left[\binom{n}{2} - m(G)\right] \\ &= \frac{n(n-1)}{4} + \frac{1}{2}m(G), \end{aligned}$$

with the equality holding if and only if $G \cong T_n(k)$. Thus, this theorem follows immediately from the formula of $H(T_n(k))$ in Theorem 4.1. □

Now we turn to the minimal Harary index of graphs from $\mathcal{W}_{n,k}$. In [29,10], one of the present authors and Gutman independently showed that the path P_n has the minimal Harary index among all the trees of order n. By the following theorem, we completely determine the graph from $\mathcal{W}_{n,k}$ with the minimal Harary index, which, in a sense, can be seen as the generalization of the case for the trees. Before doing it, we first list two related lemmas below.

Lemma 4.4 ([30])**.** *Let G be a (connected) graph with a cut vertex u such that G_1 and G_2 are two connected subgraphs of G having u as the only common vertex and $G_1 \bigcup G_2 = G$. Let $|V(G_i)| = n_i$ for $i = 1, 2$. Then $H(G) = H(G_1) + H(G_2) + \sum_{x \in V(G_1)\setminus\{u\}} \sum_{y \in V(G_2)\setminus\{u\}} \frac{1}{d_{G_1}(x,u) + d_{G_2}(u,y)}$.*

Lemma 4.5 ([24])**.** $H(P_n) = n\sum_{i=1}^{n-1} \frac{1}{i} - n + 1$, *and* $H(C_n) = \begin{cases} n\sum_{i=1}^{\frac{n-1}{2}} \frac{1}{i} & \text{if } n \text{ is odd;} \\ n\sum_{i=1}^{\frac{n-2}{2}} \frac{1}{i} + 1 & \text{if } n \text{ is even} \end{cases}$.

Theorem 4.3. *Let $G \in \mathcal{W}_{n,k}$. Then we have*

$$H(G) \geq \frac{k(k-1)}{2} + n\sum_{i=1}^{n-k} \frac{1}{i+1}$$

with the equality holding if and only if $G \cong K_{n,k}$.

Proof. Suppose that a graph G_1 from $\mathcal{W}_{n,k}$ has the smallest Harary index. From the definition of the set $\mathcal{W}_{n,k}$, G_1 contains a complete graph K_k as a subgraph. Without loss of generality, suppose that $V(K_k) = \{v_1, v_2, \ldots, v_k\}$. By Corollary 3.1 (2), G must be a graph obtained from K_k by attaching some trees rooted at some vertices of K_k. From the structure of G_1, we assume that $V_0 = \{v_i | i \in \{1, 2 \ldots, k\}, d_{G_1}(v_i) > k-1\}$ (i.e., there is a tree attached at v_i for any vertex $v_i \in V_0$) and the vertices in V_0 are labeled as $v_1, v_2, \ldots, v_t$ with $t \le k$.

In view of Corollary 2.1, we find that, in G_1, all the trees attached at some vertices of K_k must be paths. That is to say, the degrees of all vertices in V_0 of G_1 are k. Now we claim that $|V_0| = 1$. To the contrary, there are at least two vertices, say v_i and v_j, in V_0 of G_1. Let G_1' be a graph obtained from G_1 by deleting all the vertices of these two paths attaching at v_i, v_j, respectively, where v_i and v_j are not included. Note that $Q_{G_1'}(v_i) = Q_{G_1'}(v_j)$. But from Corollary 2.2, G_1 can be changed to G_0, which is a graph obtained by attaching v_i (or v_j) a path of length equal to the sum of those of paths attached at v_i and v_j, with a smaller Harary index. This is a contradiction to the choice of G_1. Therefore $G_1 \cong K_{n,k}$.

Now we calculate the Harary index of $K_{n,k}$. Recalling the definition of $K_{n,k}$, by Lemmas 4.4 and 4.5, we have

$$\begin{aligned}
H(K_{n,k}) &= H(K_k) + H(P_{n-k+1}) + \sum_{i=1}^{n-k} \frac{k-1}{i+1} \\
&= \frac{k^2-k}{2} + (n-k+1)\sum_{i=1}^{n-k}\frac{1}{i} - (n-k) + (k-1)\sum_{i=1}^{n-k}\frac{1}{i+1} \\
&= \frac{k^2+k}{2} + n\sum_{i=2}^{n-k}\frac{1}{i} - (k-1)\frac{n-k}{n-k+1} \\
&= \frac{k(k-1)}{2} + n\sum_{i=1}^{n-k}\frac{1}{i+1},
\end{aligned}$$

which finishes the proof of this theorem. □

Lemma 4.6. *Let $G \in \mathcal{X}_{n,k}$. Then for any vertex $v_i \in V(G)$,*

$$Q_G(v_i) \le \frac{n(n-k+1)}{n-k+2} - \sum_{t=1}^{n-k+1}\frac{1}{t+1} \tag{8}$$

with equality holding in (8) if and only if $G \cong K_{n,k}$ and v_i is the pendent vertex of $K_{n,k}$.

Proof. Let d be the diameter of graph G. Suppose that P_{d+1} : $v_1v_2 \ldots v_dv_{d+1}$ is a path, where the vertices v_i and v_{i+1} are adjacent for $i = 1, 2, \ldots, d$ in G. We now prove $d \le n-k+1$ by contradiction. For this, we suppose that $d \ge n-k+2$. We can use two colors to color the vertices of path P_{d+1} and at most $n-d-1$ colors to color the remaining $n-d-1$ vertices. Thus we have the chromatic number $k \le n-d+1$, that is, $d \le n-k+1$, a contradiction.

Let $Q_G(v_i) = \max_{1\le j\le n} Q_G(v_j)$. Then

$$\begin{aligned}
Q_G(v_i) &= \sum_{v_j\in V(G)} \frac{d_G(v_i,v_j)}{d_G(v_i,v_j)+1} = n-1-\sum_{v_j\in V(G)}\frac{1}{d_G(v_i,v_j)+1} \\
&\le n-1-\sum_{j=1}^{n-k+1}\frac{1}{j+1} - \frac{k-2}{n-k+2} \quad \text{as } d \le n-k+1 \text{ and } d_G(v_i,v_j) \le n-k+1,
\end{aligned} \tag{9}$$

which gives the result (8). First part of the proof is over.

Suppose that the equality holds in (8). Then the equality holds in (9). Thus we have $d = n-k+1$ and $d_G(v_i, v_j) = n-k+1$ for $j = n-k+3,\ n-k+4,\ \ldots, n$. Since G has chromatic number k, vertices $v_{n-k+1},\ v_{n-k+2},\ \ldots,\ v_n$ are completely connected and hence G is isomorphic to $K_{n,k}$ and v_i is the pendent vertex of $K_{n,k}$.

Conversely, one can see easily that the equality holds in (8) for $K_{n,k}$ and v_i is the pendent vertex of $K_{n,k}$. □

In the following theorem, we completely characterize the extremal graph from $\mathcal{X}_{n,k}$ with the minimal Harary index.

Theorem 4.4. *Let $G \in \mathcal{X}_{n,k}$. Then we have*

$$H(G) \ge \frac{k(k-1)}{2} + n\sum_{i=1}^{n-k}\frac{1}{i+1} \tag{10}$$

with the equality holding in (10) if and only if $G \cong K_{n,k}$.

Proof. If $n = k$, then the equality holds in (10). For $n = k + 1$, G is isomorphic to a graph, K_k with one vertex adjacent to some vertices in $V(K_k)$, but not all. Suppose $v_p \in V(G) \setminus V(K_k)$ and vertex v_p is adjacent to the d_p vertices in $V(K_k)$ such that $1 \leq d_p < k$. Then

$$H(G) = \frac{k(k-1)}{2} + \frac{k+d_p}{2} \geq \frac{k(k-1)}{2} + \frac{k+1}{2} = \frac{k(k-1)}{2} + n\sum_{i=1}^{n-k}\frac{1}{i+1},$$

(10) is true for $n = k + 1$. Otherwise, $n \geq k + 2$.

Let d be the diameter of graph G. Since chromatic number of G is k, there are at least one vertex of degree $k-1$. So we must have $d \leq n-k+1$. Now we will prove this theorem by induction on n. First we assume that $\chi(G - v_i) = \chi(G) - 1 = k - 1$ for any vertex $v_i \in V(G)$. In this case, we find that each color vertex v_i is adjacent to the remaining $k - 1$ colors vertices in G, that is, $d_G(v_i) \geq k - 1$, $i = 1, 2, \ldots, n$. Therefore, by induction hypothesis, we have

$$\begin{aligned} H(G) &= H(G - v_i) + \sum_{j=1, j\neq i}^{n} \frac{1}{d_G(v_i, v_j)} \\ &\geq \frac{(k-1)(k-2)}{2} + (n-1)\sum_{i=1}^{n-k}\frac{1}{i+1} + k - 1 + \left[(d_G(v_i) - k + 1) + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n - d_G(v_i)}\right] \\ &\geq \frac{k(k-1)}{2} + n\sum_{i=1}^{n-k}\frac{1}{i+1} = H\left(K_{n,k}\right), \end{aligned}$$

and (10) holds by induction.

Next we assume that there exists a vertex $v_i \in V(G)$ such that $\chi(G - v_i) = \chi(G)$. By Corollary 3.2, Lemma 4.6 and induction hypothesis, we have

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

and (10) holds by induction. Both the inequalities hold if and only if v_i is a pendent vertex of G with v_j as only one neighbor and $G \cong K_{n,k}$, by Corollary 3.2, Lemma 4.6. This completes the proof of this theorem. □

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