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ORIGINAL PAPER

On Harary index

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Abstract We report lower and upper bounds for the Harary index of a connected (molecular) graph, and, in particular, upper bounds of triangle- and quadrangle-free graphs. We also give the Nordhaus–Gaddum-type result for the Harary index.

Keywords Harary index · Harary matrix · Wiener index · Triangle-free graphs · Quandrangle-free graphs

1 Introduction

The Harary index of a molecular graph G, denoted by $\mathrm{H}(G)$, has been introduced independently in this Journal by Plavšić et al. [1] and by Ivanciuc et al. [2] in 1993 for the characterization of molecular graphs. It has been named by Plavšić et al. [1] the Harary index in honour of Professor Frank Harary on the occasion of his 70th birthday. Ivanciuc et al. [2] called it initially the reciprocal distance sum index, but later they also adopted the suggested name [3]. Nowadays the name Harary index is generally accepted (e.g., [4]).

Dedicated to the memory of Professor Frank Harary (1921–2005), the late grandmaster of both graph theory and chemical graph theory.

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The Harary index is defined as the half-sum of the elements in the reciprocal distance matrix, also called the Harary matrix [5]. This definition parallels the Hosoya definition of the Wiener index as the half-sum of the elements in the distance matrix [6]. The motivation for introduction of the Harary index was pragmatic—the aim was to design a distance index differing from the Wiener index [7] in that the contributions to it from the distant atoms in a molecule should be much smaller than from near atoms, since in many instances the distant atoms influence each other much less than near atoms.

A few years after the two initial publications on Harary index, it has been extended to heterosystems [8] and the hyper-Harary index was introduced [9]. Its modification has also been proposed [10]. The Harary index and related molecular descriptors have shown a modest success in structure-property correlations [11–15], but their use in combination with other molecular descriptors improves the correlations (e.g., [16]). The Harary index has a number of interesting properties (e.g., [8]). In this article, in continuation of our studies on the properties of the Harary index, we provide its lower and upper bounds of G, and also give the Nordhaus–Gaddum-type result [17] for it.

2 Preliminaries

We consider simple (molecular) graphs, i.e., graphs without multiple edges and loops [18]. Let G be a connected graph with the vertex-set $V(G) = \{v_1, v_2, \ldots, v_n\}$. For $v_i \in V(G)$, $\Gamma(v_i)$ denotes the set of its (first) neighbors in G and the degree of v_i is $\delta_i = |\Gamma(v_i)|$. The term $\sum_{i=1}^{n} \delta_i^2$ is known as the first Zagreb index of G, denoted by $\mathrm{M}_1(G)$ [19–23].

The distance matrix $\mathbf{D}$ of G is an $n \times n$ matrix $(\mathbf{D}_{ij})$ such that $\mathbf{D}_{ij}$ is just the distance (i.e., the number of edges of a shortest path) between the vertices v_i and v_j in G [5], denoted by $d(v_i, v_j|G)$. The reciprocal distance matrix $\mathbf{RD}$ of$G$ is an $n \times n$ matrix $(\mathbf{RD}_{ij})$ such that [5]

$$\mathbf{RD}_{ij} = \begin{cases} \frac{1}{\mathbf{D}_{ij}} & \text{if } i \neq j, \\ 0 & \text{if } i = j. \end{cases}$$

Recall the Hosoya definition of the Wiener index [6] of G, denoted by $\mathrm{W}(G)$,

$$\mathrm{W}(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \mathbf{D}_{ij} = \sum_{i<j} \mathbf{D}_{ij}.$$

The Haray index $\mathrm{H}(G)$ is defined in the similar fashion [1,2]

$$\mathrm{H}(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \mathbf{RD}_{ij} = \sum_{i<j} \mathbf{RD}_{ij}.$$

Let P_n and S_n be respectively the path and the star with n vertices. Then [24] for any tree T with n vertices, $\mathrm{H}(P_n) \le \mathrm{H}(T) \le \mathrm{H}(S_n)$ with left (right, respectively) equality if and only if $T = P_n$ ($T = S_n$, respectively). Let K_n be the complete graph with n vertices.

3 Bounds for the Harary index

First we give lower and upper bounds for the Harary index in terms of the number of vertices and the number of edges.

Proposition 1 Let G be a connected graph with $n \ge 2$ vertices. Then

$$1 + n\sum_{k=2}^{n-1}\frac{1}{k} \le \mathrm{H}(G) \le \frac{n(n-1)}{2} \tag{1}$$

with left (right, respectively) equality if and only if $G = P_n$ ($G = K_n$, respectively).

Proof It is easily seen that adding an edge to G will increase the Harary index. Thus, if $\mathrm{H}(G)$ is maximum then G is the complete graph, and if $\mathrm{H}(G)$ is minimum then G is a tree. Note that $\mathrm{H}(K_n) = \frac{n(n-1)}{2}$ and $\mathrm{H}(P_n) = \sum_{k=1}^{n-1}\frac{n-k}{k} = 1 + n\sum_{k=2}^{n-1}\frac{1}{k}$. Thus, the right inequality in (1) follows and equality holds if and only if $G = K_n$, and by Gutman's result [24] mentioned above, the left inequality in (1) follows and equality holds if and only if $G = P_n$. □

Proposition 2 Let G be a connected graph with $n \ge 2$ vertices and m edges. Then

$$\mathrm{H}(P_n) + \frac{m-n+1}{2} \le \mathrm{H}(G) \le \frac{n(n-1)}{4} + \frac{m}{2} \tag{2}$$

with left (right, respectively) equality if and only if $G = P_n$ or K_3 (G has diameter at most 2, respectively).

Proof Since there are $\binom{n}{2} = \frac{n(n-1)}{2}$ vertex pairs (at distance at least one) and the number of vertex pairs at distance one is m, we have

$$\mathrm{H}(G) \le m + \frac{1}{2}\left[\frac{n(n-1)}{2} - m\right]$$

with equality if and only if G has diameter at most 2.

If $m = n - 1$, then by Proposition 1, the left equality in (2) holds. Suppose that $m \ge n$. Note that for any connected subgraph G' of G obtained by deleting an edge $v_s v_t$ from G, we have $\mathrm{H}(G) \ge \mathrm{H}(G') + 1 - \frac{1}{2} = \mathrm{H}(G') + \frac{1}{2}$ with equality if and only if $d(v_s, v_t|G') = 2$ and $d(v_i, v_j|G') = d(v_i, v_j|G)$ for any pair of vertices $\{v_i, v_j\}$ different from $\{v_s, v_t\}$.

Let T be a spanning tree [25] of G. Then T can be obtained from G by deleting $m-n+1$ edges, say $e_1, \ldots, e_{m-n+1}$, of G outside T. Let $G_k = G_{k-1} - e_k$ for $k = 1, \ldots, m-n+1$, where $G_0 = G$ and $G_{m-n+1} = T$. Then $\mathrm{H}(G_{k-1}) \geq \mathrm{H}(G_k) + \frac{1}{2}$ for $k = 1, \ldots, m-n+1$, and so we have $\mathrm{H}(G_0) \geq \mathrm{H}(G_{m-n+1}) + (m-n+1) \cdot \frac{1}{2}$, i.e., $\mathrm{H}(G) \geq \mathrm{H}(T) + \frac{m-n+1}{2}$. By Proposition 1, $\mathrm{H}(T) \geq \mathrm{H}(P_n)$. Thus the left inequality in (2) holds. Suppose that left equality holds in (2). Then $T = P_n$ and we can add an edge between two vertices, say v_{s_0}, v_{t_0}, of distance two in $T = P_n$ to form G_{m-n} such that $d(v_i, v_j|T) = d(v_i, v_j|G_{m-n})$ for any pair of vertices $\{v_i, v_j\}$ different from $\{v_{s_0}, v_{t_0}\}$. This is only possible if $n = 3$. Thus $G = K_3$. Conversely, it is easily seen that if $G = P_n$ or K_3, then the left equality holds in (2). □

Now we consider upper bounds for the Harary index of triangle- and quadrangle-free connected graphs.

Proposition 3 Let G be a triangle- and quadrangle-free connected graph with $n \geq 2$ vertices and m edges. Then

$$\mathrm{H}(G) \leq \frac{n(n-1)}{6} + \frac{m}{2} + \frac{1}{12}\mathrm{M}_1(G) \tag{3}$$

with equality if and only if G has diameter at most 3.

Proof Note that there are $\frac{n(n-1)}{2}$ vertex pairs (at distance at least one) and the number of vertex pairs at distance one is m. Since G is triangle- and quadrangle-free, the number of vertex pairs at distance two is $\frac{1}{2}\mathrm{M}_1(G) - m$ (see [22]). Thus

$$\begin{aligned}\mathrm{H}(G) &\leq m + \frac{1}{2}\left[\frac{1}{2}\mathrm{M}_1(G) - m\right] + \frac{1}{3}\left[\frac{n(n-1)}{2} - \frac{1}{2}\mathrm{M}_1(G)\right] \\ &= \frac{n(n-1)}{6} + \frac{m}{2} + \frac{1}{12}\mathrm{M}_1(G)\end{aligned}$$

with equality if and only if G has diameter at most 3. □

Corollary 4 Let G be a triangle- and quadrangle-free connected graph with $n \geq 2$ vertices and m edges. Then

$$\mathrm{H}(G) \leq \frac{n(n-1)}{4} + \frac{m}{2} \tag{4}$$

with equality if and only if G is the star or a Moore graph of diameter 2. There are at most four Moore graphs of diameter 2 [26]: pentagon, Petersen graph, Hoffman–Singleton graph, and possibly a 57-regular graph with 3250 vertices (its existence is still an open problem).

Proof It has been shown in [23] that $\mathrm{M}_1(G) \leq n(n-1)$ with equality if and only if G is the star or a Moore graph of diameter 2. The result now follows from Proposition 3. □

We mention a connection between the Harary index and the spectrum of **RD**. Let $\lambda(G)$ be the maximum eigenvalues of **RD**. Then [27]: $\lambda(G) \geq \frac{2\mathrm{H(G)}}{n}$ with equality if and only if **RD** has equal row sums.

4 The Nordhaus–Gaddum-type result for the Harary index

Zhang and Wu [28] obtained the Nordhaus–Gaddum-type result for the Wiener index. In the following, we give the Nordhaus–Gaddum-type result for the Harary index. Note that for a graph G, $\overline{G}$ stands for its complement [29]. There is only one connected graph P_4 on 4 vertices with connected complement $\overline{P_4} = P_4$. Obviously, $\mathrm{H}(P_4) + \mathrm{H}(\overline{P_4}) = 2\mathrm{H}(P_4) = \frac{26}{3}$. For $n \geq 5$, the diameter of $\overline{P_n}$ is 2.

Lemma 5 Let G be a connected graph on $n \geq 5$ vertices with a connected $\overline{G}$. If $\overline{G}$ has diameter 2, then

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

with equality if and only if $G = P_n$.

Proof Note that both $\overline{G}$ and $\overline{P_n}$ have diameter 2. By Proposition 2,

$$\begin{aligned} \mathrm{H}(G) + \mathrm{H}(\overline{G}) &\geq \mathrm{H}(P_n) + \frac{m-n+1}{2} + \frac{n(n-1)}{4} + \frac{1}{2}\left[\frac{n(n-1)}{2} - m\right] \\ &= \mathrm{H}(P_n) + \frac{n(n-1)}{4} + \frac{1}{2}\left[\frac{n(n-1)}{2} - (n-1)\right] \\ &= \mathrm{H}(P_n) + \mathrm{H}(\overline{P_n}) \end{aligned}$$

with equality if and only if $\mathrm{H}(G) = \mathrm{H}(P_n)$, or equivalently, $G = P_n$. □

Lemma 6 Let G be a connected graph on $n \geq 5$ vertices with a connected $\overline{G}$. If both G and $\overline{G}$ have diameter 3, then $\mathrm{H}(G) + \mathrm{H}(\overline{G}) > \mathrm{H}(P_n) + \mathrm{H}(\overline{P_n})$.

Proof Let t_k and $\overline{t_k}$ be respectively the number of pairs of vertices with distance k in G and $\overline{G}$. Obviously, $t_2 + t_3 = \overline{t_1}$, $\quad \overline{t_2} + \overline{t_3} = t_1$ and $t_1 + \overline{t_1} = \frac{n(n-1)}{2}$. Then

$$\begin{aligned} \mathrm{H}(G) + \mathrm{H}(\overline{G}) &= \sum_{k=1}^{3} \frac{t_k + \overline{t_k}}{k} = t_1 + \overline{t_1} + \frac{1}{2}(t_2 + \overline{t_2} + t_3 + \overline{t_3}) - \frac{1}{6}(t_3 + \overline{t_3}) \\ &= \frac{3}{2}(t_1 + \overline{t_1}) - \frac{1}{6}(t_3 + \overline{t_3}) \\ &= \frac{3n^2 - 3n}{4} - \frac{1}{6}(t_3 + \overline{t_3}). \end{aligned}$$

Since both G and $\overline{G}$ have diameter 3, G ($\overline{G}$, respectively) has a spanning subgraph [29], say, $S_{p,n-p}$ ($S_{q,n-q}$, respectively), which is obtained by adding an edge between the centers of two vertex-disjoint stars S_p and S_{n-p} (S_q and S_{n-q}, respectively). It can be easily seen that

$$t_3 + \overline{t_3} \leq (p-1)(n-p-1) + (q-1)(n-q-1) \leq \frac{(n-2)^2}{2}.$$

Furthermore, if $n = 6$, then since $t_3 = 4$ implies that $\overline{t_3} = 1$, we have $t_3 + \overline{t_3} \leq 6$, and if $n = 5$, then since $t_3, \overline{t_3} \leq 2$ and $t_3 = 2$ imply that $\overline{t_3} = 1$, we have $t_3 + \overline{t_3} \leq 3$.

Let $f(G) = \mathrm{H}(G) + \mathrm{H}(\overline{G}) - \left[\mathrm{H}(P_n) + \mathrm{H}(\overline{P_n})\right]$. We need only to show that $f(G) > 0$. Note that

$$f(G) = \frac{3n^2 - 3n}{4} - \frac{1}{6}(t_3 + \overline{t_3}) - \left[1 + \frac{(n-1)^2}{2} + n\sum_{k=2}^{n-1}\frac{1}{k}\right]$$
$$= \frac{n^2 + n - 6}{4} - \frac{1}{6}(t_3 + \overline{t_3}) - n\sum_{k=2}^{n-1}\frac{1}{k}$$

and in particular, if $n = 6$, then $f(G) = \frac{13}{10} - \frac{1}{6}(t_3 + \overline{t_3})$, and if $n = 5$, then $f(G) = \frac{7}{12} - \frac{1}{6}(t_3 + \overline{t_3})$.

If $n = 6$, then since $t_3 + \overline{t_3} \leq 6$, we have $f(G) > 0$. If $n = 5$, then since $t_3 + \overline{t_3} \leq 3$, we have $f(G) > 0$. If $n \geq 7$, then $\sum_{k=2}^{n-1}\frac{1}{k} = \sum_{k=2}^{5}\frac{1}{k} + \sum_{k=6}^{n-1}\frac{1}{k} \leq \sum_{k=2}^{5}\frac{1}{k} + \sum_{k=6}^{n-1}\frac{1}{6} = \frac{77}{60} + \frac{n-6}{6} = \frac{17}{60} + \frac{n}{6}$, and so

$$f(G) = \frac{n^2 + n - 6}{4} - \frac{1}{6}(t_3 + \overline{t_3}) - n\sum_{k=2}^{n-1}\frac{1}{k}$$
$$\geq \frac{n^2 + n - 6}{4} - \frac{(n-2)^2}{12} - \left(\frac{17n}{60} + \frac{n^2}{6}\right)$$
$$= \frac{18n - 110}{60} = \frac{9n - 55}{30} > 0.$$

This proves the result. □

Proposition 7 Let G be a connected graph on $n \geq 5$ vertices with a connected $\overline{G}$. Then

$$1 + \frac{(n-1)^2}{2} + n\sum_{k=2}^{n-1}\frac{1}{k} \leq \mathrm{H}(G) + \mathrm{H}(\overline{G}) \leq \frac{3n(n-1)}{4} \tag{5}$$

with left (right, respectively) equality if and only if $G = P_n$ or $G = \overline{P_n}$ (both G and $\overline{G}$ have diameter 2, respectively).

Proof Let m and $\overline{m}$ be respectively the number of edges of G and $\overline{G}$. Then $m + \overline{m} = \frac{n(n-1)}{2}$. By Proposition 2,

$$\mathrm{H}(G) + \mathrm{H}(\overline{G}) \leq 2 \cdot \frac{n(n-1)}{4} + \frac{m + \overline{m}}{2} = \frac{n(n-1)}{2} + \frac{n(n-1)}{4} = \frac{3n(n-1)}{4}$$

with equality if and only if both G and $\overline{G}$ have diameter 2.

If both G and $\overline{G}$ have diameter 3, then by Lemma 6, $\mathrm{H}(G) + \mathrm{H}(\overline{G}) > \mathrm{H}(P_n) + \mathrm{H}(\overline{P_n})$. If one of them has diameter 2, then by Lemma 5, the left inequality in (5) follows, and equality holds if and only if $G = P_n$ or $G = \overline{P_n}$. □

Let G be a connected graph on $n \geq 4$ vertices with a connected $\overline{G}$. Then [27]: $\lambda(G) + \lambda(\overline{G}) > n$. By Proposition 7 and the connection between $\mathrm{H}(G)$ and $\lambda(G)$ mentioned above, this can be improved slightly as: $\lambda(G) + \lambda(\overline{G}) > n - 1 + \frac{3}{n} + 2\sum_{k=3}^{n-1} \frac{1}{k}$.

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