J Math Chem (2009) 46:1377–1393
DOI 10.1007/s10910-009-9522-8

ORIGINAL PAPER

Bounds on Harary index

Kinkar Ch. Das · Bo Zhou · N. Trinajstić

Received: 8 December 2008 / Accepted: 14 January 2009 / Published online: 30 January 2009

Abstract In this paper, we obtain the lower and upper bounds on the Harary index of a connected graph (molecular graph), and, in particular, of a triangle- and quadrangle-free graphs in terms of the number of vertices, the number of edges and the diameter. We give the Nordhaus–Gaddum-type result for Harary index using the diameters of the graph and its complement. Moreover, we compare Harary index and reciprocal complementary Wiener number for graphs.

Keywords Harary index · Triangle-free graphs · Quadrangle-free graphs · Diameter · Lower bound · Upper bound

1 Introduction

The Harary index of a molecular graph G, denoted by $H(G)$, has been introduced in 1993 in this *Journal* independently by Plavšić et al. [1] and by Ivanciuc et al. [2] for characterization of G. The Harary index is defined as the half-sum of the elements in the reciprocal distance matrix, also called the Harary matrix [3]. This definition

K. Ch. Das (✉)
Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea
e-mail: kinkar@lycos.com; kinkar@mailcity.com

B. Zhou
Department of Mathematics, South China Normal University, Guangzhou, 510631, People's Republic of China
e-mail: zhoubo@scnu.edu.cn

N. Trinajstić
The Rugjer Bošković Institute, 10002 Zagreb, Croatia
e-mail: trina@irb.hr

parallels the Hosoya definition of the Wiener index as the half-sum of the elements in the distance matrix [4]. The motivation for introduction of the Harary index was to design a distance index differing from the Wiener index [5] 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. Harary index has been extended to heterosystems [6] and the hyper-Harary index was introduced [7]. The Harary index and related molecular descriptors have shown a modest success in structure–property correlations [8–12], but their use in combination with other molecular descriptors improves the correlations (e.g., [13]). The Harary index has a number of interesting properties (e.g., [6]). The lower and upper bounds of the Harary index in terms of the number of vertices and/or the number of edges, and the Nordhaus–Gaddum-type result for Harary index were obtained in [14]. The lower and upper bounds and the Nordhaus–Gaddum-type result for the reciprocal complementary Wiener number of a connected (molecular) graph were obtained in [15].

We consider simple (molecular) graphs, that is, graphs without multiple edges and loops [16]. Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and let m be the cardinality of the edge set $E(G)$. 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 $\delta_i = |\Gamma(v_i)|$. Let $|X|$ denote the cardinality of the set X. The diameter of a graph is the maximum distance between any two vertices of G. Let d be the diameter of G. The term $\sum_{i=1}^{n} \delta_i^2$ is known as the first Zagreb index of G, denoted by $M_1(G)$ [17–22].

The distance matrix D of G is an $n \times n$ matrix (d_{ij}) such that 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 [3], denoted by $\delta(i, j|G)$. The reciprocal distance matrix RD of G is an $n \times n$ matrix (RD_{ij}) such that [3]

$$RD_{ij} = \begin{cases} \frac{1}{d_{ij}} & \text{if} \quad i \neq j, \\ 0 & \text{otherwise.} \end{cases}$$

Recall the Harary index $H(G)$ is defined in [1,2]

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

The complementary distance matrix CD of G is an $n \times n$ matrix (CD_{ij}) such that $CD_{ij} = 1 + d - d_{ij}$ if $i \neq j$, and 0 otherwise [3], where d is the diameter of the graph G. The reciprocal complementary distance matrix RCD of G is an $n \times n$ matrix (rc_{ij}) such that

$$rc_{ij} = \begin{cases} \frac{1}{c_{ij}} & \text{if} \quad i \neq j, \\ 0 & \text{otherwise.} \end{cases}$$

Recall the reciprocal complementary Wiener (RCW) number of the graph G is defined as [12]

$$RCW(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} rc_{ij} = \sum_{i<j} rc_{ij}.$$

Now we study the Harary index in more detail, especially its relationship with the diameter. The paper is organized is as follows. In Sect. 2, we present the lower and upper bounds on the Harary index of connected graph, and, in particular, lower and upper bounds of triangle- and quadrangle-free graphs in terms of the number of vertices, the number of edges and the diameter. In Sect. 3, we obtain the Nordhaus–Gaddum-type result for Harary index using the diameters of the graph and its complement. In Sect. 4, we make a comparison between Harary index and reciprocal complementary Wiener number for graphs.

2 Harary index of graphs

In [14] the following lower and upper bounds for $H(G)$ was established:

Lemma 2.1 [14] Let G be a connected graph with $n \geq 2$ vertices, and m edges. Then

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

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

From definition of Harary index, we get

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

Now we give the following Lemma 2.2 which is useful for this section and also for next section.

Lemma 2.2 *Let P_n be a path of n vertices. Then*

$$H(P_n) \leq \frac{(n-1)(n+2)}{4}.$$

Moreover, equality holds if and only if either $n = 2$ or $n = 3$.

Proof We have

$$\begin{aligned}
H(P_{n+1}) &= H(P_n) + 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n-1} + \frac{1}{n} \\
&\leq H(P_n) + 1 + \frac{1}{2} + \frac{1}{2} + \cdots + \frac{1}{2} + \frac{1}{2} \\
&\leq H(P_n) + 1 + \frac{n-1}{2},
\end{aligned}$$

that is,

$$H(P_{n+1}) - \frac{n(n+3)}{4} \leq H(P_n) - \frac{(n-1)(n+2)}{4}.$$

Now we have $H(P_2) = 1$, $H(P_3) = 2.5$ and $H(P_4) = \frac{13}{4} < 4.5$. Hence, by mathematical induction we can easily show that

$$H(P_n) \leq \frac{(n-1)(n+2)}{4},$$

with equality holds if and only if $n = 2$ or $n = 3$. □

For graph G of diameter 2,

$$H(G) = \frac{n(n-1)+2m}{4}.$$

Denoted by $G^* = (V, E)$, a graph of diameter d ($3 \leq d \leq 4$ and $|V(G^*)| \geq d+2$) such that any vertex v_i, $v_i \in V(G^*) \backslash V(P_{d+1})$, $\delta(i, j|G^*) = 1$ or $\delta(i, j|G^*) = 2$ for any vertex $v_j \in V(G^*)$, $j \neq i$, where P_{d+1} is a path of $d+1$ vertices in G^*. The two graphs depicted in Fig. 1 are of G^* type graph.

We have

$$H(G^*) = \frac{n(n-1)+2m}{4} - \frac{1}{6} \quad \text{for } d = 3$$
$$\text{and } H(G^*) = \frac{n(n-1)+2m}{4} - \frac{7}{12} \quad \text{for } d = 4.$$

Now we give lower and upper bounds for the Harary index in terms of the number of vertices n, the number of edges m and the diameter d of G.

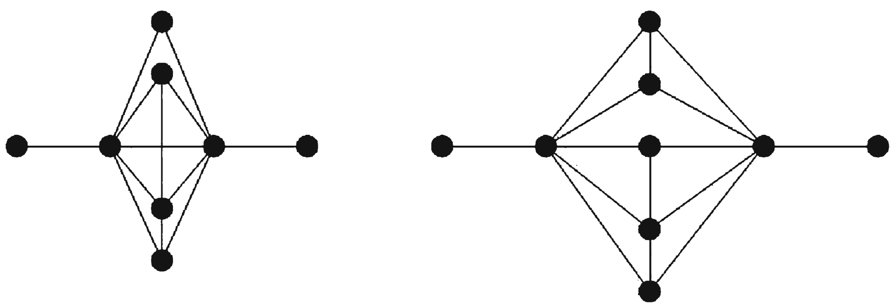


Fig. 1

Theorem 2.3 *Let G be a connected graph with $n \geq 2$ vertices, m edges, and diameter d. Then*

$$\begin{aligned} &H(P_{d+1}) + \frac{n(n-1) + 2(m-d)(d-1)}{2d} - \frac{d+1}{2} \leq H(G) \\ &\leq H(P_{d+1}) + \frac{n(n-1) + 2m}{4} - \frac{d(d+3)}{4}, \end{aligned} \tag{2}$$

with left (right, respectively) equality holds if and only if G is a graph of diameter at most 2 or G is a path P_n (G is a graph of diameter at most 2 or G is a path P_n or G is isomorphic to G^*, respectively).

Proof Since G has diameter d, G contains a path P_{d+1}. Also we have that there are $\binom{n}{2}$ vertex pairs (at distance at least one) and the number of vertex pairs at distance one is m. Thus we have

$$\begin{aligned} &H(P_{d+1}) + m - d + \left(\frac{n(n-1)}{2} - \frac{d(d+1)}{2} - (m-d)\right)\frac{1}{d} \leq H(G) \\ &\leq H(P_{d+1}) + m - d + \left(\frac{n(n-1)}{2} - \frac{d(d+1)}{2} - (m-d)\right)\frac{1}{2} \end{aligned} \tag{3}$$

$$\begin{aligned} \text{i.e.,}\quad &H(P_{d+1}) + \frac{n(n-1) + 2(m-d)(d-1)}{2d} - \frac{d+1}{2} \leq H(G) \\ &\leq H(P_{d+1}) + \frac{n(n-1) + 2m}{4} - \frac{d(d+3)}{4}. \end{aligned}$$

Now suppose that left equality holds in (2). Then the left equality holds in (3). If $d \leq 2$, then the left equality holds in (3) and hence G is a graph of diameter at most 2. Otherwise, $d \geq 3$. In this case left equality holds in (3) if and only if $\frac{n(n-1)}{2} - \frac{d(d+1)}{2} - (m-d) = 0$,

$$\text{that is,}\quad \frac{n(n-1)}{2} - \frac{d(d+1)}{2} = m - d = |E(G)\backslash E(P_{d+1})|. \tag{4}$$

We have that $m \geq d$. If $m = d$, then $d = n - 1$ as G is connected. Thus the Eq. (4) holds, and hence G is a path P_n. Otherwise, $m > d$ and so there are any vertex v_i such that $v_i \in V(G)\backslash V(P_{d+1})$, are adjacent to all the remaining vertices and diameter of G is at most 2, a contradiction.

Next we suppose that the right equality holds in (2). Then the right equality holds in (3). If $d \leq 2$, then the right equality holds in (3) and hence G is a graph of diameter at most 2. Otherwise, $d \geq 3$. Now we have $n \geq d + 1$. If $n = d + 1$, then G is a path P_n. Otherwise, $n \geq d + 2$. From right equality in (3), we conclude that any vertex v_i, $v_i \in V(G)\backslash V(P_{d+1})$, $\delta(i, j|G) = 1$ or $\delta(i, j|G) = 2$ for any vertex $v_j \in V(G)$, $j \neq i$, where P_{d+1} is a path of $d + 1$ vertices in G. So, diameter of G is less than or equal to 4. Hence G is isomorphic to a graph G^*.

Conversely, one can see easily that the left (right, respectively) equality holds in (2) for a graph of diameter at most 2 or a path P_n (a graph of diameter at most 2 or a path P_n or a graph isomorphic to G^*, respectively). $\square$

Remark 2.4 If G has diameter at most 2, then our lower bound in (2) is always better than the lower bound in (1). Now,

$$\begin{aligned}
H(P_n) &= H(P_{d+1}) \\
&\quad +\Big(\frac{1}{d+1}+\frac{1}{d+2}+\cdots+\frac{1}{n-1}\Big)+\Big(\frac{1}{d}+\frac{1}{d+1}+\cdots+\frac{1}{n-2}\Big) \\
&\quad +\Big(\frac{1}{d-1}+\frac{1}{d}+\cdots+\frac{1}{n-3}\Big)+\cdots+\Big(1+\frac{1}{2}+\cdots+\frac{1}{n-d-1}\Big) \\
&= H(P_{d+1})+\underbrace{1+1+\cdots+1}_{d+1}+\Big(\frac{d+1}{d+2}+\frac{d+1}{d+3}+\cdots+\frac{d+1}{n-d-1}\Big) \\
&\quad +\Big(\frac{d}{n-d}+\frac{d-1}{n-d+1}+\cdots+\frac{1}{n-1}\Big) \\
&< H(P_{d+1})+d+1+\frac{(d+1)(n-2d-2)}{d}+\frac{d(d+1)}{2d}.
\end{aligned}$$

Now we will see that the lower bound in (2) is better than the lower bound in (1) for $2 < d \leq \frac{n-2}{2}$. For this we have to show that

$$\begin{aligned}
&H(P_{d+1})+d+1+\frac{(d+1)(n-2d-2)}{d}+\frac{d(d+1)}{2d} \\
&\quad +\frac{m-n+1}{2} \leq H(P_{d+1})+\frac{n(n-1)}{2d} \\
&\quad +\frac{m(d-1)}{d}-\frac{3}{2}d+\frac{1}{2}
\end{aligned}$$

which is equivalent to

$$n(n-d-3)+(d-2)(m-2d+1)+2 \geq 0,$$

which is true for $2 < d \leq \frac{n-2}{2}$.

Remark 2.5 By Lemma 2.2, the upper bound in (2) is always better than the upper bound in (1).

Remark 2.6 The lower and upper bounds given by (2) are equal when G is a graph of diameter at most 2 or G is a path P_n.

Denoted by $G^{**} = (V, E)$, a triangle- and quadrangle-free graph of diameter 4 with $|V(G^{**})| \geq 6$ such that any vertex v_i, $v_i \in V(G^{**})\backslash V(P_{d+1})$, $\delta(i, j|G^{**}) = 1$ or $\delta(i, j|G^{**}) = 2$ or $\delta(i, j|G^{**}) = 3$ for any vertex $v_j \in V(G^{**})$, $j \neq i$, where P_{d+1} is a path of $d+1$ vertices. The two graphs depicted in Fig. 2 are of G^{**} type graph.

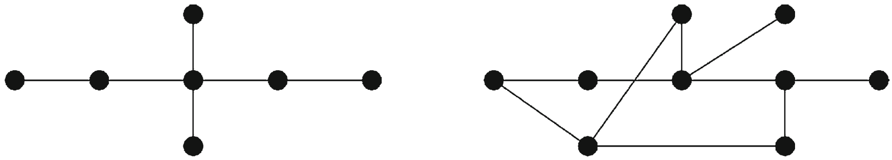


Fig. 2

We have

$$H(G^{**}) = \frac{1}{6}n(n-1) + \frac{1}{12}M_1(G^{**}) + \frac{1}{2}m - \frac{1}{12}.$$

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

Theorem 2.7 *Let G be a triangle- and quadrangle-free connected graph with $n \geq 2$ vertices, m edges and diameter d. Then*

$$H(G) \geq H(P_{d+1}) + \frac{d-2}{4d}M_1(G) - 2(d-1) + \frac{n(n-1)-2}{2d} + \frac{m}{2} \quad (5)$$

and $$H(G) \leq H(P_{d+1}) + \frac{1}{12}M_1(G) + \frac{n(n-1)}{6} + \frac{m}{2} - \frac{d^2}{6} - d + \frac{1}{6}. \quad (6)$$

Moreover, the equality holds in (5) if and only if G is a graph of diameter at most 3 or G is a path P_n, and the equality holds in (6) if and only if G is a graph of diameter at most 3 or G is a path P_n or G is isomorphic to a graph G^{**}.

Proof Since G has diameter d, path P_{d+1} contains in G. Also we have that there are $\binom{n}{2}$ vertex pairs (at distance at least one), the number of vertex pairs at distance one is m and the number of vertex pairs at distance two is $\frac{1}{2}M_1(G) - m$. Thus we have

$$\begin{aligned} H(G) \geq\ & H(P_{d+1}) + m - d + \left(\frac{1}{2}M_1(G) - m - d + 1\right)\frac{1}{2} \\ & + \left(\frac{n(n-1)}{2} - \frac{d(d+1)}{2} - (m-d) - \frac{1}{2}M_1(G) + m + d - 1\right)\frac{1}{d} \quad (7) \end{aligned}$$

and

$$\begin{aligned} H(G) \leq\ & H(P_{d+1}) + m - d + \left(\frac{1}{2}M_1(G) - m - d + 1\right)\frac{1}{2} \\ & + \left(\frac{n(n-1)}{2} - \frac{d(d+1)}{2} - (m-d) - \frac{1}{2}M_1(G) + m + d - 1\right)\frac{1}{3} \quad (8) \end{aligned}$$

i.e., $$H(G) \geq H(P_{d+1}) + \frac{d-2}{4d}M_2(G) - 2(d-1) + \frac{n(n-1)-2}{2d} + \frac{m}{2}$$

and $$H(G) \leq H(P_{d+1}) + \frac{1}{12}M_1(G) + \frac{n(n-1)}{6} + \frac{m}{2} - \frac{d^2}{6} - d + \frac{1}{6}.$$

Now suppose that equality holds in (5). Then the equality holds in (7). If $d \leq 3$, then the equality holds in (7) and G is a graph of diameter at most 3. Otherwise, $d \geq 4$. So we must have

$$\frac{n(n-1)}{2} - \frac{d(d+1)}{2} - \frac{1}{2}M_1(G) + 2d - 1 = 0$$

Now we have $n \geq d+1$. If $n = d+1$, then G is a path P_n. Otherwise, $n \geq d+2$. Since G is connected, from equality in (7), we have that any vertex v_i, $v_i \in V(G)\backslash V(P_{d+1})$, $\delta(i, j|G) = 1$ or $\delta(i, j|G) = 2$ for any vertex $v_j \in V(G)$, $j \neq i$, where P_{d+1} is a path of $d+1$ vertices in G. Using this we conclude that there are no graph of diameter greater than or equal to 4, as G is triangle- and quadrangle-free. Thus diameter of G is less than or equal to 3, a contradiction.

Next suppose that equality holds in (6). Then the equality holds in (8). If $d \leq 3$, then the equality holds in (8) and G is a graph of diameter at most 3. Otherwise, $d \geq 4$. Again we have $n \geq d+1$. If $n = d+1$, then G is a path P_n. Otherwise, $n \geq d+2$. From equality in (8), we conclude that any vertex v_i, $v_i \in V(G)\backslash V(P_{d+1})$, $\delta(i, j|G) = 1$ or $\delta(i, j|G) = 2$ or $\delta(i, j|G) = 3$ for any vertex $v_j \in V(G)$, $j \neq i$, where P_{d+1} is a path of $d+1$ vertices in G. Using this we conclude that graph G has diameter less than or equal to 4, as G is triangle- and quadrangle-free. Thus diameter of G is equal to 4. Hence G is isomorphic to G^{**}.

Conversely, one can see easily that the equality holds in (5) for a graph of diameter at most 3 or a path P_n and the equality holds in (6) for a graph of diameter at most 3 or a path P_n or a graph isomorphic to G^{**}. □

Corollary 2.8 [14] *Let G be a triangle- and quadrangle-free connected graph with $n \geq 2$ vertices and m edges. Then*

$$H(G) \leq \frac{1}{12}M_1(G) + \frac{n(n-1)}{6} + \frac{m}{2}$$

with equality holding if and only if G is a graph of diameter at most 3.

Proof We have

$$\begin{aligned}
H(P_{d+1}) &= d + \left(\frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{d}\right) + \left(\frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{d-1}\right) \\
&\quad + \cdots + \left(\frac{1}{2} + \frac{1}{3}\right) + \frac{1}{2} \\
&= d + \frac{d-1}{2} + \frac{d-2}{3} + \cdots + \frac{2}{d-1} + \frac{1}{d} \\
&\leq d + \frac{d-1}{2} + \frac{(d-1)(d-2)}{6} \\
&= d + \frac{d^2}{6} - \frac{1}{6}.
\end{aligned}$$

The result now follows from Theorem 2.7. □

Corollary 2.9 *Let G be a triangle- and quadrangle-free connected graph with $n \geq 2$ vertices, m edges and diameter d. Then*

$$H(G) \leq H(P_{d+1}) + \frac{1}{4}n(n-1) + \frac{m}{2} - \frac{d^2}{6} - d + \frac{1}{6}. \tag{9}$$

Moreover, the equality holds in (9) if and only if G is a star $K_{1,n-1}$ or G is a Moore graph of diameter 2. There are at most four Moore graphs of diameter 2: pentagon, Petersen graph, Hoffman-Singleton graph, and possibly a 57-regular graph with 3250 vertices [23].

Proof In [21], we have that $M_1(G) \leq n(n-1)$ with equality holding if and only if G is the star $K_{1,n-1}$ or G is a Moore graph of diameter 2. The result (9) follows from Theorem 2.7. □

Remark 2.10 The lower and upper bounds given by (5) and (6), respectively, are equal when G is a graph of diameter at most 3 or G is a path P_n.

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

Zhou et al. [14] obtained the Nordhaus–Gaddum-type result for the Harary index in the following Lemma 3.1.

Lemma 3.1 *Let G be a connected graph on $n \geq 5$ vertices with a connected $\overline{G}$. Then*

$$1 + \frac{(n-1)^2}{2} + n\sum_{k=2}^{n-1}\frac{1}{k} \leq H(G) + H(\overline{G}) \leq \frac{3}{4}n(n-1) \tag{10}$$

with left (right, respectively) equality holds in (10) if and only if $G = P_n$ or $G = \overline{P}_n$ (both G and $\overline{G}$ have diameter 2, respectively).

Now we give a lower bound for $H(G) + H(\overline{G})$:

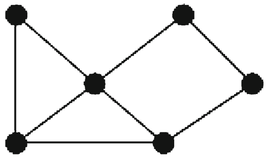
Theorem 3.2 *Let G be a connected graph on $n \geq 2$ vertices with a connected $\overline{G}$. Then*

$$H(G) + H(\overline{G}) \geq H(P_{k+1}) + \frac{n(n-1)}{2}\left(1 + \frac{1}{k}\right) - 3k + \frac{7}{2}, \tag{11}$$

where $k = \max\{d, \overline{d}\}$, d and $\overline{d}$ are diameter of G and $\overline{G}$, respectively. Moreover, the equality holds in (11) if and only if both G and $\overline{G}$ have diameter 2.

Proof By Theorem 2.3,

$$H(G) \geq H(P_{d+1}) + m + \frac{\overline{m}}{d} - \frac{3}{2}d + \frac{1}{2},$$



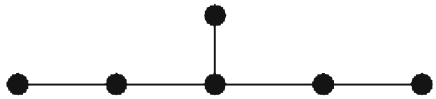


Fig. 3

where $\overline{m}$ is the number of edges in $\overline{G}$. Using above result, we get

$$\begin{aligned} H(G)+H(\overline{G}) &\geq H(P_{d+1})+H(P_{\overline{d}+1})+m+\overline{m}+\frac{\overline{m}}{d}+\frac{m}{\overline{d}} \\ &\quad -\frac{3}{2}(d+\overline{d})+1 \qquad (12) \\ &\geq H(P_{d+1})+H(P_{\overline{d}+1})+(m+\overline{m})\left(1+\frac{1}{k}\right)-3k+1 \\ &\quad \text{as } k=\max\{d,\overline{d}\} \qquad (13) \\ &\geq H(P_{k+1})+\frac{n(n-1)}{2}\left(1+\frac{1}{k}\right)-3k+\frac{7}{2} \\ &\quad \text{as } k=\max\{d,\overline{d}\} \text{ and } d,\overline{d}\geq 2 \qquad (14) \end{aligned}$$

Now suppose that equality holds in (11). Then all inequalities in the above argument must be equalities. Then from equality in (12), we get G is a graph of diameter 2 or G is a path P_n, and $\overline{G}$ is a graph of diameter 2 or $\overline{G}$ is a path P_n. From equality in (13), we get $k=d=\overline{d}$. Also from equality in (14), we get either $d=2$ or $\overline{d}=2$. Hence both G and $\overline{G}$ have diameter 2.

Conversely, one can easily check that the equality holds in (11) for both G and $\overline{G}$ of diameter 2. □

Remark 3.3 For graph G_1 (Fig. 3), the lower bound (11) for $H(G)+H(\overline{G})$ is 31.5 better than 29.15, the lower bound given in (10). But for graph G_2, the lower bound (10) is 21.2 better than our lower bound 16.67, given in (11). So the lower bounds are given in (10) and (11), are not comparable.

Now we give upper bound for $H(G)+H(\overline{G})$ in terms of the number of vertices n and the diameter d in G.

Theorem 3.4 *Let G be a connected graph on $n\geq 2$ vertices with a connected $\overline{G}$. If G has diameter d, then*

$$H(G)+H(\overline{G})\leq H(P_{d+1})+\frac{3n(n-1)}{4}-\frac{d(d+3)}{4}. \qquad (15)$$

Moreover, the equality holds if and only if both G and $\overline{G}$ have diameter 2 or G is a path P_n.

Proof Since G and $\overline{G}$ are connected, $d \geq 2$ and $\overline{d} \geq 2$. By Theorem 2.3, we get

$$H(G) + H(\overline{G}) \leq H(P_{d+1}) + \frac{n(n-1)+2m}{4} - \frac{d(d+3)}{4} + H(P_{\overline{d}+1}) + \frac{n(n-1)+2\overline{m}}{4} - \frac{\overline{d}(\overline{d}+3)}{4}, \tag{16}$$

where $\overline{m}$ is the number of edges in $\overline{G}$ and $\overline{d}$ is the diameter in $\overline{G}$.

Using Lemma 2.2 in above result, we get

$$H(G) + H(\overline{G}) \leq H(P_{d+1}) + \frac{3n(n-1)}{4} - \frac{d(d+3)}{4}, \quad \text{as } 2\overline{m} = n(n-1) - 2m. \tag{17}$$

Now suppose that equality holds in (15). Then the equality holds in (16) and (17). From equality in (16), we have G is a graph of diameter at most 2 or G is a path P_n and $\overline{G}$ is a graph of diameter at most 2 or $\overline{G}$ is a path P_n.

From equality in (17), we must have

$$H(P_{\overline{d}+1}) = \frac{\overline{d}(\overline{d}+3)}{4}.$$

By Lemma 2.2, $\overline{d} = 2$ as $\overline{d} \neq 1$. Hence both G and $\overline{G}$ have diameter 2 or G is a path P_n.

Conversely, one can see easily that the equality holds in (15) for both G and $\overline{G}$ have diameter 2 or for $G = P_n$. □

Remark 3.5 By Lemma 2.2, one can see easily that (15) is always better than the upper bound given in (10).

Remark 3.6 The lower and upper bounds given by (11) and (15), respectively, are equal when both G and $\overline{G}$ have diameter 2.

Theorem 3.7 *Let G be a triangle- and quadrangle-free connected graph of $n \geq 2$ vertices, m edges with a connected $\overline{G}$. Then*

$$H(G) + H(\overline{G}) \leq \frac{1}{6}M_1(G) + \frac{7n(n-1)}{12} + \frac{n(n-1)^2}{12} - \frac{m(n-1)}{3}. \tag{18}$$

Moreover, the equality holds if and only if both G and $\overline{G}$ have diameter at most 3.

Proof By Corollary 2.8, we get

$$H(G) \leq \frac{1}{12}M_1(G) + \frac{n(n-1)}{6} + \frac{m}{2}$$

with equality holding if and only if G is a graph of diameter at most 3. Thus

$$\begin{aligned} H(G) + H(\overline{G}) &\leq \frac{1}{12}M_1(G) + \frac{1}{12}M_1(\overline{G}) + \frac{n(n-1)}{3} + \frac{n(n-1)}{4} \\ &= \frac{1}{6}M_1(G) + \frac{7n(n-1)}{12} + \frac{n(n-1)^2}{12} - \frac{m(n-1)}{3} \qquad (19) \\ &\text{as } M_1(\overline{G}) = \sum_{i=1}^{n}(n-1-\delta_i)^2. \end{aligned}$$

Hence the equality holds in (18) if and only if both G and $\overline{G}$ have diameter at most 3.
□

4 Comparison between Harary index and reciprocal complementary Wiener number

In this section we compare between Harary index and reciprocal complementary Wiener number. For star $K_{1,n-1}$, we have $H(K_{1,n-1}) \leq RCW(K_{1,n-1})$ and for path P_n, we have $H(P_n) \geq RCW(P_n)$. Denote by DS_{n_1,n_2} $(n_1 \geq n_2)$, double star which is constructed by joining the central vertices of two stars K_{1,n_1} and K_{1,n_2}. We can see easily that $H(DS_{1,1}) > RCW(DS_{1,1})$, $H(DS_{2,1}) > RCW(DS_{2,1})$, $H(DS_{2,2}) > RCW(DS_{2,2})$ and $H(DS_{n_1,1}) > RCW(DS_{n_1,1})$. But we have the following theorem:

Theorem 4.1 *Let DS_{n_1,n_2} be a double star with $n_1 \geq 3$ and $n_2 \geq 2$. Then*

$$H(DS_{n_1,n_2}) \leq RCW(DS_{n_1,n_2}) \qquad (20)$$

with equality holding if and only if G is isomorphic to a graph $DS_{3,2}$.

Proof We have

$$\begin{aligned} 2H(DS_{n_1,n_2}) &= \left(n_1 + 1 + \frac{n_2}{2}\right) + \left(n_2 + 1 + \frac{n_1}{2}\right) + n_1\left(1 + \frac{1}{2} + \frac{n_2}{3}\right) \\ &\quad + \frac{n_1(n_1-1)}{2} + n_2\left(1 + \frac{1}{2} + \frac{n_1}{3}\right) + \frac{n_2(n_2-1)}{2} \\ &= \frac{1}{2}(n_1^2 + n_2^2) + \frac{2}{3}n_1n_2 + \frac{5}{2}(n_1 + n_2) + 2. \qquad (21) \end{aligned}$$

and

$$\begin{aligned} 2RCW(DS_{n_1,n_2}) &= \left(\frac{n_1}{3} + \frac{1}{3} + \frac{n_2}{2}\right) + \left(\frac{n_2}{3} + \frac{1}{3} + \frac{n_1}{2}\right) + \frac{n_1(n_1-1)}{2} \\ &\quad + n_1\left(\frac{1}{3} + \frac{1}{2} + n_2\right) + \frac{n_2(n_2-1)}{2} + n_2\left(\frac{1}{3} + \frac{1}{2} + n_1\right) \\ &= \frac{1}{2}(n_1^2 + n_2^2) + 2n_1n_2 + \frac{7}{6}(n_1 + n_2) + \frac{2}{3}. \qquad (22) \end{aligned}$$

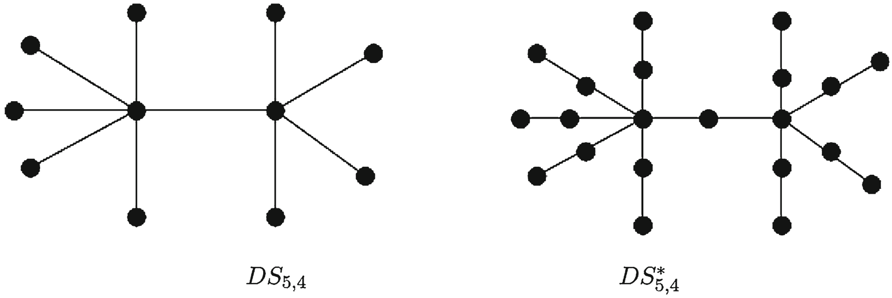


Fig. 4

We have to prove that $H(DS_{n_1,n_2}) \le RCW(DS_{n_1,n_2})$, that is,

$$\begin{aligned}\frac{1}{2}(n_1^2+n_2^2)+\frac{2}{3}n_1n_2+\frac{5}{2}(n_1+n_2)+2 &\le \frac{1}{2}(n_1^2+n_2^2)\\ &+2n_1n_2+\frac{7}{6}(n_1+n_2)+\frac{2}{3}, \quad \text{by (21) and (22),}\\ \text{i.e.,}\quad (n_1-1)(n_2-1)\ge 2,&\ \text{which is true.}\end{aligned} \tag{23}$$

Hence the first part of the proof is over.

Now, the equality holds in (23) if and only if $n_1 = 3$ and $n_2 = 2$ as $n_1 \ge n_2$. One can easily see that the equality holds in (20) if and only if G is isomorphic to a graph $DS_{3,2}$. Hence the theorem. □

Now we construct a graph $DS^*_{n_1,n_2}$ from a graph DS_{n_1,n_2} by replacing each edge of a path of length two. For example, $DS^*_{5,4}$ is a graph depicted in Fig. 4.

Theorem 4.2 *Let $DS^*_{n_1,n_2}$ be a tree with $n_1 \ge 8n_2$. Then*

$$RCW(DS^*_{n_1,n_2}) \le H(DS^*_{n_1,n_2}). \tag{24}$$

Proof We have

$$\begin{aligned}2H(DS^*_{n_1,n_2}) &= \left(n_1+\frac{n_1}{2}+1+\frac{1}{2}+\frac{n_2}{3}+\frac{n_2}{4}\right)+\left(2+\frac{n_1}{2}+\frac{n_1}{3}+\frac{n_2}{2}+\frac{n_2}{3}\right)\\ &\quad+\left(n_2+\frac{n_2}{2}+1+\frac{1}{2}+\frac{n_1}{3}+\frac{n_1}{4}\right)+n_1\left(2+\frac{n_1}{2}+\frac{n_1}{3}+\frac{n_2}{4}+\frac{n_2}{5}\right)\\ &\quad+n_1\left(1+\frac{1}{2}+\frac{n_1}{3}+\frac{n_1}{4}+\frac{n_2}{5}+\frac{n_2}{6}\right)\\ &\quad+n_2\left(2+\frac{n_2}{2}+\frac{n_2}{3}+\frac{n_1}{4}+\frac{n_1}{5}\right)\\ &\quad+n_2\left(1+\frac{1}{2}+\frac{n_2}{3}+\frac{n_2}{4}+\frac{n_1}{5}+\frac{n_1}{6}\right)\\ &= \frac{17}{12}(n_1^2+n_2^2)+\frac{49}{30}n_1n_2+\frac{77}{12}(n_1+n_2)+5.\end{aligned} \tag{25}$$

and

$$
\begin{aligned}
2RCW(DS^*_{n_1,n_2}) &= \left(\frac{n_1}{6}+\frac{n_1}{5}+\frac{1}{6}+\frac{1}{5}+\frac{n_2}{4}+\frac{n_2}{3}\right) \\
&\quad+\left(\frac{2}{6}+\frac{n_1}{5}+\frac{n_1}{4}+\frac{n_2}{5}+\frac{n_2}{4}\right)+\left(\frac{n_2}{6}+\frac{n_2}{5}\right. \\
&\quad\left.+\frac{1}{6}+\frac{1}{5}+\frac{n_1}{4}+\frac{n_1}{3}\right)+n_1\left(\frac{2}{6}+\frac{n_1}{5}+\frac{n_1}{4}+\frac{n_2}{3}+\frac{n_2}{2}\right) \\
&\quad+n_1\left(\frac{1}{6}+\frac{1}{5}+\frac{n_1}{4}+\frac{n_1}{3}+\frac{n_2}{2}+n_2\right)+n_2\left(\frac{2}{6}+\frac{n_2}{5}+\frac{n_2}{4}\right. \\
&\quad\left.+\frac{n_1}{3}+\frac{n_1}{2}\right)+n_2\left(\frac{1}{6}+\frac{1}{5}+\frac{n_2}{4}+\frac{n_2}{3}+\frac{n_1}{2}+n_1\right) \\
&= \frac{31}{30}(n_1^2+n_2^2)+\frac{14}{3}n_1n_2+\frac{63}{30}(n_1+n_2)+\frac{16}{15}. \qquad (26)
\end{aligned}
$$

We have to prove that

$$H(DS^*_{n_1,n_2}) \geq RCW(DS^*_{n_1,n_2}),$$

that is,

$$
\begin{aligned}
&\frac{17}{12}(n_1^2+n_2^2)+\frac{49}{30}n_1n_2+\frac{77}{12}(n_1+n_2)+5 \geq \frac{31}{30}(n_1^2+n_2^2)+\frac{14}{3}n_1n_2 \\
&\quad+\frac{63}{30}(n_1+n_2)+\frac{16}{15} \\
&\quad\Leftrightarrow n_1^2+n_2^2-\frac{182}{23}n_1n_2+\frac{259}{23}(n_1+n_2)+\frac{236}{23} \geq 0 \\
&\quad\Leftrightarrow n_1^2+n_2^2-8n_1n_2+11(n_1+n_2)+10 \geq 0 \\
&\quad\Leftrightarrow n_2^2+11(n_1+n_2)+10 \geq 0, \text{ as } n_1 \geq 8n_2,
\end{aligned}
$$

which, evidently, is always obeyed. Hence the theorem. □

Remark 4.3 For $n_1 = n_2 > 5$, $RCW(DS^*_{n_1,n_2}) \geq H(DS^*_{n_1,n_2})$. In order to see this note that

$$
\begin{aligned}
&n_1^2+n_2^2-\frac{182}{23}n_1n_2+\frac{259}{23}(n_1+n_2)+\frac{236}{23} \leq 0 \\
&\quad\Leftrightarrow -5n_1^2+24n_1+11 \leq 0,
\end{aligned}
$$

which is true for $n_1 > 5$.

Remark 4.4 In Theorem 4.1, we have $H(DS_{n_1,n_2}) \leq RCW(DS_{n_1,n_2})$ for $n_1 \geq 3$ and $n_2 \geq 2$, but $H(DS^*_{n_1,n_2}) \geq RCW(DS^*_{n_1,n_2})$ for $n_1 \geq 8n_2$.

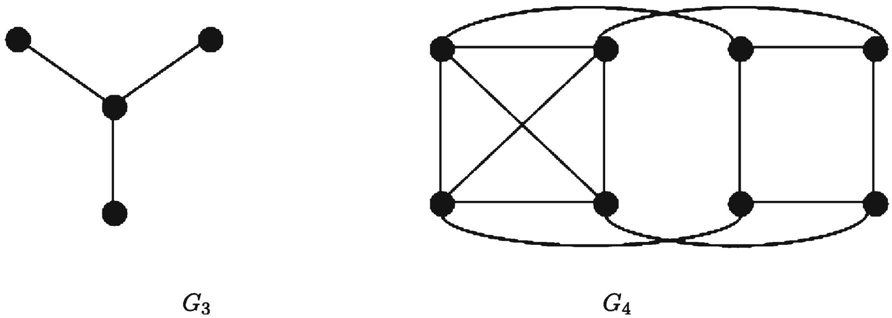


Fig. 5

Now we find the characterization for which $H(G) = RCW(G)$. We have that diameter is one for complete graph K_n and $H(K_n) = RCW(K_n)$. Now we begin the characterization for graph of diameter 2.

Theorem 4.5 *Let G be a graph of diameter 2. If $H(G) = RCW(G)$, then either n or $n-1$ is divisible by 4.*

Proof Since diameter of G is 2, either $\delta(i, j|G) = 1$ or $\delta(i, j|G) = 2$ for each pair (v_i, v_j). Since m is the number of edges in G, we have

$$H(G) = m + \frac{1}{2}\Big(\frac{n(n-1)}{2} - m\Big) \text{ and } RCW(G) = \frac{1}{2}m + \Big(\frac{n(n-1)}{2} - m\Big).$$

$$m + \frac{1}{2}\Big(\frac{n(n-1)}{2} - m\Big) = \frac{1}{2}m + \Big(\frac{n(n-1)}{2} - m\Big),$$
$$\text{i.e., } m = \frac{n(n-1)}{4}.$$

Since m is an integer, either n or $n-1$ must be divisible by 4. □

Example 1 For the two graphs depicted in Fig. 5, $H(G) = RCW(G)$ and n is divisible by 4.

Theorem 4.6 *Let G be a triangle- and quadrangle-free connected graph of diameter 3. If $H(G) = RCW(G)$, then the first Zagreb index $M_1(G)$ is equal to the two times of the number of edges in the complement of G.*

Proof Since diameter of G is 3, either $\delta(i, j|G) = 1$ or $\delta(i, j|G) = 2$ or $\delta(i, j|G) = 3$ for each pair (v_i, v_j). Since m is the number of edges in G, the number of vertex pairs at distance two is $\frac{1}{2}M_1(G) - m$. Thus

$$H(G) = m + \frac{1}{2}\Big(\frac{1}{2}M_1(G) - m\Big) + \frac{1}{3}\Big(\frac{n(n-1)}{2} - \frac{1}{2}M_1(G)\Big)$$
$$\text{and } RCW(G) = \Big(\frac{n(n-1)}{2} - \frac{1}{2}M_1(G)\Big) + \frac{1}{2}\Big(\frac{1}{2}M_1(G) - m\Big) + \frac{1}{3}m.$$

So we have

$$m+\frac{1}{2}\Big(\frac{1}{2}M_1(G)-m\Big)+\frac{1}{3}\Big(\frac{n(n-1)}{2}-\frac{1}{2}M_1(G)\Big)=\Big(\frac{n(n-1)}{2}-\frac{1}{2}M_1(G)\Big)$$
$$+\frac{1}{2}\Big(\frac{1}{2}M_1(G)-m\Big)+\frac{1}{3}m,$$

i.e., $M_1(G)=n(n-1)-2m=2\overline{m}$, where $\overline{m}$ is the number of edges in $\overline{G}$.

Hence the theorem. □

Acknowledgements K. Ch. D., B. Z., and N. T. thank, respectively, for support by Sungkyunkwan University BK21 Project, BK21 Math Modeling HRD Div., Sungkyunkwan University, Suwon, Republic of Korea, the Guangdong Provincial Natural Science Foundation of China (Grant No. 8151063101000026), and the Ministry of Science, Education and Sports of Croatia (Grant No. 098-1770495-2919).

References

1. D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, On the Harary index for the characterization of chemical graphs. J. Math. Chem. **12**, 235–250 (1993)
2. O. Ivanciuc, T.S. Balaban, A.T. Balaban, Reciprocal distance matrix, related local vertex invariants and topological indices. J. Math. Chem. **12**, 309–318 (1993)
3. D. Janežič, A. Miličević, S. Nikolić, N. Trinajstić, *Graph Theoretical Matrices in Chemistry*, Mathematical Chemistry Monographs No. 3, University of Kragujevac, Kragujevac (2007)
4. H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. Bull. Chem. Soc. Jpn. **44**, 2332–2339 (1971)
5. H. Wiener, Structural determination of paraffin boiling points. J. Am. Chem. Soc. **69**, 17–20 (1947)
6. O. Ivanciuc, T. Ivanciuc, A.T. Balaban, Design of topological indices. Part 10. Parameters based on electronegativity and vovalent radius for the computation of molecular graph descriptors for heteroatom-containing molecules. J. Chem. Inf. Comput. Sci. **38**, 395–401 (1998)
7. M.V. Diudea, Indices of reciprocal properties or Harary indices. J. Chem. Inf. Comput. Sci. **37**, 292–299 (1997)
8. B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, Harary index-twelve years later. Croat. Chem. Acta **75**, 847–868 (2002)
9. J. Devillers, A.T. Balaban (eds.), *Topological Indices and Related Descriptors in QSAR and QSPR* (Gordon & Breach, Amsterdam, 1999)
10. R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors* (Wiley-VCH, Weinheim, 2000)
11. Z. Mihalić, N. Trinajstić, A graph-theoretical approach to structure-property relationships. J. Chem. Educ. **69**, 701–712 (1999)
12. O. Ivanciuc, QSAR comparative study of Wiener descriptors for weighted molecular graphs. J. Chem. Inf. Comput. Sci. **40**, 1412–1422 (2000)
13. N. Trinajstić, S. Nikolić, S.C. Basak, I. Lukovits, Distance indices and their hyper-counterparts: intercorrelation and use in the structure-property modeling. SAR QSAR Environ. Res. **12**, 31–54 (2001)
14. B. Zhou, X. Cai, N. Trinajstić, On Harary index. J. Math. Chem. **44**, 611–618 (2008)
15. B. Zhou, X. Cai, N. Trinajstić, On reciprocal complementary Wiener number. Discrete Appl. Math. (in press). doi:10.1016/j.dam.2008.09.010
16. N. Trinajstić, *Chemical Graph Theory*, 2nd revised edn. (CRC Press, Boca Raton, 1992)
17. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. III. Total π-electron energy of alternant hydrocarbons. Chem. Phys. Lett. **17**, 535–538 (1972)
18. I. Gutman, B. Ruščić, N. Trinajstić, C.F. Wilcox, Jr., Graph theory and molecular orbitals. XII. Acyclic polyenes. J. Chem. Phys. **62**, 3399–3405 (1975)
19. S. Nikolić, G. Kovačević, A. Mihalić, N. Trinajstić, The Zagreb indices 30 years after. Croat. Chem. Acta **76**, 113–124 (2003)
20. I. Gutman, K.C. Das, The first Zagreb index 30 years after. MATCH Commun. Math. Comput. Chem. **50**, 83–92 (2004)

21. B. Zhou, D. Stevanović, A note on Zagreb indices. MATCH Commun. Math. Comput. Chem. **56**, 571–578 (2006)
22. K.C. Das, I. Gutman, B. Zhou, New upper bounds on Zagreb indices. J. Math. Chem. doi:10.1007/s10910-008-9475-3.
23. D.M. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs-Theory and Application* (Johann Ambrosius Barth, Heidelberg, 1995)