**MATCH**
*Communications in Mathematical and in Computer Chemistry*

MATCH Commun. Math. Comput. Chem. **70** (2013) 301-314

ISSN 0340 - 6253

# On Zagreb and Harary Indices

**Kinkar Ch. Das**[a], **Kexiang Xu**[b], **Ivan Gutman**[c],

[a]*Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea*
kinkardas2003@googlemail.com

[b]*College of Science, Nanjing University of Aeronautics & Astronautics, Nanjing, PR China*
xukexiang0922@yahoo.cn

[c]*Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia,*
gutman@kg.ac.rs

(Received October 20, 2012)

**Abstract**

The first $(M_1)$ and second $(M_2)$ Zagreb indices and the Harary index $(H)$ are graph invariants that found applications in chemistry. We present several new estimates for $M_1$ and $M_2$ and characterize the extremal trees. Lower and upper bounds on Harary index are obtained in terms of independence and matching numbers, as well as $M_1$ and $M_2$, and the extremal trees are characterized.

# 1 Introduction

In this paper we are concerned with finite and simple graphs. Let $G$ be such 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 $d_i$, is the number of vertices in $G$ adjacent to $v_i$. The minimum and maximum vertex degree are denoted by $\delta$ and $\Delta$, respectively. Let $N_i(G)$ be the neighbor set of the vertex $v_i \in V(G)$. The average of the degrees of the vertices in $N_i(G)$ is denoted by $m_i$.

For a subset $W$ of $V(G)$, let $G \setminus W$ be the subgraph of $G$ obtained by deleting the vertices of $W$ together with the incident edges. Given a graph $G$, a subset $S$ of $V(G)$ is said to be an *independent set* of $G$ if the subgraph $G[S]$, induced by $S$, is a graph with $|S|$ isolated vertices. The *independence number* $\alpha(G)$ of $G$ is the number of vertices in the largest independent set of $G$.

Two distinct edges in a graph $G$ are independent if they do not share a common vertex in $G$. A set of pairwise independent edges in $G$ is called a matching in $G$, while a matching of maximum cardinality is a maximum matching in $G$. The *matching number* $\beta(G)$ of $G$ is the cardinality of a maximum matching of $G$.

For other undefined notations and terminology from graph theory, the readers are referred to [1].

A graph invariant named *Harary index* was first time introduced in 1992 by Mihalić and Trinajstić [13]. They defined this index as

$$H_{old}(G) = \sum_{k \geq 1} \frac{1}{k^2}\,\gamma(G,k)$$

where the notation is same as in Eq. (1). This index was named in honor of Frank Harary, on the occasion of his 70th birthday.

In 1993 the same authors changed their minds [14], and defined the Harary index via Eq. (1). In the same year, Ivanciuc et al. [11] independently considered the same quantity.

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 $d$.

For mathematical research on $H$ see the recent papers [7, 10, 16–20] and the references cited therein.

The first and second Zagreb indices, $M_1(G)$ and $M_2(G)$, of a graph $G$ are among the oldest and the most studied graph invariants in mathematical chemistry. They are defined as [8, 9]:

$$M_1(G) = \sum_{v_i \in V(G)} d_i^2 \qquad \text{and} \qquad M_2(G) = \sum_{v_iv_j \in E(G)} d_i\, d_j\ .$$

For more details on these indices see the recent papers [4–6, 12, 15] and the references therein.

The paper is organized as follows. In Section 2 we offer some new estimates of the Zagreb indices. In Section 3 are given upper bounds on $M_1$ and $M_2$ for trees in terms of

$n$ and $\alpha$, and characterized the extremal trees. In Section 4 we establish a relationship between the Harary index and the two Zagreb indices of trees in terms of order $n$ and diameter $d$, and characterize the equality cases. Two earlier known results [10] can now be easily deduced from this relationship. In Section 5 some related open problems are posed.

## 2 Estimating the first Zagreb index

Let $v_i$ be a vertex of the graph $G$ and let $m_i$ be the average degree of the vertices adjacent to $v_i$. Denote by $\mu$ and $\nu$ the maximum and minimum of $m_i$. Then

$$M_1(G) = \sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} d_i\, m_i \tag{2}$$

$$M_2(G) = \frac{1}{2} \sum_{i=1}^{n} d_i^2\, m_i\ . \tag{3}$$

For $1 \leq \alpha \leq n-1$, the *complete split graph* $CS(n, \alpha)$, is the graph on $n$ vertices consisting of a clique on $n - \alpha$ vertices and a stable set on the remaining $\alpha$ vertices in which each vertex of the clique is adjacent to each vertex of the stable set.

**Theorem 2.1.** *Let $G$ be a connected graph of order $n$ with $m$ edges. Then*

$$\frac{2m[2m - (\Delta - \nu)(n-1)]}{n + \nu - \Delta} \leq M_1(G) \leq \frac{2m[2m + (\mu - \delta)(n-1)]}{n + \mu - \delta} \tag{4}$$

*where $\delta$, $\Delta$ are the minimum degree and the maximum degree, respectively. Equality on the left–hand side of (4) holds if and only if $G$ regular. The right–hand side equality holds in (4) if and only if $G$ is either a regular graph or $G \cong CS(n, \alpha)$.*

Proof: Let $p_i$ be the average degree of the vertices not adjacent to the vertex $v_i$. Then, $2m - d_i\, m_i - d_i = (n - d_i - 1)p_i$. Since $\delta \leq p_i \leq \Delta$,

$$(n - d_i - 1)\delta \leq 2m - d_i\, m_i - d_i \leq (n - d_i - 1)\Delta \tag{5}$$

that is,

$$\left(1 - \frac{d_i}{n-1}\right)\delta \leq \frac{2m}{n-1} - \frac{d_i\, m_i}{n-1} - \frac{d_i}{n-1} \leq \left(1 - \frac{d_i}{n-1}\right)\Delta\ . \tag{6}$$

One can easily check that equality on the left–hand side of (4) holds if $G$ is regular, and that equality on the right–hand side holds if either $G$ is regular or $G \cong CS(n, \alpha)$.

Equality on the left–hand side of (6) holds if and only if either $d_i = n-1$ or $d_j = \delta$ for $v_i v_j \notin E(G)$ , $j \neq i$. Equality on the right–hand side holds if and only if either $d_i = n-1$ or $d_j = \Delta$ for $v_i v_j \notin E(G)$ , $j \neq i$.

From the left–hand side inequality in (6) we get

$$\begin{aligned} d_i + m_i &\leq \frac{2m}{n-1} + \frac{n-2}{n-1} d_i + \left(1 - \frac{d_i}{n-1}\right)(m_i - \delta) \\ &\leq \frac{2m}{n-1} + \frac{n-2}{n-1} d_i + \left(1 - \frac{d_i}{n-1}\right)(\mu - \delta) \end{aligned} \tag{7}$$

because $m_i \leq \mu$ . Multiplying both sides by $d_i$ and by summation from $i = 1$ to $n$ (using (2)), we get

$$2M_1(G) \leq \frac{4m^2}{n-1} + \frac{n-2}{n-1} M_1(G) + \left(2m - \frac{M_1(G)}{n-1}\right)(\mu - \delta)$$

which yields the right–hand side inequality in (4).

The left–hand side of (4) is obtained analogously, bearing in mind that $m_i \geq \nu$.

Suppose now that equality holds on the right–hand side of (4). Then the left–hand side equality holds in (5) and (6), and equality holds in (7). From the left–hand side equality in (6), we get that either $d_i = n-1$ or $d_j = \delta$ for $v_i v_j \notin E(G)$ , $j \neq i$ .

From equality in (7) it follows that $m_i = \mu$ and $d_i \neq n-1$. From these results we conclude that either $G$ is isomorphic to a regular graph or $G$ is the complete split graph $CS(n, \alpha)$.

Finally, we consider the case when equality holds on the left–hand side of (4). Then the right–hand side equality holds in (5) and (6). Equality on the right–hand side of (6) implies that either $d_i = n-1$ or $d_j = \Delta$ for $v_i v_j \notin E(G)$ , $j \neq i$. Moreover, $m_i = \nu$, $d_i \neq n-1$. From these results we conclude that $G$ is a regular graph. ■

Theorem 2.1 generalizes a previously reported upper bound for $M_1$ :

**Corollary 2.2.** [3] *Let $G$ be a connected graph of order $n$ with $m$ edges. Then*

$$M_1(G) \leq \frac{2m[2m + (\Delta - \delta)(n-1)]}{n + \Delta - \delta} \, .$$

*Equality holds if and only if $G$ is either regular or $G \cong CS(n, \alpha)$.*

We now offer one more estimate for $M_1(G)$.

**Theorem 2.3.** *Let $G$ be a connected graph of order $n$ with $m$ edges. Then*

$$2m(n+\Delta-1)-(n-1)n\Delta \le M_1(G) \le 2m(n+\delta-1)-(n-1)n\delta \ . \tag{8}$$

*Equality on the left–hand side of (8) holds if and only if $G$ regular. The right–hand side equality holds in (8) if and only if $G$ is either a regular graph or $G \cong CS(n,\alpha)$.*

Proof: By summation from $i=1$ to $n$ in (5) we get

$$n(n-1)\delta - 2m\delta \le 2mn - M_1(G) - 2m \le n(n-1)\Delta - 2m\Delta$$

which gives the required result. The equality cases are established in the same way as in Theorem 2.1. ■

**Theorem 2.4.** *Let $G$ be a connected graph of order $n$ with $m$ edges. Then*

$$M_1(G)(\Delta-1) - 2M_2(G) \le 2m[(n-1)\Delta - 2m] \ . \tag{9}$$

*Equality holds if and only if $G$ is regular.*

Proof: Multiplying the right–hand side inequality (5) by $d_i$, summing from $i=1$ to $n$, and taking into account relation (3), we get

$$4m^2 - M_1(G) - 2M_2(G) \le 2m(n-1)\Delta - M_1(G)\Delta$$

which gives the required result.

Equality in (9) holds if and only if either $d_i = n-1$ or $d_j = \Delta$ for $v_iv_j \notin E(G)$ , $j \neq i$, for all $i$. Thus equality holds in (9) if and only if $G$ is regular. ■

# 3 Upper bounds on Zagreb indices for trees

As usual, $K_{1,n-1}$ and $P_n$ denote, respectively, the star and the path on $n$ vertices.

Denote by $S_{n,\alpha}$ a tree obtained from the star $K_{1,\alpha}$ by attaching a pendent edge to its $n-\alpha-1$ pendent vertices. Recall that $S_{n,\alpha}$ is called *spur*. If $\Delta = \alpha$ in a tree $T$ of order $n$ with independence number $\alpha$, then $T \cong S_{n,\alpha}$.

The first and second Zagreb indices and the Harary index of $S_{n,\alpha}$ are readily calculated:

$$\begin{aligned} M_1(S_{n,\alpha}) &= \alpha^2 - 3\alpha + 4n - 4 \\ M_2(S_{n,\alpha}) &= n\alpha - 3\alpha + 2n - 2 \\ H(S_{n,\alpha}) &= \frac{1}{24}\left(3n^2 + \alpha^2 + 2n\alpha + 19n - 9\alpha - 22\right) . \end{aligned}$$

**Theorem 3.1.** *Let $T$ be a tree of order $n$ with independence number $\alpha$. Then*

$$M_1(T) \le \alpha^2 - 3\alpha + 4n - 4 \tag{10}$$

*with equality holding if and only if $T \cong S_{n,\alpha}$.*

Proof: By direct checking we verify that for $T \cong S_{2,1}$ ($\equiv P_2$), $T \cong S_{3,2}$ ($\equiv P_3$), and $T \cong S_{4,2}$ ($\equiv P_4$), the equality holds in (10). For $T \cong P_n$ ($n \ge 5$), the inequality in (10) is strict. Otherwise, $\Delta \ge 3$. Let $S(T)$ be the largest independent set in $T$. Then $\alpha(T) = |S(T)|$. Also let $d$ be the diameter of the tree $T$. Then there exists a path $P_{d+1} : v_1 v_2 \dots v_{d+1}$ of length $d$. Since $T$ is a tree, both vertices $v_1$ and $v_{d+1}$ are pendent.

We have $n \ge \alpha + 1$. For $n = \alpha + 1$, $T \cong K_{1,n-1}$ and hence the equality holds in (10).

We now prove the theorem by induction on $n$. Assume that (10) is true for a positive integer $n - 1$. We demonstrate that it remains true when $n$ is replaced by $n + 1$.

First we assume that $\alpha(T \setminus \{v_1\}) = \alpha(T) - 1$. By the induction hypothesis,

$$\begin{aligned} M_1(T) &= M_1(T \setminus \{v_1\}) + 2d_2 \qquad \text{because } v_1 v_2 \in E(T) \\ &\le (\alpha - 1)^2 - 3(\alpha - 1) + 4(n - 1) - 4 + 2d_2 \qquad (11) \\ &= \alpha^2 - 3\alpha + 4n - 4 - 2(\alpha - d_2) \\ &\le \alpha^2 - 3\alpha + 4n - 4 \qquad (12) \end{aligned}$$

because $\alpha \ge \Delta \ge d_2$. Therefore (10) holds by induction. Equalities in (11) and (12) hold if and only if the pendent vertex $v_1$ is adjacent to a vertex $v_2$ and $d_2 = \alpha$. Thus we have $d_2 = \alpha = \Delta$, that is, $T \cong S_{n,\alpha}$.

Next we assume that $\alpha(T \setminus \{v_1\}) = \alpha(T)$. Since the vertex $v_2$ is adjacent to vertex $v_1$, it must be $v_2 \in S(T)$ as $S(T)$ is the largest independent set in $T$. By contradiction, we show that $v_2$ is of degree 2, that is, $d_2 = 2$. For this we can assume that $d_2 \ge 3$. Since the path $P_{d+1} : v_1 v_2 \dots v_{d+1}$ is of length $d$ ($d$ is the diameter of $T$), then there exists a pendent vertex $v_1'$ such that $v_1'v_2 \in E(T)$ as $d_2 \geq 3$. Since $v_2 \in S(T)$, $v_1, v_1' \notin S(T)$. Now, $|\{S(T) \cup \{v_1, v_1'\}\} \setminus \{v_2\}| > |S(T)|$, a contradiction as $S(T)$ is the largest independent set in $T$. Thus we have $d_2 = 2$. Similarly, as before, by the induction hypothesis,

$$M_1(T) = M_1(T \setminus \{v_1\}) + 4 \leq \alpha^2 - 3\alpha + 4n - 4$$

and (10) holds by induction. This inequality is strict as the pendent vertex $v_1$ is adjacent to a vertex $v_2$ and $d_2 = 2 < \Delta$. This completes the proof of this theorem. ■

**Theorem 3.2.** *Let $T$ be a tree of order $n$ with independence number $\alpha$. Then*

$$M_2(T) \leq n\alpha - 3\alpha + 2n - 2 \tag{13}$$

*with equality holding in (13) if and only if $T \cong S_{n,\alpha}$.*

Proof: For $T \cong S_{2,1}$ ($\equiv P_2$) or $T \cong S_{3,2}$ ( $\equiv P_3$) or $T \cong S_{4,2}$ ($\equiv P_4$), the equality holds in (13). For $T \cong P_n$ ($n \geq 5$), the inequality in (13) is strict. Otherwise, $\Delta \geq 3$.

For a vertex $v_j$ of the tree $T$ we have $d_j \leq \Delta \leq \alpha$. Therefore,

$$\begin{aligned}
d_j\, m_j + d_j &= \sum_{k=1}^{n} d_k - \sum_{v_k v_j \notin E(T)\,,\, k \neq j} d_k \\
&\leq 2(n-1) - (n - d_j - 1) \qquad \text{because } d_k \geq 1 \text{ for } v_k v_j \notin E(T)\,,\ k \neq j \\
&\leq 2(n-1) - (n - \alpha - 1) \qquad \text{because } d_j \leq \alpha \\
&= n + \alpha - 1\,. 
\end{aligned} \tag{14}$$

Moreover, $d_j\, m_j + d_j = n + \alpha - 1$ if and only if the vertex $v_j$ is of degree $\alpha$ and the vertices not adjacent to $v_j$ are pendent, i.e., if and only if $T \cong S_{n,\alpha}$.

We have $n \geq \alpha + 1$. For $n = \alpha + 1$, $T \cong K_{1,n-1}$ and hence the equality holds in (13).

We now prove the theorem by induction on $n$. Assume that (13) is true for a positive integer $n-1$ and we demonstrate that it remains true when $n$ is replaced by $n+1$.

In Theorem 3.1 we considered a path $P_{d+1} : v_1 v_2 \ldots v_{d+1}$ of length $d$. Thus the vertex $v_2$ of degree $d_2$ is adjacent to the pendent vertex $v_1$. First we assume that $\alpha(T \setminus \{v_1\}) = \alpha(T) - 1$. By the induction hypothesis and by bearing in mind relation (14),

$$M_2(T) = M_2(T \setminus \{v_1\}) + d_2\, m_2 + d_2 - 1$$

as the pendent vertex $v_1$ is adjacent to $v_2$, and further

$$\begin{aligned} M_2(T) &\leq (n-1)(\alpha-1) - 3(\alpha-1) + 2(n-1) - 2 + d_2\, m_2 + d_2 - 1 \\ &= n\alpha - 3\alpha + 2n - 2 - [n + \alpha - 1 - (d_2\, m_2 + d_2)] \\ &\leq n\alpha - 3\alpha + 2n - 2 \; . \end{aligned}$$

Then the inequality (13) holds by induction. Equality holds if and only if $T \cong S_{n,\alpha}$ .

Next we assume that $\alpha(T \setminus \{v_1\}) = \alpha(T)$. Since $v_2$ is adjacent to $v_1$, by Theorem 3.1 we have $d_2 = 2$. Similarly, as before, from the induction hypothesis it follows

$$M_2(T) = M_2(T \setminus \{v_1\}) + d_2\, m_2 + d_2 - 1 \leq n\alpha - 3\alpha + 2n - 2$$

because $d_2 = 2$ and $d_2\, m_2 \geq 3$. Then (13) holds by induction. Since $d_2 = 2 < \Delta \leq \alpha$, this inequality is strict. Hence $d_2\, m_2 + d_2 < n + \alpha - 1$. ■

# 4 Bounds on Harary index of trees

**Theorem 4.1.** *Let $T$ be a tree of order $n$ with diameter $d$. Then*

$$H(T) \geq \left(\frac{1}{3} - \frac{1}{d}\right) M_2 + \left(\frac{1}{2d} - \frac{1}{12}\right) M_1 + \frac{1}{2d}\, n^2 + \left(\frac{5}{6} - \frac{3}{2d}\right) n + \frac{1}{d} - \frac{5}{6} \qquad (15)$$

$$H(T) \leq \frac{1}{12}\, M_2 + \frac{1}{24}\, M_1 + \frac{1}{8}\, n^2 + \frac{11}{24}\, n - \frac{7}{12} \; . \qquad (16)$$

*Equality holds both in (15) and (16) if and only if $T$ is a tree of diameter at most 4.*

Proof: Since $T$ is a tree, we have $\gamma(T,1) = n-1$. Also, in view of Eq. (2),

$$\gamma(T,2) = \frac{1}{2} \sum_{i=1}^{n} \sum_{v_j \in N_i} (d_j - 1) = \frac{1}{2} \sum_{i=1}^{n} (d_i\, m_i - d_i) = \frac{1}{2}\, M_1 - n + 1 \; .$$

Denote by $\gamma(T, v_i, 3)$, the number of vertex pairs at distance three from the vertex $v_i$. Then

$$\begin{aligned} \gamma(T, v_i, 3) &= \sum_{v_j \in N_i} \left[ \sum_{v_k \in N_j} (d_k - 1) - (d_i - 1) \right] \\ &= \sum_{v_j \in N_i} [d_j\, m_j - d_j - d_i + 1] \qquad \text{since} \sum_{v_k \in N_j} d_k = d_j\, m_j \\ &= \sum_{v_j \in N_i} d_j\, m_j - d_i\, m_i - d_i^2 + d_i \; . \end{aligned}$$

Using the identities (2), (3), and

$$\sum_{i=1}^{n} \sum_{v_j \in N_i} d_j\, m_j = \sum_{i=1}^{n} d_i^2\, m_i$$

we have

$$\gamma(T,3) = \frac{1}{2} \sum_{i=1}^{n} \gamma(T, v_i, 3) \;=\; \frac{1}{2} \sum_{i=1}^{n} \left[ \sum_{v_j \in N_i} d_j\, m_j - d_i\, m_i - d_i^2 + d_i \right]$$

$$= \frac{1}{2} \sum_{i=1}^{n} d_i^2\, m_i - M_1 + n - 1 = M_2 - M_1 + n - 1 \; .$$

There are $\binom{n}{2}$ vertex pairs and the diameter of $T$ is $d$. Bearing in mind the definition (1) of the Harary index, the above results imply

$$H(T) \;\geq\; n - 1 + \frac{1}{2}\left(\frac{1}{2}\, M_1 - n + 1\right) + \frac{1}{3}\,(M_2 - M_1 + n - 1)$$
$$+\; \frac{1}{d}\left(\frac{n(n-1)}{2} - M_2 + \frac{1}{2}\, M_1 - n + 1\right)$$

and

$$H(T) \;\leq\; n - 1 + \frac{1}{2}\left(\frac{1}{2}\, M_1 - n + 1\right) + \frac{1}{3}\,(M_2 - M_1 + n - 1)$$
$$+\; \frac{1}{4}\left(\frac{n(n-1)}{2} - M_2 + \frac{1}{2}\, M_1 - n + 1\right) \; .$$

Inequalities (15) and (16) follow straightforwardly. The conditions for equality are also immediately recognized. ■

Substituting (10) and (13) back into (16), we obtain an earlier known result:

**Corollary 4.2.** [10] *Let $T$ be a tree of order $n$ with independence number $\alpha$. Then*

$$H(T) \leq \frac{1}{24}\,(3n^2 + \alpha^2 + 2n\alpha + 19n - 9\alpha - 22) \; .$$

*Equality holds if and only if $T \cong S_{n,\alpha}$ .*

By $\beta(G)$ we denote the matching number of the graph $G$. It is well known [1] that for any bipartite graph $G$ of order $n$, $\alpha(G) + \beta(G) = n$. Therefore the following corollary is immediate.

**Corollary 4.3.** [10] *Let $T$ be a tree of order $n$ with matching number $\beta$. Then*

$$H(T) \leq \frac{1}{24}\left(6n^2 + \beta^2 - 4n\beta + 10n + 9\beta - 22\right) .$$

*Equality holds in if and only if $T \cong S_{n,n-\beta}$ .*

For the complete split graph $CS(n, \alpha)$ we have

$$H(CS(n,\alpha)) = \frac{\alpha(\alpha-1)}{4} + \frac{(n-\alpha)\alpha}{2} + \frac{n(n-1)}{4} .$$

**Theorem 4.4.** *Let $G$ be a connected graph of order $n$ with independence number $\alpha$. Then*

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

*with equality holding if and only if $G \cong CS(n, n-\alpha)$.*

Proof: It is well-known that Harary index strictly increases if two vertices are joined by an edge in graph $G$. Using this result one can see easily that $H(G) \leq H(CS(n, n-\alpha))$ and the upper bound is attained if and only if $G \cong CS(n, n-\alpha)$ as graph $G$ has independence number $\alpha$. ■

**Lemma 4.5.** [20] *Let $G$ be a (connected) graph with a cut vertex $v_k$ such that $G_1$ and $G_2$ are two connected subgraphs of $G$ having $v_k$ as the only common vertex. Let $|V(G_i)| = n_i$ for $i = 1, 2$. Then*

$$H(G) = H(G_1) + H(G_2) + \sum_{v_i \in V(G_1)\backslash\{v_k\}} \sum_{v_j \in V(G_2)\backslash\{v_k\}} \frac{1}{d_{G_1}(v_i, v_k) + d_{G_2}(v_k, v_j)} .$$

The dumbbell $D(n, a, b)$ consists of the path $P_{n-a-b}$ together with $a$ independent vertices adjacent to one pendent vertex of the path and $b$ independent vertices adjacent to the other pendent vertex. The graph $D(n, a, b)$ is said to be a *balanced dumbbell* if $|a - b| \leq 1$. We now calculate the Harary index of $D(n, a, b)$, where $a = \left\lceil \frac{2\alpha-n+1}{2} \right\rceil$, $b = \left\lfloor \frac{2\alpha-n+1}{2} \right\rfloor$. For this we assume that the vertex of degree $a + 1$ in $D(n, a, b)$ is labelled as $v_k$. By $B_{n,k}$, usually called *broom*, we denote the graph obtained from path $P_{n-k+1}$ by attaching $k-1$ pendant vertices to one end vertex $v_r$ of $P_{n-k+1}$. By Lemma 4.5, we have

$$\begin{aligned} H\left(B_{n-a,b}\right) &= H\left(K_{1,b}\right)+H(P_{n-a-b}) \\ &+ \sum_{v_s\in V\left(K_{1,b}\right)\setminus\{v_r\}}\ \sum_{v_t\in V(P_{n-a-b})\setminus\{v_r\}} \frac{1}{d_{K_{1,b}}(v_s,v_r)+d_{P_{n-a-b}}(v_r,v_t)} \\ &= \frac{b(b-1)}{4}+b+\sum_{i=1}^{n-a-b-1}\left(1+\frac{1}{2}+\cdots+\frac{1}{n-a-b-i}\right) \\ &+ b\left(\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{n-a-b}\right) . \end{aligned}$$

Now,

$$\begin{aligned} & H\left(D(n,a,b)\right) = H\left(K_{1,a}\right)+H\left(B_{n-a,b}\right) \\ + & \sum_{v_i\in V(K_{1,a})\setminus\{v_k\}}\ \sum_{v_j\in V\left(B_{n-a-1,b}\right)\setminus\{v_k\}} \frac{1}{d_{K_{1,a}}(v_i,v_k)+d_{B_{n-a-1,b}}(v_k,v_j)} \\ = & \frac{a(a-1)}{4}+a+\frac{b(b-1)}{4}+b+\sum_{i=1}^{n-a-b-1}\left(1+\frac{1}{2}+\cdots+\frac{1}{n-a-b-i}\right) \\ + & b\left(\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{n-a-b}\right)+a\left(\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{n-a-b}+\frac{b}{n-a-b+1}\right) \\ = & \frac{a(a-1)+b(b-1)}{4}+\frac{ab}{n-a-b+1}+(a+b)\sum_{i=1}^{n-a-b}\frac{1}{i}+\sum_{i=1}^{n-a-b-1}\sum_{j=1}^{n-a-b-i}\frac{1}{j} . \end{aligned}$$

Thus we have

$$\begin{aligned} & D\left(n,\left\lceil\frac{2\alpha-n+1}{2}\right\rceil,\left\lfloor\frac{2\alpha-n+1}{2}\right\rfloor\right) = \frac{1}{4}\left(2\alpha-n+1\right)^2 \\ - & \frac{n-\alpha-1}{2(n-\alpha)}\left\lceil\frac{2\alpha-n+1}{2}\right\rceil\left\lfloor\frac{2\alpha-n+1}{2}\right\rfloor-\frac{1}{4}\left(2\alpha-n+1\right) \\ + & \left(2\alpha-n+1\right)\sum_{i=1}^{2n-2\alpha-1}\frac{1}{i}+\sum_{i=1}^{2n-2\alpha-2}\sum_{j=1}^{2n-2\alpha-i-1}\frac{1}{j} . \end{aligned}$$

In [2] it was shown that the balanced dumbbell $D\left(n,\left\lceil\frac{2\alpha-n+1}{2}\right\rceil,\left\lfloor\frac{2\alpha-n+1}{2}\right\rfloor\right)$ has maximal Wiener index among trees with $n$ vertices and independence number $\alpha$. Inspired from above result, initially we thought that the same dumbbell has the minimal Harary index among trees with $n$ vertices and independence number $\alpha$. Here we give a counterexample for the above statement.

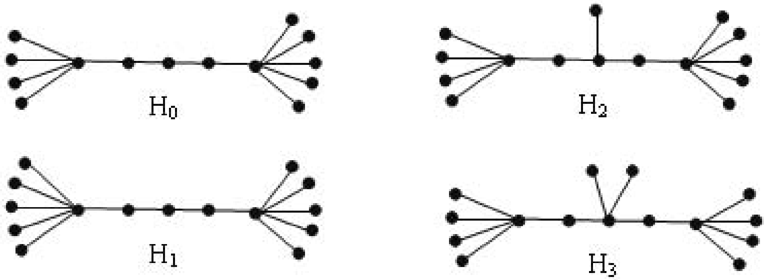


Fig. 1. Trees providing counterexamples for the dumbbell conjecture.

Note that the trees $H_i$ , $i = 1, 2, 3$, depicted in Fig. 1, are of order 15 and have independence number 12. Direct calculation yields:

$$\begin{aligned} H(H_1) &= H(H_0) + 3 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{5} + \frac{5}{6} \\ H(H_2) &= H(H_0) + 3 + \frac{2}{3} + \frac{5}{4} \end{aligned}$$

implying that $H(H_1) > H(H_2)$. From this we conclude that the balanced dumbbell is not the tree with minimal Harary index among trees for given $n$ and $\alpha$.

In addition, by simple calculation we find that

$$\begin{aligned} M_1(H_1) &= 94 > 88 = M_1(H_2) \\ M_2(H_1) &= 92 > 84 = M_2(H_3) \ . \end{aligned}$$

which shows that the balanced dumbbell is not the tree with minimal (first and second) Zagreb index among trees with given $n$ and $\alpha$.

# 5 Concluding remarks

In this paper we discussed bounds on the Zagreb indices and the Harary index of trees and characterize extremal graphs. Here we pose three related problems.

**Problem 1.** Characterize the extremal tree with minimal Harary index among trees of order $n$ and independence number $\alpha$.

**Problem 2.** Characterize the extremal tree with minimal (first or second) Zagreb index among trees of order $n$ and independence number $\alpha$.

**Problem 3.** Find some nice relationship between Harary index and Zagreb index for general graphs, or for some special graphs.

*Acknowledgement.* K. Ch. D. thanks for support by Sungkyunkwan University BK21 Project, BK21 Math Modeling HRD Div. Sungkyunkwan University, Suwon, Republic of Korea. K. X. thanks for support by the NNSF of China (grant No. 11201227).

# References

[1] J. A. Bondy, U. S. R. Murty, *Graph Theory with Applications*, Macmillan, New York, 1976.

[2] P. Dankelmann, Average distance and independence number, *Discr. Appl. Math.* **51** (1994) 75–83.

[3] K. C. Das, Maximizing the sum of the squares of the degrees of a graph, *Discr. Math.* **285** (2004) 57–66.

[4] K. C. Das I. Gutman, B. Horoldagva, Comparing Zagreb indices and coindices of trees, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 189–198.

[5] K. C. Das, I. Gutman, B. Zhou, New upper bounds on Zagreb indices, *J. Math. Chem.* **46** (2009) 514–521.

[6] T. Došlić, B. Furtula, A. Graovac, I. Gutman, S. Moradi, Z. Yarahmadi, On vertex–degree–based molecular structure descriptors, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 613–626.

[7] L. Feng, A. Ilić, Zagreb, Harary and hyper–Wiener indices of graphs with a given matching number, *Appl. Math. Lett.* **23** (2010) 943–948.

[8] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[9] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total $\pi$-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[10] A. Ilić, G. Yu, L. Feng, The Harary index of trees, *Util. Math.*, in press.

[11] O. Ivanciuc, T. S. Balaban, A. T. Balaban, Reciprocal distance matrix, related local vertex invariants and topological indices, *J. Math. Chem.* **12** (1993) 309–318.

[12] B. Liu, Z. You, A survey on comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 581–593.

[13] Z. Mihalić, N. Trinajstić, A graph–theoretical approach to structure–property relationships, *J. Chem. Educ.* **69** (1992) 701–712.

[14] D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, On the Harary index for the characterization of chemical graphs, *J. Math. Chem.* **12** (1993) 235–250.

[15] T. Réti, On the relationships between the first and second Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 169–188.

[16] S. Wagner, H. Wang, X. Zhang, Distance–based graph invariants of trees and the Harary index, *Filomat* **27** (2013) 39–48.

[17] K. Xu, Trees with the seven smallest and eight greatest Harary indices, *Discr. Appl. Math.* **160** (2012) 321–331.

[18] K. Xu, K. C. Das, On Harary index of graphs, *Discr. Appl. Math.* **159** (2011) 1631–1640.

[19] K. Xu, K. C. Das, Extremal unicyclic and bicyclic graphs with respect to Harary index, *Bull. Malaysian Math. Sci. Soc.*, in press.

[20] K. Xu, N. Trinajstić, Hyper–Wiener and Harary indices of graphs with cut edges, *Util. Math.* **84** (2011) 153-163.