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The Hyper-Zagreb Index of Trees and Unicyclic Graphs

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Abstract. Topological indices are widely used as mathematical tools to analyze different types of graphs emerged in a broad range of applications. The Hyper-Zagreb index (HM) is an important tool because it integrates the first two Zagreb indices. In this paper, we characterize the trees and unicyclic graphs with the first four and first eight greatest HM-value, respectively.

Keywords: Hyper-Zagreb index, Vertex degree, Unicyclic graphs, Trees.

2000 Mathematics subject classification: 05C05, 05C07, 05C35.

1. Introduction

A nonnegative number is assigned to a graph G to define an associated topological index if it is the same for every isomorphic graph of G, i.e., it is graph invariant. Topological indices are appropriate tools to mathematically investigate and properly comprehend molecular structures and their properties

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such as complexity [9, 10]. The first topological index is proposed by Wiener [24] in order to examine chemical features of paraffin. Since trees demonstrate a remarkable importance in various applications, authors in [4] specifically investigate this index for this setting. Moreover, In [20], the extremal unicyclic graphs with respect to Wiener index is studied. The Hyper-Wiener index for acyclic structures is due to Randic, where later [15] extends this notion so that it applies applied for any connected graphs. An interested reader can explore some chemical applications of the Hyper-Wiener index in [12]. Zagreb indices were first suggested by Gutman et al. [13] in the 1970s, which absorbed attention of many scientists in different fields. The reader is encouraged to consult with [1, 3, 11, 14, 21, 25, 27] for more useful information. A comprehensive study on relations between the mentioned indices is found in [26].

All graphs in this paper are simple, finite and undirected. The vertex and edge sets of a graph G are shown by $V(G)$ and $E(G)$, respectively. Also, $n(G)$ denotes the number of vertices of G, which is called its order.

For a graph G, the *Hyper-Zagreb index* of G is defined as the following

$$HM(G) = \sum_{xy\in E(G)} \left(d_G(x) + d_G(y)\right)^2, \tag{1.1}$$

where $d_G(x)$ is the degree of vertex x. For the edge $xy \in E(G)$, if consider $h_G(xy) := \left(d_G(x) + d_G(y)\right)^2$. Then, the above formulation can be equivalently written as

$$HM(G) = \sum_{xy\in E(G)} h_G(xy).$$

This was initially presented by Shirdel et al. [23] in 2013. They consider two simply connected graphs and compute this distance-based index for the resulted Cartesian product, composition, join and disjunction graphs. Gao et al. [7] discuss acyclic, unicyclic, and bicyclic graphs and find sharp bounds for their Hyper-Zagreb index. The degree of vertices is the main part of some other graph invariants such as irregularity and total irregularity, see [6, 17, 18, 19]. There is an extensive literature on this topic including [2, 5, 8, 22, 16].

2. Preliminaries and lemmas

In this section, we first bring several notations and definitions. Then, we propose different propositions which are essential for the subsequent section.

Unicylcic graph G of order n with circuit $C_m = x_1x_2\dots x_mx_1$ of length m is denoted by $C_m^{u_1,u_2,\dots,u_k}(T_1, T_2, \dots, T_k)$ in which trees T_i's for $i = 1, 2, \dots, k$ are all nontrivial components of $G - E(C_m)$ and u_i $(i = 1, 2, \dots, k)$ is the common vertex of T_i and C_m. Specially, $G = C_n$ for $k = 0$. For convenience, we denote $C_m^{u_1,u_2,\dots,u_k}(T_1, T_2, \dots, T_k)$ by $C_m(T_1, T_2, \dots, T_k)$, for any integer number $k \geq 1$. Let $n(T_i) = l_i + 1$, $i = 1, 2, \dots, k$, then $l = \sum_{i=1}^{k} l_i = n - m$. Also, if

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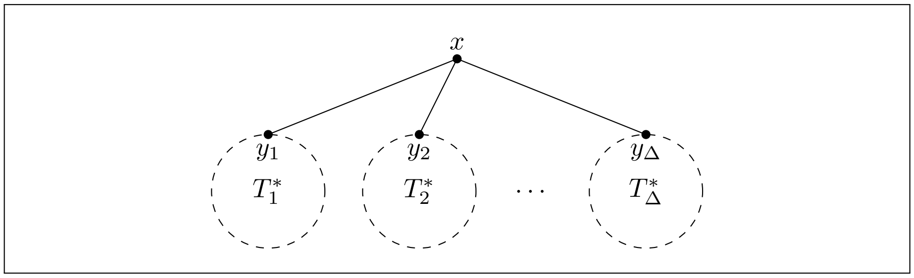

FIGURE 1. Tree $T^x(T_1, T_2, \ldots, T_\Delta)$.

a tree T_i is the star S_{l_i+1} then we replace it by l_i, for example we denote $C_4(T_1, S_5, T_3, S_9)$ by $C_4(T_1, 4, T_3, 8)$.

Let T be a *tree* with n vertices ($n \geq 2$) such that $x \in V(T)$ and x has a maximum degree of vertices in graph T, i.e. $\Delta = d_T(x) = \max\{d_T(u), u \in V(T)\}$. T is shown by $T^x(T_1, T_2, \ldots, T_\Delta)$, where $T_i = T_i^* + \{y_i x\}$, $i = 1, 2, \ldots, \Delta$, and $T_1^*, T_2^*, \ldots, T_\Delta^*$ are trees with disjoint vertex sets and $n_1, n_2, \ldots, n_\Delta$ are numbers of their vertices, respectively. Therefore, we have $|V(T_i)| = |V(T_i^*)| + 1 = n_i + 1$, $i = 1, 2, \ldots, \Delta$, and $n = |V(T)| = \sum_{i=1}^{\Delta} n_i + 1$ and $y_i \in V(T_i^*)$. Moreover, $E(T_i) = E(T_i^*) \cup \{y_i x\}$ and $V(T_i) = V(T_i^*) \cup \{x\}$ (see Figure 1).

The *coalescence* of G and H is denoted by $G(u)oH(v)$ and obtained by identifying the vertex u of G with the vertex v of H.

Lemma 2.1. *Assume that $z \in V(H)$ and $\{u, w\} \subseteq V(G)$ such that the following conditions hold:*

(a) $d_G(u) \leq d_G(w)$,

(b) $\displaystyle\sum_{x \in N_G(u)\setminus\{w\}} d_G(x) \leq \sum_{x \in N_G(w)\setminus\{u\}} d_G(x)$.

Moreover, let $G_1 = G(u)oH(z)$ and $G_2 = G(w)oH(z)$, where G_1 and G_2 are as shown in Figure 2 . Then, $HM(G_2) \geq HM(G_1)$, with the equality if and only if equality holds in both given conditions.

Proof. Recall that

$$\sum_{x \in N_G(w)\setminus\{u\}} h_{G_1}(xw) = \sum_{x \in N_G(w)\setminus\{u\}} \left(d_G(x) + d_G(w)\right)^2,$$
$$\sum_{x \in N_H(z)} h_{G_1}(xz) = \sum_{x \in N_H(z)} \left(d_H(z) + d_G(u) + d_H(x)\right)^2$$

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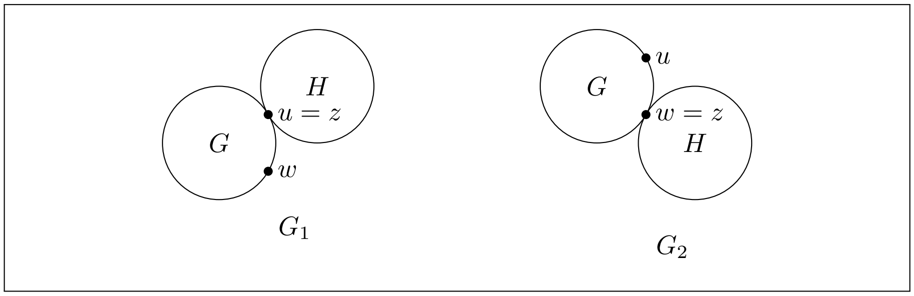

Figure 2. The transformation of two graphs.

and $h_{G_1}(uw) = h_{G_2}(uw) = (d_G(z) + d_G(w) + d_H(x))^2$. In addition, one has

$$\sum_{x\in N_H(z)} h_{G_2}(zx) = \sum_{x\in N_H(z)} (d_H(z) + d_G(w) + d_H(x))^2,$$

$$\sum_{x\in N_G(u)\setminus\{w\}} h_{G_2}(xu) = \sum_{x\in N_G(u)\setminus\{w\}} (d_G(u) + d_G(x))^2$$

and

$$\sum_{x\in N_G(w)\setminus\{u\}} h_{G_2}(xw) = \sum_{x\in N_G(w)\setminus\{x\}} (d_G(w) + d_G(x) + d_H(z))^2.$$

We consider two cases where either $uw \in E(G)$ or $uw \notin E(G)$. First, suppose that $uw \in E(G)$. For $i = 1$ and 2, we have

$$HM(G_i) = \sum_{\substack{xy\in E(G)\\ x,y\notin\{u,w\}}} h_G(xy) + \sum_{x\in N_G(u)\setminus\{w\}} h_{G_i}(xu) + \sum_{x\in N_G(w)\setminus\{u\}} h_{G_i}(xw) + h_{G_i}(uw) + \sum_{x,y\neq z} h_H(xy) + \sum_{x\in N_H(z)} h_{G_i}(xz).$$

On the other hand,

$$\sum_{x\in N_G(u)\setminus\{w\}} h_{G_1}(xu) = \sum_{x\in N_G(u)\setminus\{w\}} (d_G(u) + d_G(x) + d_H(x))^2.$$

Therefore,

$$\begin{aligned} &HM(G_2) - HM(G_1)\\ =&\sum_{x\in N_G(u)\setminus\{w\}} \left((d_G(u) + d_G(x))^2 - (d_G(u) + d_G(x) + d_H(z))^2\right)\\ &+\sum_{x\in N_G(w)\setminus\{u\}} \left((d_G(w) + d_G(x) + d_H(z))^2 - (d_G(w) + d_G(u))^2\right)\\ &+\sum_{x\in N_H(z)} \left((d_H(z) + d_G(w) + d_H(x))^2 - (d_H(z) + d_G(u) + d_H(w))^2\right)\end{aligned}$$

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this implies that

$$\begin{aligned}HM(G_2) - HM(G_1) \geq & 2d_H(z)\left(d_G(u)\left(d_G(w)-1\right) - d_G(u)\left(d_G(u)-1\right)\right) \\ & + 2d_H(z)\left(\sum_{x\in N_G(w)\setminus\{u\}} d_G(u) - \sum_{x\in N_G(w)\setminus\{w\}} d_G(x)\right) \\ \geq & 0.\end{aligned}$$

Now, suppose that $uw \notin E(G)$. Then, for $i = 1$ and 2, we have

$$\begin{aligned}HM(G_i) = & \sum_{\substack{xy\in E(G)\\ x,y\notin\{u,w\}}} h_G(xy) + \sum_{x\in N_G(u)} h_{G_i}(xu) + \sum_{x\in N_G(w)} h_{G_i}(xw) \\ & + \sum_{x,y\neq z} h_H(xy) + \sum_{x\in N_{G_i}} h_{G_i}(xz).\end{aligned}$$

Also, in this case one has

$$\sum_{x\in N_G(w)\setminus\{u\}} d_G(x) = \sum_{x\in N_G(w)} d_G(x), \quad \sum_{x\in N_G(u)\setminus\{w\}} d_G(x) = \sum_{x\in N_G(u)} d_G(x).$$

Hence, a similar approach as the previous case can be used to prove the result. □

Lemma 2.2. *Suppose u and v are vertices of graphs G_1 and G_2, respectively. Let G be the graph obtained by joining $u \in V(G_1)$ to $v \in V(G_2)$ by an edge, and G' be the graph obtained by identifying $u \in V(G_1)$ with $v \in V(G_2)$ and attaching a pendent vertex to the common vertex as shown in Figure 3. Then if $d_G(u), d_{G'}(v) \geq 2$, we have $HM(G) < HM(G')$.*

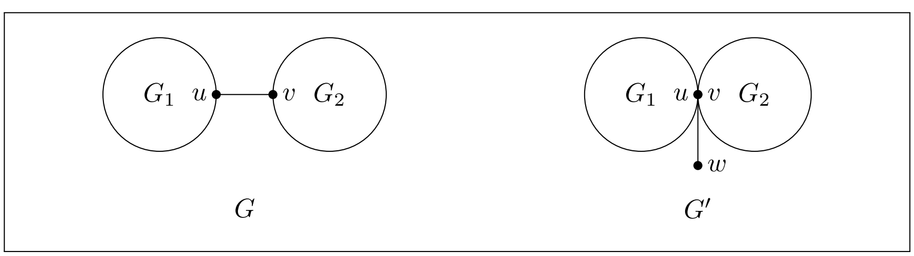

FIGURE 3. An illustration of graphs in Lemma 2.2.

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Proof. Assume that the graph G' is obtained by identifying $u \in V(G_1)$ with $v \in V(G_2)$ and attaching a pendent vertex w to the common vertex. Then,

$$HM(G) = h_G(uv) + \sum_{x \in N_{G_1}(u)} h_G(ux) + \sum_{x \in N_{G_2}(v)} h_G(vx) + \sum_{\substack{xy \in E(G_1) \\ u \notin \{x,y\}}} h_{G_1}(xy) + \sum_{xy \in E(G_2), v \notin \{x,y\}} h_{G_2}(xy)$$

and

$$HM(G') = h_{G'}(uw) + \sum_{x \in N_{G_1}(u)} h_{G'}(ux) + \sum_{x \in N_{G_2}(v)} h_{G'}(vx) + \sum_{\substack{xy \in E(G_1) \\ u \notin \{x,y\}}} h_{G_1}(xy) + \sum_{\substack{xy \in E(G_2) \\ v \notin \{x,y\}}} h_{G_2}(xy).$$

Since $d_G(u) = d_{G_1}(u) + 1,\ d_G(v) = d_{G_1}(v) + 1,\ d_{G'}(w) = 1$ and $d_{G'}(u) = d_{G'}(v) = d_{G_1}(u) + d_{G_2}(v) + 1$ we have

$$\sum_{x \in N_{G_1}(u)} h_G(ux) < \sum_{x \in N_{G_1}(u)} h_{G'}(ux), \qquad \sum_{x \in N_{G_2}(v)} h_G(vx) < \sum_{x \in N_{G_2}(v)} h_{G'}(vx)$$

and $h_G(uv) = h_{G'}(uw) = (d_{G_1}(u) + d_{G_2}(v) + 2)^2$. Hence,

$$HM(G') - HM(G) = \sum_{x \in N_{G_1}(u)} h_{G'}(ux) - \sum_{x \in N_{G_1}(u)} h_G(ux) + \sum_{x \in N_{G_2}(v)} h_{G'}(vx) - \sum_{x \in N_{G_2}(v)} h_G(vx) > 0.$$

□

Corollary 2.3. *Let T be a tree with n vertices. Then, $HM(T) \leq HM(S_n)$, with the equality if and only if $T \cong S_n$.*

Corollary 2.4. *Let $G = C_m(T_1, T_2, \ldots, T_k)$ be a unicyclic graph and $n(T_i) = l_i + 1$. Then, $HM(G) \leq HM(C_m(l_1, l_2, \ldots, l_k))$, with the equality if and only if $T_i \cong S_{l_i+1}$, $i = 1, 2, \ldots, k$.*

Lemma 2.5. *Let $G_1 = C_m(l_1, l_2, \ldots, l_k)$ be a unicyclic graph and $y_1u_i, u_iu_{i+1} \in E(C_m)$ such that $d_{G_1}(y_1), d_{G_1}(u_i) \leq d_{G_1}(u_{i+1})$, then for $G_2 = C_m(l_1, \ldots, l_{i-1}, l_{i+1} + l_i, l_{i+2}, \ldots, l_k)$ one has that $HM(G_1) < HM(G_2)$.*

Proof. Let $G = C_m(l_1, \ldots, l_{i-1}, l_{i+1}, l_{i+2}, \ldots, l_k)$, then $2 = d_G(u_i) < 3 \leq d_G(u_{i+1})$; meaning that the condition *(a)* in Lemma 2.1 holds. Hence, we now

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show that the second condition in this Lemma is also satisfied. Suppose that $y_2u_{i+1} \in E(C_m)$. By a simple calculation one can check that

$$\begin{aligned}\sum_{x\in N_G(u_i)\setminus\{u_{i+1}\}} d_G(x) =& d_G(y_1),\\ \sum_{x\in N_G(u_{i+1})\setminus\{u_i\}} d_G(x) =& \sum_{\substack{x\in N_G(u_{i+1})\setminus\{u_i\}\\ x\in V(C_m)}} d_G(x) + \sum_{\substack{x\in N_G(u_{i+1})\setminus\{u_i\}\\ x\notin V(C_m)}} d_G(x)\\ =& d_G(y_2) + \sum_{\substack{x\in N_G(u_{i+1})\setminus\{u_i\}\\ x\notin V(C_m)}} 1\\ =& d_G(y_2) + d_G(u_{i+1}) - 2.\end{aligned}$$

Moreover, $d_{G_1}(u_{i+1}) = d_G(u_{i+1})$ and $d_G(y_1) = d_{G_1}(y_1)$. On the other hand, since $y_2 \in V(C_m)$ then $d_G(y_2) \geq 2$; implying that $d_G(y_2) - 2 \geq 0$. So, we have

$$\textstyle\sum_{x\in N_G(u_i)\setminus\{u_{i+1}\}} d_G(x) = d_G(y_1) = d_{G_1}(y_1) \leq d_{G_1}(u_{i+1}) = d_G(u_{i+1}) \leq \sum_{x\in N_G(u_{i+1})\setminus\{u_i\}} d_G(x).$$

Therefore, the condition *(b)* of Lemma 2.1 holds, which completes the proof. □

Lemma 2.6. *Let $G = C_m^{u_1,u_2,\ldots,u_k}(l_1, l_2, \ldots, l_k)$ be a unicyclic graph and $k > 1$. Then if $u_iu_{i+1} \in E(C_m)$, $i = 1, 2, \ldots, k-1$, then $HM(G) < HM(C_m(n-m))$. Otherwise, there exist positive integers $l'_1, l'_2, \ldots, l'_r$ $(r \leq k)$, such that $HM(G) < HM(G') < HM(G'')$, where $G' = C_m^{v_1,v_2,\ldots,v_r}(l'_1, l'_2, \ldots, l'_r)$, $G'' = C_m^{v_2,v_3,\ldots,v_r}(l'_1 + l'_2, l'_3, \ldots, l'_r)$, $d_{G'}(v_i, v_j) \geq 2$ for $1 \leq i < j \leq r$ and $\{v_1, v_2, \ldots, v_r\} \subseteq \{u_1, u_2, \ldots, u_k\}$.*

Proof. $HM(G) < HM(G')$ is straightforward in light of Lemma 2.5. Now, by considering $u = v_1, w = v_2$, $H = S_{l'_1+1}$ and $G = C_m^{v_2,v_3,\ldots,v_r}(l'_2, l'_3, \ldots, l'_r)$ and using Lemma 2.1 we can conclude that $HM(G') < HM(G'')$, as desired. □

Lemma 2.7. *Let $G = C_m(l_1, l_2, \ldots, l_k)$ be a unicyclic graph of order n. Then $HM(G) \leq HM(C_m(n-m))$, with equality if and only if $k = 1$.*

Proof. The proof is obtained by applying Lemmas 2.5 and 2.6. □

Corollary 2.8. *Let $G = C_m(T_1, T_2, \ldots, T_k)$ be a unicyclic graph and $n(T_i) = l_i + 1$, $i = 1, 2, \ldots, k$. Then,*

$$HM(G) \leq HM(C_m(l_1, l_2, \ldots, l_k)) \leq HM(C_m(n-m)),$$

with left equality if and only if $T_i \cong S_{l_i+1}$, $i = 1, 2, \ldots, k$, and right equality if and only if $k = 1$.

Lemma 2.9. *Let $G_1 = C_m(n-m)$ and $G_2 = C_{m-1}(n-m+1)$, $m \geq 4$, be unicyclic graphs of order n. Then, $HM(G_1) < HM(G_2)$.*

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Proof. By a simple calculation we have

$$\begin{aligned} HM(G_1) =& 4\left(m-2\right)+2\left(n-m+4\right)^2+\left(n-m\right)\left(n-m+3\right)^2 \\ <& 4\left(m-3\right)+2\left(n-m+5\right)^2+\left(n-m+1\right)\left(n-m+4\right)^2 \\ =& HM(G_2). \end{aligned}$$

As desired. □

Lemma 2.10. *Let $G = C_m\left(T_1, T_2, \ldots, T_k\right)$ be a unicyclic graph. Then,*

$$HM(G) = \sum_{i=1}^{k} \sum_{xy\in E(T_i)} h_G(xy) + \sum_{xy\in E(C_m)} h_G(xy).$$

Proof. The proof is trivial by the Hyper-Zagreb index definition (1.1). □

3. Main Results

In this section, we characterize the trees and unicyclic graphs with the first four and first eight greatest HM-value, respectively.

Theorem 3.1. *Let T be a tree with n vertices. If $T \ncong S_n, T_n^1$ or T_2^n, then*

$$HM(T) \leq HM\left(T_n^3\right) < HM\left(T_n^2\right) < HM\left(T_n^1\right) < HM\left(S_n\right),$$

with the equality if and if $T \cong T_3^n$, where T_n^1, T_n^2 and T_n^3 are given as in Figure 4.

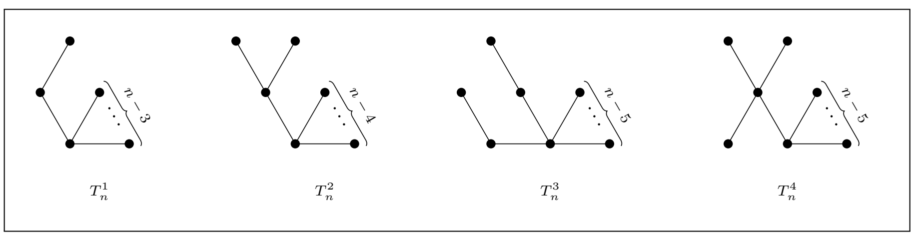

Figure 4. Some trees with large Hyper-Zagreb values.

Graph	HM-value
S_n	n^3-n^2
T_1^n	n^3-4n^2+7n+6
T_2^n	$n^3-7n^2+20n+16$
T_3^n	n^3-7n^2+20n

Table 1. Trees with large Hyper-Zagreb values.

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Proof. Using Table 1, we have $HM(S_n) > HM\left(T_n^1\right) > HM\left(T_n^2\right) > HM\left(T_n^3\right)$. Hence, we need to prove that $HM(T) < HM\left(T_n^3\right)$ when $T \ncong T_n^3$. Let $T = T^x(T_1, T_2, \ldots, T_\Delta)$, where $\Delta = d_T(x)$. By Corollary 2.3, we have $HM(T_i) \leq HM(S_{n_i})$, $i = 1, 2, \ldots, \Delta$. Moreover, let $T' = T^x(T_1', T_2', \ldots . T_\Delta')$, where $T_i'^* = S_{n_i}$, $i = 1, 2, \ldots, \Delta$, then we have $HM(T) \leq HM(T')$. To complete the proof, we consider three different cases as follows:

Case 1: assume that $d_T(y_i) = 1$, $i = 1, 2, \ldots, \Delta$, then $T = S_n$. This is a contradiction to the assumption.

Case 2: assume that there exists y_t for $t = 1, 2, \ldots, \Delta$ such that $d_T(y_t) \geq 2$ and $d_T(y_i) = 1$ for $i = 1, 2, \ldots, \Delta$ and $i \neq t$. In this case, there are three subcases that can happen:

(i) If $|V(T_t^*)| = 2$, then $T \cong T_1^n$. This is clearly a contradiction.

(ii) If $|V(T_t^*)| = 3$, then we must consider that $d_T(y_t) = 2$ or 3. The case $d_T(y_t) = 3$ implies that $T \cong T_n^2$, which is a contradiction. If $d_T(y_t) = 2$, then

$$\begin{aligned} HM(T) = &(n-4)(n-2)^2 + (n-1)^2 + 16 + 9 \\ =&n^3 - 7n^2 + 18n + 10 \\ <&n^3 - 7n^2 + 20n \\ =&HM\left(T_n^3\right). \end{aligned}$$

(iii) If $|V(T_t^*)| \geq 4$, then $T = T^x\left(\overbrace{S_2, \ldots, S_2}^{t-1\ times},\ T_t,\ \overbrace{S_2, \ldots, S_2}^{\Delta-t\ times}\right)$. By Corollary 2.3, the Hyper-Zagreb index for T is maximum when $T_t^* = S_{n_t}$. On the other hand, it follows from Lemma 2.1 that if $n_t = 4$ than T has maximum HM-value, i.e. in this case T has maximum HM-value when $T \cong T_n^4$ (see Figure 4). Hence, applying Lemma 2.1, it is clear that $HM(T) \leq HM\left(T_n^4\right) < HM\left(T_n^3\right)$.

Case 3: Suppose that there exist $1 \leq s, t \leq \Delta$ such that $d_T(y_s), d_T(y_t) \geq 2$. Similar to previous, applying Corollary 2.3 and Lemma 2.1, it can concluded that $HM(T) < HM\left(T_n^3\right)$. □

Theorem 3.2. *Let G be a unicylcic graph of order $n \geq 15$. If $G \ncong C_3(n-3)$, $C_3(1, n-4)$, $C_3\left(T_{n-2}^1\right)$, $C_4(n-2)$, $C_3(2, n-5)$, $C_3(1, 1, n-5)$ and $C_3\left(T_{n-2}^2\right)$. Then,*

$$\begin{aligned} HM(G) \leq &HM\left(C_3\left(T_{n-2}^3\right)\right) < HM\left(C_3\left(T_{n-2}^2\right)\right) < HM\left(C_3(1, 1, n-5)\right) \\ <&HM\left(C_3(2, n-5)\right) < HM\left(C_4(n-4)\right) < HM\left(C_3\left(T_{n-2}^1\right)\right) \\ <&HM\left(C_3(1, n-4)\right) < HM\left(C_3(n-3)\right), \end{aligned}$$

with the equality if and only if $G \cong C_3\left(T_{n-2}^3\right)$ or $G \cong C_3(P_3, 10)$ for $n = 15$ (see Figure 5).

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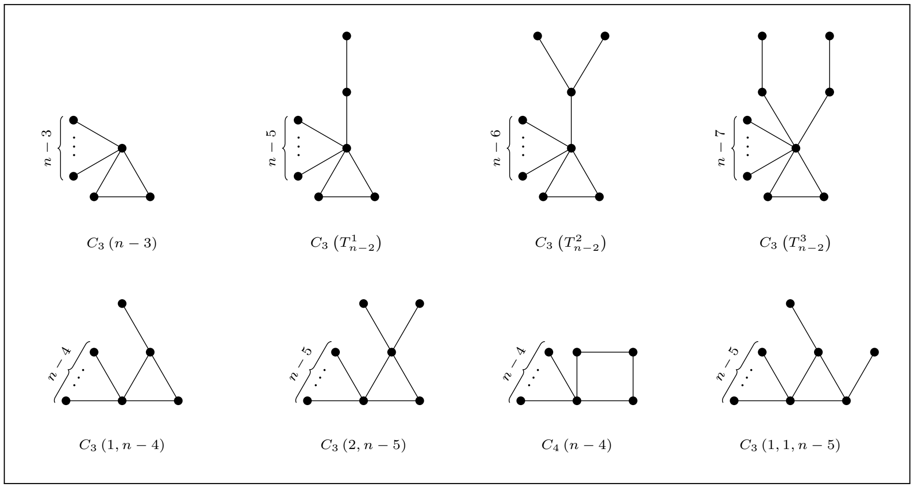

FIGURE 5. The unicyclic graphs with the first eight greatest Hyper-Zagreb.

Graph	HM-value
$C_3\,(n-3)$	$n^3 - n^2 + 4n + 18$
$C_3\,(1, n-4)$	$n^3 - 4n^2 + 11n + 38$
$C_3\left(T^1_{n-2}\right)$	$n^3 - 4n^2 + 11n + 20$
$C_4\,(n-4)$	$n^3 - 4n^2 + 9n + 28$
$C_3\,(2, n-5)$	$n^3 - 7n^2 + 24n + 68$
$C_3\,(1, 1, n-5)$	$n^3 - 7n^2 + 24n + 48$
$C_3\left(T^2_{n-2}\right)$	$n^3 - 7n^2 + 24n + 26$
$C_3\left(T^3_{n-2}\right)$	$n^3 - 7n^2 + 24n + 10$

TABLE 2. Unicyclic graphs with large Hyper-Zagreb values.

Proof. Assume that $G = C_m\,(T_1, T_2, \ldots, T_k)$ be a unicyclic graph and $n(T_i) = l_i + 1,\ i = 1, 2, \ldots, k$. The given Table 2 provides the Hyper-Zagreb index of some graphs by which the result is trivial. It is enough to discuss about the equality case. If $G \cong C_3\left(T^3_{n-2}\right)$, then $HM(G) = HM\left(C_3\left(T^3_{n-2}\right)\right)$. Also, if $G \cong C_3\,(P_3, 10)$ for $n = 15$, then $HM(G) = 2170 = HM\left(C_3\left(T^3_{13}\right)\right)$. We now prove that $HM(G) < HM\left(C_3\left(T^3_{n-2}\right)\right)$, where $G \ncong C_3\,(n-3),\ C_3\,(1, n-4)$, $C_3\left(T^1_{n-2}\right),\ C_4\,(n-2),\ C_3\,(2, n-5),\ C_3\,(1, 1, n-5)$ and $C_3\left(T^2_{n-2}\right)$. We examine three cases of $m = 3, 4$ and 5 for $G = C_m\,(T_1, T_2, \ldots, T_k)$ as follows:

Case 1: $m = 3$. We need to discuss three subcases that $k = 1, 2$ and 3.

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(i) $k = 1$, then $G = C_3(T_1)$. By assumption, we know that $T_1 \ncong S_{n-2}, T^1_{n-2}, T^2_{n-2}$ and T^3_{n-2}. So, Theorem 3.1 implies that $HM(T_1) < HM(T^3_{n-2})$. By Lemma 2.10, we get $HM(G) < HM\left(C_3\left(T^3_{n-2}\right)\right)$.

(ii) $k = 2$, then $G = C_3(T_1, T_2)$. By assumption, $G \ncong C_3(1, n-4)$ and $C_3(2, n-5)$. By Corollaries 2.3, 2.4 and Lemmas 2.1, 2.10, the maximum value of $HM(G)$ happens when $G \cong C_3(3, n-6)$ or $C_3(P_3, n-5)$. The first case yields that

$$HM(G) \leq HM(C_3(3, n-6)) = n^3 - 10n^2 + 43n + 108.$$

Hence, we have (for $n \geq 15$) that

$$\begin{aligned} HM\left(C_3\left(T^3_{n-3}\right)\right) - HM(G) \geq & HM\left(C_3\left(T^3_{n-3}\right)\right) - HM(C_3(3, n-6)) \\ = & \left(n^3 - 7n^2 + 24n + 10\right) \\ & - \left(n^3 - 10n^2 + 43n + 108\right) \\ = & 3n^2 - 19n - 98 \\ > & 0. \end{aligned}$$

Similarly, for the second case we have

$$\begin{aligned} HM\left(C_3\left(T^3_{n-3}\right)\right) - HM(G) \geq & HM\left(C_3\left(T^3_{n-3}\right)\right) - HM(C_3(P_3, n-5)) \\ = & \left(n^3 - 7n^2 + 24n + 10\right) - \left(n^3 - 7n^2 + 22n + 40\right) \\ = & 2n - 30 \\ > & 0. \end{aligned}$$

This means that in both cases $HM(G) < HM\left(C_3\left(T^3_{n-2}\right)\right)$.

(iii) $k = 3$, then $G = C_3(T_1, T_2, T_3)$. By Corollary 2.4, it is simple to see that $HM(G) \leq HM(C_3(l_1, l_2, l_3))$. On the other hand, since by assumption $G \ncong C_3(1, 1, n-5)$, the Hyper-Zagreb index attains its maximum when
$G \cong C_3(1, 2, n-6)$. Hence,

$$\begin{aligned} HM\left(C_3\left(T^3_{n-3}\right)\right) - HM(G) \geq & HM\left(C_3\left(T^3_{n-3}\right)\right) - HM(C_3(1, 2, n-6)) \\ = & \left(n^3 - 7n^2 + 24n + 10\right) - \left(n^3 - 10n^2 + 43n + 62\right) \\ > & 0. \end{aligned}$$

Case 2: $m = 4$. This needs to be analyzed for $k = 1, 2, 3$ and 4.

(i) $k = 1$, then $G = C_4(T_1)$. Since $G \ncong C_4(n-4)$, we have $T_1 \ncong S_{n-3}$. Note that G has a maximum value of the Hyper-Zagreb index if $T_1 \cong T^1_{n-3}$ by Theorem 3.1 and Lemma 2.10. Moreover, we have (for $n \geq 15$)

$$\begin{aligned} HM\left(C_3\left(T^3_{n-3}\right)\right) - HM(G) \geq & HM\left(C_3\left(T^3_{n-3}\right)\right) - HM\left(C_4\left(T^1_{n-3}\right)\right) \\ = & \left(n^3 - 7n^2 + 24n + 10\right) - \left(n^3 - 7n^2 + 22n + 20\right) \\ > & 0. \end{aligned}$$

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(ii) $k=2$, then $G=C_4^{u_1,u_2}(T_1,T_2)_\alpha = C_4\left(T_1,T_2\right)_\alpha$, where $\alpha = d_G(u_1,u_2)$. By Lemma 2.1, G attains maximum HM-value if $G \cong C_4\left(l_1,l_2\right)_{\alpha=1}$. This lemma also implies that

$$HM\left(C_4\left(l_1,l_2\right)\right)_{\alpha=1} \leq HM\left(C_4\left(1,n-5\right)\right)_{\alpha=1} = n^3-7n^2+22n+38.$$

Therefore, for $n \geq 15$, we have

$$HM(G) \leq n^3-7n^2+22n+38 < n^3-7n^2+24n+10 = HM\left(C_3\left(T^3_{n-2}\right)\right).$$

(iii) $k=3$, then G is considered as $C_4\left(T_1,T_2,T_3\right)$. By Corollary 2.4 and Lemmas 2.1, 2.10, for $n \geq 15$ we have

$$\begin{aligned} HM\left(C_3\left(T^3_{n-2}\right)\right) - HM(G) \geq & HM\left(C_3\left(T^3_{n-2}\right)\right) - HM\left(C_4\left(l_1,l_2,l_3\right)\right) \\ > & HM\left(C_3\left(T^3_{n-2}\right)\right) - HM\left(C_4\left(1,n-5\right)\right)_{\alpha=1} \\ = & \left(n^3-7n^2+24n+10\right) - \left(n^3-7n^2+22n+38\right) \\ > & 0. \end{aligned}$$

(iv) $k=4$, then $G=C_4(T_1,T_2,T_3,T_4)$. In a similar way, one can see easily that $HM(G) < HM\left(C_3\left(T^3_{n-2}\right)\right)$; completing the proof of the second case.

Case 3: $m \geq 5$. Using Lemmas 2.9, 2.10 and Corollaries 2.3, 2.8, we conclude that (for $n \geq 15$)

$$\begin{aligned} HM\left(C_3\left(T^3_{n-2}\right)\right) - HM(G) \geq & HM\left(C_3\left(T^3_{n-2}\right)\right) - HM\left(C_m\left(l_1,l_2,\ldots,l_k\right)\right) \\ \geq & HM\left(C_3\left(T^3_{n-2}\right)\right) - HM\left(C_m\left(n-m\right)\right) \\ \geq & HM\left(C_3\left(T^3_{n-2}\right)\right) - HM\left(C_5\left(n-5\right)\right) \\ = & \left(n^3-7n^2+24n+10\right) - \left(n^3-7n^2+20n+30\right) \\ > & 0. \end{aligned}$$

□

4. Conclusion

In this paper, we studied the Hyper-Zagreb index and characterized the trees and unicyclic graphs with the first four and first eight greatest HM-value. It would be of interest to investigate its behavior on other classes of graphs with simple connectivity patterns and cyclic structures.

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