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Ordering the Zagreb Coindices of Connected Graphs [1]

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Abstract

In this paper, we give a simple approach to order the first Zagreb indices of connected graphs and the second Zagreb coindices of trees and unicyclic graphs, respectively. As an application of our new method, we determine the first eight smallest and the first three largest (respectively, first eight smallest and first three largest, first seven smallest and first two largest) values of the first Zagreb coindices in the class of trees (respectively, unicyclic graphs, bicyclic graphs) on n vertices, and we also determine the first eleven (respectively, thirteen) smallest values of the second Zagreb coindices in the class of trees (respectively, unicyclic graphs) on n vertices. Furthermore, we also identify the smallest value of the first Zagreb coindices in the class of chemical trees on $n \geq 8$ vertices, partially giving an answer to a question of Ashrafi, Došlić and Hamzeh.

1 Introduction

Throughout this paper, we only consider undirected simple graphs. Suppose G has n vertices and m edges. If $m = n + c - 1$, then G is called a c-cyclic graph. Specially, when m is equal to $n - 1$, n and $n + 1$, then G is called a tree, a unicyclic graph and a bicyclic

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graph, respectively. We use the notations $\mathbb{T}_n$ (respectively, $\mathbb{U}_n$ and $\mathbb{B}_n$) to denote the class of trees (respectively, unicyclic and bicyclic graphs) on n vertices.

Let $d(u)$ be the degree of u. Specially, $\Delta = \Delta(G)$ denotes the maximum degree of vertices of G. The sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G if $d_i = d(v)$ holds for some $v \in V(G)$. In the sequel, we enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$. Let $\pi(G)$ be the degree sequence of G, and let $\Gamma(\pi)$ define the class of connected simple graphs with degree sequence π.

The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ are two famous important topological indices, where $M_1(G)$ and $M_2(G)$ are defined as [11]:

$$M_1(G) = \sum_{v \in V(G)} d(v)^2, \qquad M_2(G) = \sum_{uv \in E(G)} d(u)d(v). \tag{1}$$

Recent research showed that they have been closely correlated with many chemical and mathematical properties [3, 4, 9, 10, 16, 19, 20].

Recently, Došlić [5] defined two new graphical invariants $\overline{M_1(G)}$ and $\overline{M_2(G)}$, where

$$\overline{M_1} = \overline{M_1(G)} = \sum_{uv \notin E(G)} (d(u) + d(v)), \qquad \overline{M_2} = \overline{M_2(G)} = \sum_{uv \notin E(G)} d(u)d(v). \tag{2}$$

One can easily discover that

$$M_1(G) = \sum_{uv \in E(G)} (d(u) + d(v)).$$

Thus, Ashrafi et al. [1, 2] called $\overline{M_1}$ and $\overline{M_2}$ the first Zagreb coindex and second Zagreb coindex of G, respectively. These two new topological indices received much attention quickly [1, 2, 7, 17, 18].

In this paper, we give a simple approach to order the first Zagreb coindices of connected graphs (respectively, trees and unicyclic graphs). As an application of this new ordering method, we determine the first eight smallest and the first three largest (respectively, first eight smallest and first three largest, first seven smallest and first two largest) values of the first Zagreb coindices in the class of trees (respectively, unicyclic graphs, bicyclic graphs) on n vertices, and we also determine the first eleven (respectively, thirteen) smallest values of the second Zagreb coindices in the class of trees (respectively, unicyclic graphs) on n vertices. Furthermore, we also identify the smallest value of the first Zagreb coindices in the class of chemical trees on $n \geq 8$ vertices, partially giving an answer to a question of Ashrafi, Došlić and Hamzeh.

2 The main results

Suppose $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ are two different non-increasing graphic degree sequences, we write $\pi \lhd \pi'$ if and only if $\pi \neq \pi'$, $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, \ldots, n$. Such an ordering is sometimes called *majorization* (see [8, 13]).

Recently, the following majorization theorems of the Zagreb indices were proved.

Lemma 2.1. [12] *Let $\pi = (d_1, d_2, \ldots, d_n)$ with $G \in \Gamma(\pi)$ and let $\pi' = (d'_1, d'_2, \ldots, d'_n)$ with $G' \in \Gamma(\pi')$. If $\pi \lhd \pi'$, then $M_1(G) < M_1(G')$.*

Lemma 2.2. [13, 15] *Let $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ be two degree sequences of trees (respectively, unicyclic graphs). Suppose G and G' have the largest second Zagreb indices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $\pi \lhd \pi'$, then $M_2(G) < M_2(G')$.*

For the relation between M_1 and $\overline{M_1}$ (respectively, M_2 and $\overline{M_2}$), it is well-known that

Lemma 2.3. [1] *Let G be a connected graph with n vertices and m edges. Then,*

$$(1)\ \overline{M_1(G)} = 2m(n-1) - M_1(G), \qquad (2)\ \overline{M_2(G)} = 2m^2 - M_2(G) - \frac{1}{2}M_1(G).$$

Remark 2.4. By (1) of Lemma 2.3, if G and G' are two graphs of $\Gamma(\pi)$, then $\overline{M_1(G)} = \overline{M_1(G')}$. By (2) of Lemma 2.3, G has the largest second Zagreb index in $\Gamma(\pi)$ if and only if G has the smallest second Zagreb coindex in $\Gamma(\pi)$.

Theorem 2.5. *Let $\pi = (d_1, d_2, \ldots, d_n)$ with $G \in \Gamma(\pi)$ and let $\pi' = (d'_1, d'_2, \ldots, d'_n)$ with $G' \in \Gamma(\pi')$. If $\pi \lhd \pi'$, then $\overline{M_1(G)} > \overline{M_1(G')}$.*

Proof. Since $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$, G and G' contains exactly m edges and n vertices, respectively. So, the result clearly follows from Lemmas 2.1 and 2.3 (1). ■

With the similar reason, by Lemmas 2.1–2.2 and 2.3 (2), and Remark 2.4 we have

Theorem 2.6. *Let $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ be two degree sequences of trees (respectively, unicyclic graphs). Suppose G and G' have the smallest second Zagreb coindices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $\pi \lhd \pi'$, then $\overline{M_2(G)} > \overline{M_2(G')}$.*

In [2], Ashrafi et al. determined the largest and smallest values of $\overline{M_1(G)}$ and $\overline{M_2(G)}$ in the class of trees on n vertices. In the following, as an application of the majorization theorems of the Zagreb coindices, we shall determine the first eight smallest and first three largest (respectively, first eleven smallest) values of the first (respectively, second) Zagreb coindices in the class of trees on n vertices.

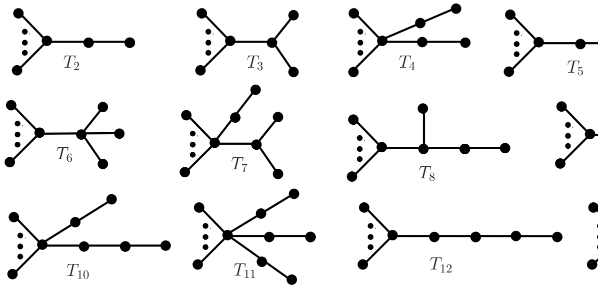

Figure 1: The trees $T_2, T_3, \ldots, T_{13}$.

Let T_1 be the star and $T_2, T_3, \ldots, T_{13}$ be the trees on n vertices as shown in Fig. 1.

Theorem 2.7. (1) *Suppose* $T \in \mathbb{T}_n \setminus \{T_1, T_2, \ldots, T_{13}\}$ *and* $n \geq 13$. *Then,* $\overline{M_1(T_1)} < \overline{M_1(T_2)} < \overline{M_1(T_3)} < \overline{M_1(T_4)} = \overline{M_1(T_5)} < \overline{M_1(T_6)} < \overline{M_1(T_7)} = \overline{M_1(T_8)} = \overline{M_1(T_9)} < \overline{M_1(T_{10})} = \overline{M_1(T_{11})} = \overline{M_1(T_{12})} < \overline{M_1(T_{13})} < \overline{M_1(T)}$;

(2) *Suppose* $T \in \mathbb{T}_n \setminus \{T_1, T_2, \ldots, T_8, T_{10}, T_{11}, T_{13}\}$ *and* $n \geq 22$. *Then,* $\overline{M_2(T_1)} < \overline{M_2(T_2)} < \overline{M_2(T_3)} < \overline{M_2(T_4)} < \overline{M_2(T_5)} < \overline{M_2(T_6)} < \overline{M_2(T_7)} < \overline{M_2(T_{11})} < \overline{M_2(T_8)} < \overline{M_2(T_{10})} < \overline{M_2(T_{13})} < \overline{M_2(T)}$.

Proof. Obviously, T_1 is the unique tree with $\Delta = n-1$, T_2 is the unique tree with $\Delta = n-2$, T_3, T_4, T_5 are all the trees with $\Delta = n-3$, $T_6, \ldots, T_{12}$ are all the trees with $\Delta = n-4$. Recall that $T \in \mathbb{T}_n \setminus \{T_1, T_2, \ldots, T_{13}\}$. So, $\Delta(T) \leq n-5$. Since $\pi(T_{13}) = (n-5, 5, 1, \ldots, 1)$ and $\Gamma(\pi(T_{13})) = \{T_{13}\}$, we have $\pi(T) \lhd \pi(T_{13})$. By Theorems 2.5–2.6, it follows that $\overline{M_1(T_{13})} < \overline{M_1(T)}$ and $\overline{M_2(T_{13})} < \overline{M_2(T)}$.

By an elementary computation, we have $\overline{M_1(T_5)} = n^2+n-12$, $\overline{M_1(T_6)} = n^2+3n-28$, $\overline{M_1(T_{12})} = n^2+3n-22$, $\overline{M_1(T_{13})} = n^2+5n-46$, $\overline{M_2(T_4)} = \frac{1}{2}(n^2+5n-24)$, $\overline{M_2(T_5)} = \frac{1}{2}(n^2+7n-34)$, $\overline{M_2(T_6)} = \frac{1}{2}(n^2+9n-58)$, $\overline{M_2(T_7)} = \frac{1}{2}(n^2+9n-46)$, $\overline{M_2(T_8)} = \frac{1}{2}(n^2+11n-60)$, $\overline{M_2(T_9)} = \frac{1}{2}(n^2+13n-70)$, $\overline{M_2(T_{10})} = \frac{1}{2}(n^2+11n-52)$, $\overline{M_2(T_{11})} = \frac{1}{2}(n^2+9n-40)$, $\overline{M_2(T_{12})} = \frac{1}{2}(n^2+13n-64)$, $\overline{M_2(T_{13})} = \frac{1}{2}(n^2+13n-94)$.

Note that $\pi(T_5) = \pi(T_4) \lhd \pi(T_3) \lhd \pi(T_2) \lhd \pi(T_1)$. By the above values and Theorem 2.6, (2) follows when $n \geq 22$. Now, we turn to prove (1). It is easily checked that $\pi(T_{12}) = \pi(T_{11}) = \pi(T_{10}) \lhd \pi(T_9) = \pi(T_8) = \pi(T_7) \lhd \pi(T_6)$ and $\pi(T_5) = \pi(T_4) \lhd \pi(T_3) \lhd \pi(T_2) \lhd \pi(T_1)$. So, (1) follows from Theorem 2.5 and Lemma 2.3 (1). ■

Theorem 2.8. *In the class of trees on n vertices, the path has the largest first Zagreb coindex, the trees with degree sequence* $(3, 2, 2, \ldots, 2, 1, 1, 1)$ *have the second largest first Zagreb coindex, and the trees with degree sequence* $(3, 3, 2, \ldots, 2, 1, 1, 1, 1)$ *have the third largest first Zagreb coindex.*

Proof. Suppose $T \in \mathbb{T}(n)$. Let $\pi_1 = (2, 2, 2, \ldots, 2, 1, 1)$, $\pi_2 = (3, 2, 2, \ldots, 2, 1, 1, 1)$ and $\pi_3 = (3, 3, 2, \ldots, 2, 1, 1, 1, 1)$. Suppose $\pi(T) \notin \{\pi_1, \pi_2, \pi_3\}$. Then, $\pi_1 \lhd \pi_2 \lhd \pi_3 \lhd \pi(T)$. By Theorem 2.5, the result follows. ■

Ashrafi et al. [2] also determined the smallest and largest values of $\overline{M_1(G)}$ in the class of unicyclic graphs and bicyclic graphs on n vertices. In the following, we shall identify the first eight smallest and the first three largest (respectively, the first seven smallest and the first two largest) values of the first Zagreb coindices in the class of unicyclic (respectively, bicyclic) graphs on n vertices, and we also determine the first thirteen smallest values of the second Zagreb coindices in the class of unicyclic graphs on n vertices.

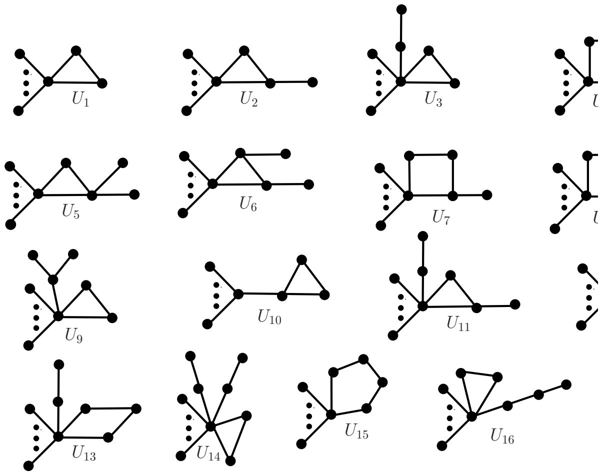

Figure 2: The unicyclic graphs U_1, U_2, $\ldots$, U_{17}.

Let $U_1, \ldots, U_{17}$ be the unicyclic graphs on n vertices as shown in Fig. 2.

Theorem 2.9. (1) *If* $n \geq 12$ *and* $U \in \mathbb{U}(n) \setminus \{U_1, \ldots, U_{17}\}$, *then* $\overline{M_1(U_1)} < \overline{M_1(U_2)} < \overline{M_1(U_3)} = \overline{M_1(U_4)} < \overline{M_1(U_5)} < \overline{M_1(U_6)} < \overline{M_1(U_7)} = \overline{M_1(U_8)} = \overline{M_1(U_9)} = \overline{M_1(U_{10})} = \overline{M_1(U_{11})} = \overline{M_1(U_{12})} < \overline{M_1(U_{13})} = \overline{M_1(U_{14})} = \overline{M_1(U_{15})} = \overline{M_1(U_{16})} < \overline{M_1(U_{17})} < \overline{M_1(U)}$;

(2) *If* $n \geq 23$ *and* $U \in \mathbb{U}(n) \setminus \{U_1, \ldots, U_7, U_9, U_{12}, U_{13}, U_{14}, U_{16}, U_{17}\}$*, then* $\overline{M_2(U_1)} < \overline{M_2(U_2)} < \overline{M_2(U_3)} < \overline{M_2(U_4)} < \overline{M_2(U_5)} < \overline{M_2(U_6)} < \overline{M_2(U_{11})} < \overline{M_2(U_9)} < \overline{M_2(U_{14})} < \overline{M_2(U_{12})} < \overline{M_2(U_7)} < \overline{M_2(U_{13})} = \overline{M_2(U_{16})} < \overline{M_2(U_{17})} < \overline{M_2(U)}$*.*

Proof. Clearly, U_1 is the unique unicyclic graph with $\Delta = n-1$, U_2, U_3, U_4 are all the unicyclic graphs with $\Delta = n-2$, and $U_5, U_6, \ldots, U_{16}$ are all the unicyclic graphs with $\Delta(G) = n-3$. If $U \in \mathbb{U}(n) \setminus \{U_1, \ldots, U_{17}\}$, then $\Delta(G) \leq n-4$. Since $\Gamma(\pi(U_{17})) = \{U_{17}\}$, we have $\pi(U) \lhd \pi(U_{17})$. By Theorems 2.5–2.6, $\overline{M_1(U_{17})} < \overline{M_1(U)}$ and $\overline{M_2(U_{17})} < \overline{M_2(U)}$.

By an elementary computation, we have $\overline{M_1(U_4)} = n^2 + n - 12$, $\overline{M_1(U_5)} = n^2 + 3n - 26$, $\overline{M_1(U_{16})} = n^2 + 3n - 20$, $\overline{M_1(U_{17})} = n^2 + 5n - 42$, $\overline{M_2(U_3)} = \frac{1}{2}(n^2 + 5n - 20)$, $\overline{M_2(U_4)} = \frac{1}{2}(n^2 + 7n - 28)$, $\overline{M_2(U_5)} = \frac{1}{2}(n^2 + 9n - 52)$, $\overline{M_2(U_6)} = \frac{1}{2}(n^2 + 9n - 48)$, $\overline{M_2(U_7)} = \frac{1}{2}(n^2 + 11n - 48)$, $\overline{M_2(U_8)} = \frac{1}{2}(n^2 + 13n - 58)$, $\overline{M_2(U_9)} = \frac{1}{2}(n^2 + 9n - 36)$, $\overline{M_2(U_{10})} = \frac{1}{2}(n^2 + 13n - 60)$, $\overline{M_2(U_{11})} = \frac{1}{2}(n^2 + 9n - 38)$, $\overline{M_2(U_{12})} = \frac{1}{2}(n^2 + 11n - 50)$, $\overline{M_2(U_{13})} = \frac{1}{2}(n^2 + 11n - 40)$, $\overline{M_2(U_{14})} = \frac{1}{2}(n^2 + 9n - 30)$, $\overline{M_2(U_{15})} = \frac{1}{2}(n^2 + 13n - 50)$, $\overline{M_2(U_{16})} = \frac{1}{2}(n^2 + 11n - 40)$, $\overline{M_2(U_{17})} = \frac{1}{2}(n^2 + 13n - 84)$.

Note that $\pi(U_4) = \pi(U_3) \lhd \pi(U_2) \lhd \pi(U_1)$. By the above values and Theorem 2.6, (2) follows when $n \geq 23$. Now, we turn to prove (1). It is easy to see that $\pi(U_{16}) = \pi(U_{15}) = \pi(U_{14}) = \pi(U_{13}) \lhd \pi(U_{12}) = \pi(U_{11}) = \pi(U_{10}) = \pi(U_9) = \pi(U_8) = \pi(U_7) \lhd \pi(U_6) \lhd \pi(U_5)$ and $\pi(U_4) = \pi(U_3) \lhd \pi(U_2) \lhd \pi(U_1)$. Therefore, (1) follows from Theorem 2.5 and Lemma 2.3 (1). ■

With the similar reason as Theorem 2.8, it follows that

Theorem 2.10. *In the class of unicyclic graphs on* n *vertices, the cycle has the largest first Zagreb coindex, the unicyclic graphs with degree sequence* $(3, 2, 2, \ldots, 2, 1)$ *have the second largest first Zagreb coindex, and the unicyclic graphs with degree sequence* $(3, 3, 2, \ldots, 2, 1, 1)$ *have the third largest first Zagreb coindex.*

Theorem 2.11. *Suppose* $n \geq 11$ *and* $B \in \mathbb{B}(n) \setminus \{B_1, \ldots, B_{12}\}$*, where* $B_1, \ldots, B_{12}$ *are the bicyclic graphs on* n *vertices as shown in Fig. 3. Then,* $\overline{M_1(B_1)} < \overline{M_1(B_2)} < \overline{M_1(B_3)} < \overline{M_1(B_4)} = \overline{M_1(B_5)} < \overline{M_1(B_6)} = \overline{M_1(B_7)} = \overline{M_1(B_8)} = \overline{M_1(B_9)} < \overline{M_1(B_{10})} = \overline{M_1(B_{11})} < \overline{M_1(B_{12})} < \overline{M_1(B)}$*.*

Proof. It is easy to check that B_1, B_2 are all the bicyclic graphs with $\Delta = n-1$, $B_3, \ldots, B_{11}$ are all the bicyclic graphs with $\Delta = n-2$. Since $B \in \mathbb{B}(n) \setminus \{B_1, \ldots, B_{12}\}$, $\Delta(G) \leq n-3$. Note that $\pi(B_{12}) = (n-3, 5, 2, 2, 1, ..., 1)$ and $\Gamma(\pi(B_{12})) = \{B_{12}\}$. Then, $\pi(B) \lhd \pi(B_{12})$, which implies that $\overline{M_1(B_{12})} < \overline{M_1(B)}$ by Theorem 2.5.

It is easily checked that $\pi(B_{11}) = \pi(B_{10}) \lhd \pi(B_9) = \pi(B_8) = \pi(B_7) = \pi(B_6) \lhd \pi(B_5) = \pi(B_4) \lhd \pi(B_3)$ and $\pi(B_2) \lhd \pi(B_1)$. Furthermore, by an elementary computation, we have $\overline{M_1(B_2)} = n^2 + n - 14 < n^2 + 3n - 26 = \overline{M_1(B_3)}$, and $\overline{M_1(B_{11})} = n^2 + 3n - 20 < n^2 + 5n - 40 = \overline{M_1(B_{12})}$. Thus, by Theorem 2.5 and Lemma 2.3 (1), the result follows. ■

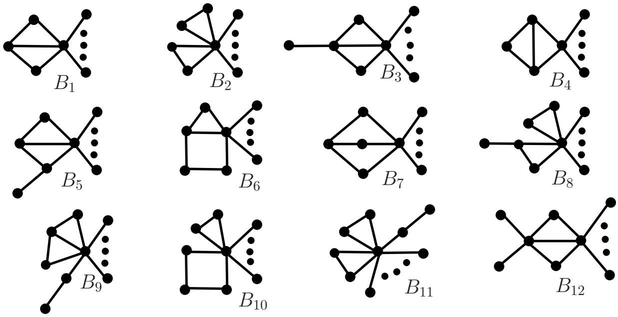

Figure 3: The bicyclic graphs B_1, B_2, …, B_{12}.

Theorem 2.12. *In the class of bicyclic graphs on n vertices, the bicyclic graphs with degree sequence $(3, 3, 2, 2, \ldots, 2)$ have the largest first Zagreb coindex, and the bicyclic graphs with degree sequence $(3, 3, 3, 2, \ldots, 2, 1)$ or $(4, 2, 2, \ldots, 2)$ have the second largest first Zagreb coindex.*

Proof. Suppose $B \in \mathbb{B}(n)$. Let $\pi_1 = (3, 3, 2, 2, \ldots, 2)$, $\pi_2 = (3, 3, 3, 2, \ldots, 2, 1)$, and $\pi_3 = (4, 2, 2, \ldots, 2)$. Since $B \in \mathbb{B}(n)$, $\Delta(B) \geq 3$. If $\Delta(B) = 3$, $\pi_1 \lhd \pi_2 \lhd \pi(B)$. If $\Delta(B) \geq 4$, $\pi_1 \lhd \pi_3 \lhd \pi(B)$.

Suppose $G_i \in \Gamma(\pi_i)$, where $i = 1, 2, 3$. Since $M_1(G_2) = 4n+12 = M_1(G_3)$, by Theorem 2.5 and Lemma 2.3 (1), we have $\overline{M_1(G_1)} > \overline{M_1(G_2)} = \overline{M_1(G_3)} > \overline{M_1(B)}$. ■

For integers n, c, k with $c \geq 0$ and $0 \leq k \leq n - 2c - 1$, let $\mathcal{G}_n(c, k)$ be the class of connected c-cyclic graphs with n vertices and k pendant vertices.

Theorem 2.13. *In the class of $\mathcal{G}_n(c, k)$, where $c \geq 0$ and $1 \leq k \leq n - 2c - 1$, the graphs with degree sequence $(2c+k, \underbrace{2, 2, \ldots, 2}_{n-k-1}, \underbrace{1, 1, \ldots, 1}_{k})$ have the largest first Zagreb coindices.*

Proof. Let $\pi_1 = (2c + k, \underbrace{2, 2, \ldots, 2}_{n-k-1}, \underbrace{1, 1, \ldots, 1}_{k})$. Suppose $G \in \mathcal{G}_n(c, k)$ with $\pi(G) = (d_1, d_2, \ldots, d_n)$. If $\pi(G) \neq \pi_1$, then $d_{n-k+1} = d_{n-k+2} = \cdots = d_n = 1$ and $d_2 \geq d_3 \geq \cdots \geq d_{n-k} \geq 2$. Thus, $\pi(G) \lhd \pi_1$.

Now, the result follows from Theorem 2.5 and Lemma 2.3 (1). ■

3 Concluding remarks

In this note, we prove that the majorization theorem also holds for the first Zagreb coindices of connected graphs and the second Zagreb coindices of trees and unicyclic graphs, namely, Theorems 2.5–2.6. The proofs are based on the corresponding majorization theorems of the first Zagreb index and the second Zagreb index, i.e., Lemmas 2.1–2.2. Actually, if the majorization theorem also holds for the second Zagreb index of the other c-cyclic graphs, then it also holds to the second Zagreb coindex.

As shown in [6, 12, 14] and also illustrated in the former section, the majorization theorem is a good tool to deal with the ordering of (signless Laplacian) spectral radii and/or the topological indices. But the majorization theorem cannot hold to all the topological indices [13]. Thus, it is a good question to find out which topological index also obey the majorization theorem (The known results show that such topological index are always closely related with the degree sequence of the graph).

In the end of this paper, we shall apply Theorem 2.5 to determine the smallest value of the first Zagreb coindices over chemical trees on n vertices, which partially answers an open problem asked in [2].

Theorem 3.1. *In the class of chemical trees on $n \geq 8$ vertices, the trees with degree sequence π_0 have the smallest first Zagreb coindices, where π_0 is defined as follows:*

(1) *If $n \equiv 0 \pmod 3$, then $\pi_0 = (4, \ldots, 4, 2, 1, \ldots, 1)$, where the cardinality of 1 in π_0 is $\frac{2n}{3}$,*

(2) *If $n \equiv 1 \pmod 3$, then $\pi_0 = (4, \ldots, 4, 3, 1, \ldots, 1)$, where the cardinality of 1 in π_0 is $\frac{2n+1}{3}$,*

(3) *If $n \equiv 2 \pmod 3$, then $\pi_0 = (4, \ldots, 4, 1, \ldots, 1)$, where the cardinality of 1 in π_0 is $\frac{2n+2}{3}$.*

Proof. Let $\pi_1 = (4, \ldots, 4, 1, \ldots, 1)$, $\pi_2 = (4, \ldots, 4, 3, 1, \ldots, 1)$ and $\pi_3 = (4, \ldots, 4, 2, 1, \ldots, 1)$. Suppose T is a chemical tree on n vertices. Here we only prove the case of $n \equiv 0 \pmod 3$, since the other cases can be shown by using the similar argument.

Suppose that $n \equiv 0 \pmod 3$. If $\pi(T) = \pi_1$, we assume that the cardinality of 4 in $\pi(T)$ is x. Then, $4x + n - x = 2(n-1)$, which contradicts $n \equiv 0 \pmod 3$. So, $\pi(T) \neq \pi_1$. Similarly, $\pi(T) \neq \pi_2$. If $\pi(T) \neq \pi_3$, since $\Delta(T) \leq 4$, we have $\pi(T) \lhd \pi_3$.

Now, the result follows from Theorem 2.5 and Lemma 2.3 (1). ■

Remark 3.2. In [2], Ashrafi et al. also asked the smallest value of the second Zagreb coindices over chemical trees on n vertices. By Theorem 2.6 and the proof of Theorem 3.1, we can conclude that the smallest value of the second Zagreb coindices among $\Gamma(\pi_0)$, where π_0 is denoted as in Theorem 3.1, is also the smallest value of the second Zagreb coindices over chemical trees on $n \geq 8$ vertices.

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