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A Simple Approach to Order the First Zagreb Indices of Connected Graphs*

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Abstract: This paper presents a simple approach to order the first Zagreb indices of connected graphs. Moreover, by the application of this simple approach, we extend the known ordering of the first Zagreb indices for some class of connected graphs.

1 Introduction

In this paper, $G = (V, E)$ is a connected undirected simple graph with $|V| = n$ and $|E| = m$. If $m = n - 1$, $m = n$ or $m = n + 1$, then G is called a tree, a unicyclic graph or a bicyclic graph, respectively. Let $d(u)$ denote the degree of u. Specially, $\Delta = \Delta(G)$ denotes the maximum degree of vertices of G. Suppose the degree of vertex v_i equals d_i for $i = 1, 2, ..., n$, then $\pi(G) = (d_1, ..., d_n)$ is called the *degree sequence* of G. Throughout this paper, we enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$.

The Zagreb indices was first introduced by Gutman and Trinajstić [1], it is an important molecular descriptor and has been closely correlated with many chemical properties [1−2]. Thus, it attracted more and more attention from chemists and mathematicians [3−9,12−18]. The *first Zagreb index* $M_1(G)$ is defined as [1]:

$$M_1(G) = \sum_{v \in V} d(v)^2.$$

In this paper, we give a simple approach to order the first Zagreb indices of connected graphs. Moreover, we illustrate the application of the approach and extend the known ordering of the first Zagreb indices for some class of connected graphs.

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2 Main results

We recall the notation of *majorization* (see [10,11]). Suppose $(x) = (x_1, x_2, ..., x_n)$ and $(y) = (y_1, y_2, ..., y_n)$ are two non-increasing sequences of real numbers, we say (x) is majorized by (y), denoted by $(x) \trianglelefteq (y)$, if and only if $\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$, and $\sum_{i=1}^{j} x_i \leq \sum_{i=1}^{j} y_i$ for all $j = 1, 2, ..., n$. Furthermore, by $(x) \triangleleft (y)$ we mean that $(x) \trianglelefteq (y)$ and $(x) \neq (y)$. A real valued function $f(x)$ defined on a convex set D is said to be convex if

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda)f(y) \tag{1}$$

for all $0 \leq \lambda \leq 1$ and all x, $y \in D$. If inequality (1) is always strict for $0 < \lambda < 1$ and $x \neq y$, then f is called strictly convex. It has been shown that

Lemma 2.1 [10] *Suppose $(x) = (x_1, x_2, ..., x_n)$ and $(y) = (y_1, y_2, ..., y_n)$ are non–increasing sequences of real numbers. If $(x) \trianglelefteq (y)$, then for any convex function φ, $\sum_{i=1}^{n} \varphi(x_i) \leq \sum_{i=1}^{n} \varphi(y_i)$. Furthermore, if $(x) \triangleleft (y)$ and φ is a strictly convex function, then $\sum_{i=1}^{n} \varphi(x_i) < \sum_{i=1}^{n} \varphi(y_i)$.*

Theorem 2.1 *Let G be a connected graph with degree sequence $(a) = (d_1, d_2, ..., d_n)$ and G' be a connected graph with degree sequence $(b) = (d'_1, d'_2, ..., d'_n)$. If $(a) \trianglelefteq (b)$, then $M_1(G) \leq M_1(G')$, where equality holds if and only if $(a) = (b)$.*

Proof. Observe that for $x > 0$, x^2 is a strictly convex function. Since $(a) \trianglelefteq (b)$, then $M_1(G) \leq M_1(G')$ follows from Lemma 2.1. Also, Lemma 2.1 implies that equality holds if and only if $(a) = (b)$.

In the following, the symbol $\mathcal{T}_n$ is used to denote the class of trees of order n. The tree $S(n, i)$ on n vertices is called a double star graph, which is obtained by joining the center of $K_{1,i-1}$ to that of $K_{1,n-1-i}$ by an edge, where $i \geq \lceil \frac{n}{2} \rceil$. Particularly, $S(n, n-1) = K_{1,n-1}$. Let $\mathcal{T}_n^s = \{T \in \mathcal{T}_n | \Delta(T) = s\}$.

Corollary 2.1 *Let T be a tree in $\mathcal{T}_n^s$, where $s \geq \lceil \frac{n}{2} \rceil$. Then, $M_1(T) \leq M_1(S(n, s))$, where equality holds if and only if $T \cong S(n, s)$.*

Proof. Note that the tree degree sequence $(s, n-s, 1, ..., 1)$ is maximal in the class of $\mathcal{T}_n^s$, i.e., the ordering $\triangleleft$. Since $S(n, s)$ is the unique tree with $(s, n-s, 1, ..., 1)$ as its degree sequence, thus the statement immediately follows from Theorem 2.1.

Let G be a connected undirected simple graph with n vertices and m edges. If $m = n + c - 1$, then G is called a $c-$*cyclic* graph. 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, and $\mathcal{S}_n(c,k)$ be the class of connected graphs on n vertices obtained by attaching c cycles at a unique common vertex, says v_1, and then attaching k paths at v_1, i.e., $\mathcal{S}_n(c,k)$ denotes the class of connected graphs with $(2c+k, \underbrace{2,2,...,2}_{n-k-1}, \underbrace{1,1,...,1}_{k})$ as their degree sequences. Obviously, $\mathcal{S}_n(c,k) \subseteq \mathcal{G}_n(c,k)$. For example, let U_3, U_4 be the unicyclic graphs as shown in Fig. 2, and B_{10}, B_{11} be the bicyclic graphs as depicted in Fig. 3. By definition, $U_3, U_4 \in \mathcal{S}_n(1, n-4)$ and $B_{10}, B_{11} \in \mathcal{S}_n(2, n-6)$. If G',$G \in \mathcal{S}_n(c,k)$, since they share the same degree sequences, then we have

Proposition 2.1 *If G' and G are graphs in $\mathcal{S}_n(c,k)$, where $c \geq 0$ and $1 \leq k \leq n-2c-1$, then $M_1(G) = M_1(G')$.*

Theorem 2.2 *Let G' and G be the graphs in $\mathcal{S}_n(c,k)$ and $\mathcal{G}_n(c,k) \setminus \mathcal{S}_n(c,k)$, respectively, where $c \geq 0$ and $1 \leq k \leq n-2c-1$. Then, $M_1(G) < M_1(G')$.*

Proof. Clearly, G', $G \in \mathcal{G}_n(c,k)$. Thus, there are exactly k elements 1 in their degree sequences. Since $G' \in \mathcal{S}_n(c,k)$, we have $\pi(G') = (d'_1, d'_2, ..., d'_{n-k}, \underbrace{1,1,...,1}_{k}) = (2c + k, \underbrace{2,2,...,2}_{n-k-1}, \underbrace{1,1,...,1}_{k})$. Let $\pi(G) = (d_1, d_2, ..., d_{n-k}, \underbrace{1,1,...,1}_{k})$, where $d_1 \geq d_2 \geq \cdots \geq d_{n-k} \geq 2$. Since $\sum_{i=1}^{n-k} d_i = 2(n+c-1) - k$, then $d_1 \leq 2c+k$. Suppose $d_1 = 2c+k$, then $d_2 = d_3 = \cdots = d_{n-k} = 2$, which implies that $G \in \mathcal{S}_n(c,k)$, a contradiction. Thus, $d_1 < 2c+k$. Since $d_i \geq 2$ holds for $1 \leq i \leq n-k$, then $\sum_{l=1}^{i} d_l = 2(n+c-1) - k - d_{i+1} - d_{i+2} - \cdots - d_{n-k} \leq 2(n+c-1) - k - 2(n-k-i) = \sum_{l=1}^{i} d'_l$ holds for $1 \leq i \leq n-k$. Thus, $\pi(G) \trianglelefteq \pi(G')$ but $\pi(G) \neq \pi(G')$. Now by Theorem 2.1, the result follows.

Theorem 2.3 *Let G and G' be graphs with the greatest first Zagreb index in $\mathcal{G}_n(c,k)$ and $\mathcal{G}_n(c,k+1)$, respectively, where $c \geq 0$ and $1 \leq k \leq n-2c-2$. Then, $M_1(G) < M_1(G')$.*

Proof. By Theorem 2.2, it follows that $G \in \mathcal{S}_n(c,k)$ and $G' \in \mathcal{S}_n(c,k+1)$. Thus, $\pi(G) = (2c+k, \underbrace{2,2,...,2}_{n-k-1}, \underbrace{1,1,...,1}_{k})$ and $\pi(G') = (2c+k+1, \underbrace{2,2,...,2}_{n-k-2}, \underbrace{1,1,...,1}_{k+1})$. It is easy to check that $\pi(G) \trianglelefteq \pi(G')$ but $\pi(G) \neq \pi(G')$, which implies that $M_1(G) < M_1(G')$ by Theorem 2.1.

Let U_n^t denote the unicyclic graph obtained from the cycle C_t by attaching $n-t$ pendant edges to the same vertex on C_t. By Theorems 2.2-2.3, it follows immediately that

Corollary 2.2 [9] *Let G be a unicyclic graph of order n and girth t. If G is different from U_n^t, then $M_1(G) < M_1(U_n^t)$.*

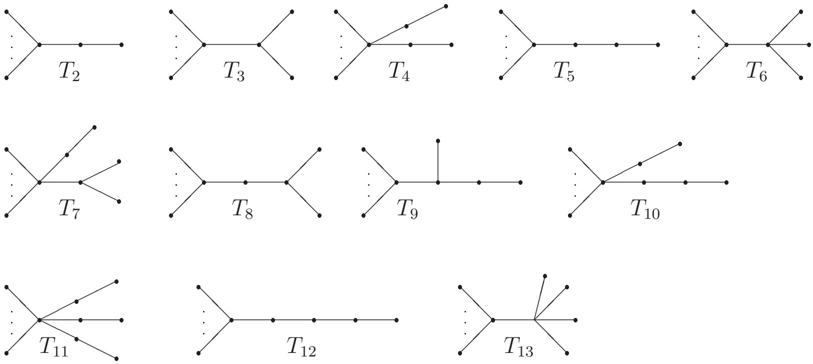

Fig. 1. The trees T_2, ..., T_{13}.

Let $T_1 = K_{1,n-1}, T_2, T_3, ..., T_{13}$ be the trees on n vertices as shown in Fig. 1. In [9, 12], the five trees with the first through fourth greatest first Zagreb indices among all trees of order n were given. The next result extends this ordering by determining the fifth up to eighth greatest first Zagreb indices together with the corresponding trees among all trees of order n.

Theorem 2.4 *Suppose $T \in \mathcal{T}_n \setminus \{T_1, T_2, ..., T_{13}\}$ and $n \geq 13$, then $M_1(T_1) > M_1(T_2) > M_1(T_3) > M_1(T_4) = M_1(T_5) > M_1(T_6) > M_1(T_7) = M_1(T_8) = M_1(T_9) > M_1(T_{10}) = M_1(T_{11}) = M_1(T_{12}) > M_1(T_{13}) > M_1(T)$.*

Proof. By an elementary computation, we have $M_1(T_1) = n^2 - n$, $M_1(T_2) = n^2 - 3n + 6$, $M_1(T_3) = n^2 - 5n + 16$, $M_1(T_4) = M_1(T_5) = n^2 - 5n + 14$, $M_1(T_6) = n^2 - 7n + 30$, $M_1(T_7) = M_1(T_8) = M_1(T_9) = n^2 - 7n + 26$, $M_1(T_{10}) = M_1(T_{11}) = M_1(T_{12}) = n^2 - 7n + 24$, $M_1(T_{13}) = n^2 - 9n + 48$. Thus, $M_1(T_1) > M_1(T_2) > M_1(T_3) > M_1(T_4) = M_1(T_5) > M_1(T_6) > M_1(T_7) = M_1(T_8) = M_1(T_9) > M_1(T_{10}) = M_1(T_{11}) = M_1(T_{12}) > M_1(T_{13})$. Next we only need to show that if $T \in \mathcal{T}_n \setminus \{T_1, T_2, ..., T_{13}\}$, then $M_1(T_{13}) > M_1(T)$.

Clearly, 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 the all trees with $\Delta = n - 3$, $T_6, ...$ T_{12} are the all trees with $\Delta = n - 4$. Since $T \in \mathcal{T}_n \setminus \{T_1, T_2, ..., T_{13}\}$, then $\Delta(T) \leq n - 5$.

Let $(a) = (d_1, d_2, ..., d_n)$ be the degree sequence of T. Note that the degree sequence of T_{13} is $(b) = (n - 5, 5, 1, ..., 1)$, it is easy to see that $(a) \trianglelefteq (b)$ and $(a) \neq (b)$ because T_{13}

is the unique tree with (b) as its degree sequence. Thus, $M_1(T_{13}) > M_1(T)$ follows from Theorem 2.1.

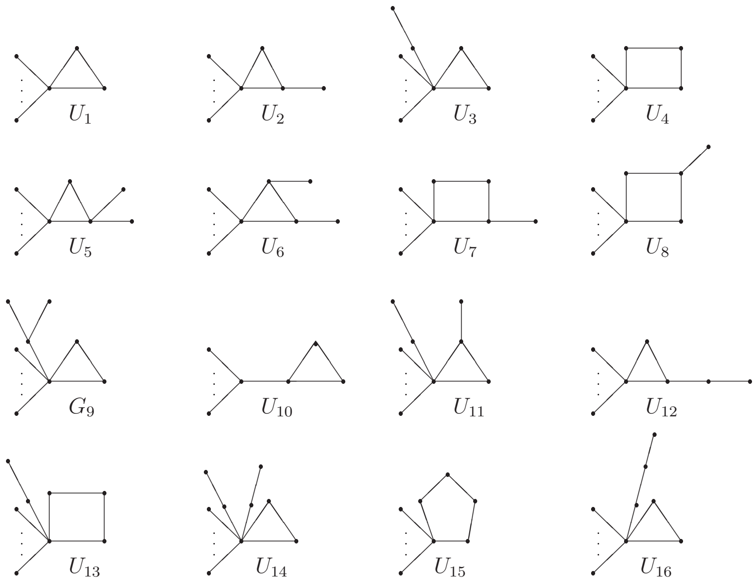

Fig. 2. The unicyclic graphs U_1, ..., U_{16}.

Let $\mathbb{U}(n)$ denote the class of connected unicyclic graphs of order n. Let U_1, ..., U_{16} be the unicyclic graphs as shown in Fig. 2. In [11], we have determined the four unicyclic graphs with the first through third greatest first Zagreb indices among the class of connected unicyclic graphs of order n. The next result extends this ordering by determining the fourth up to seventh greatest first Zagreb indices together with the corresponding unicyclic graphs among the class of connected unicyclic graphs of order n.

Theorem 2.5 *If* $G \in \mathbb{U}(n) \setminus \{U_1, ..., U_{16}\}$ *and* $n \geq 12$, *then* $M_1(U_1) > M_1(U_2) > M_1(U_3) = M_1(U_4) > M_1(U_5) > M_1(U_6) > M_1(U_7) = M_1(U_8) = M_1(U_9) = M_1(U_{10}) = M_1(U_{11}) = M_1(U_{12}) > M_1(U_{13}) = M_1(U_{14}) = M_1(U_{15}) = M_1(U_{16}) > M_1(G)$.

Proof. By an elementary computation, we have $M_1(U_1) = n^2 - n + 6$, $M_1(U_2) = n^2 - 3n + 14$, $M_1(U_3) = M_1(U_4) = n^2 - 3n + 12$, $M_1(U_5) = n^2 - 5n + 26$, $M_1(U_6) = n^2 - 5n + 24$, $M_1(U_7) = M_1(U_8) = M_1(U_9) = M_1(U_{10}) = M_1(U_{11}) = M_1(U_{12}) = n^2 - 5n + 22$, and $M_1(U_{13}) = M_1(U_{14}) = M_1(U_{15}) = M_1(U_{16}) = n^2 - 5n + 20$. Thus, $M_1(U_1) > M_1(U_2) > M_1(U_3) = M_1(U_4) > M_1(U_5) > M_1(U_6) > M_1(U_7) = M_1(U_8) = M_1(U_9) = M_1(U_{10}) =$

$M_1(U_{11}) = M_1(U_{12}) > M_1(U_{13}) = M_1(U_{14}) = M_1(U_{15}) = M_1(U_{16})$. Next we only need to prove that if $G \in \mathbb{U}(n) \setminus \{U_1, ..., U_{16}\}$, then $M_1(U_{16}) > M_1(G)$.

It is easy to check that U_1 is the unique unicyclic graph with $\Delta = n-1$, U_2, U_3, U_4 are the all unicyclic graphs with $\Delta = n-2$, and $U_5, U_6, ..., U_{16}$ are the all unicyclic graphs with $\Delta(G) = n-3$. If $G \in \mathbb{U}(n) \setminus \{U_1, ..., U_{16}\}$, then $\Delta(G) \leq n-4$. Suppose the degree sequence of G is $(a) = (d_1, d_2, d_3, ..., d_n)$, since $G \in \mathbb{U}(n)$, then G has exactly one cycle. This implies that $n-4 \geq d_1 \geq d_2 \geq d_3 \geq 2$. Let $(b) = (n-4, 5, 2, 1, ..., 1)$, then $(a) \trianglelefteq (b)$. By Theorem 2.1, we can conclude that

$$M_1(G) \leq (n-4)^2 + 5^2 + 2^2 + n - 3 = n^2 - 7n + 42 < n^2 - 5n + 20 = M_1(U_{16}).$$

This completes the proof of this result.

Let $\mathbb{B}(n)$ be the class of connected bicyclic graphs of order n. Let B_1,..., B_{11} be the bicyclic graphs as shown in Fig. 3.

Theorem 2.6 *If $G \in \mathbb{B}(n) \setminus \{B_1, ..., B_{11}\}$ and $n \geq 11$, then $M_1(B_1) > M_1(B_2) > M_1(B_3) > M_1(B_4) = M_1(B_5) > M_1(B_6) = M_1(B_7) = M_1(B_8) = M_1(B_9) > M_1(B_{10}) = M_1(B_{11}) > M_1(G)$.*

Proof. By an element computation, we have $M_1(B_1) = n^2-n+14$, $M_1(B_2) = n^2-n+12$, $M_1(B_3) = n^2 - 3n + 24$, $M_1(B_4) = M_1(B_5) = n^2 - 3n + 22$, $M_1(B_6) = M_1(B_7) = M_1(B_8) = M_1(B_9) = n^2 - 3n + 20$, $M_1(B_{10}) = M_1(B_{11}) = n^2 - 3n + 18$. Thus, $M_1(B_1) > M_1(B_2) > M_1(B_3) > M_1(B_4) = M_1(B_5) > M_1(B_6) = M_1(B_7) = M_1(B_8) = M_1(B_9) > M_1(B_{10}) = M_1(B_{11})$. Next we only need to prove that if $G \in \mathbb{B}(n) \setminus \{B_1, ..., B_{11}\}$, then $M_1(B_{11}) > M_1(G)$.

It is easy to check that B_1, B_2 are the all bicyclic graphs with $\Delta = n-1$, $B_3, ..., B_{11}$ are the all bicyclic graphs with $\Delta = n-2$. If $G \in \mathbb{B}(n) \setminus \{B_1, ..., B_{11}\}$, then $\Delta(G) \leq n-3$. Suppose the degree sequence of G is $(a) = (d_1, d_2, d_3, ..., d_n)$, since $G \in \mathbb{B}(n)$, then $n-3 \geq d_1 \geq d_2 \geq d_3 \geq d_4 \geq 2$. Let $(b) = (n-3, 5, 2, 2, 1, ..., 1)$, then $(a) \trianglelefteq (b)$. By Theorem 2.1, we can conclude that

$$M_1(G) \leq (n-3)^2 + 5^2 + 2^2 \times 2 + n - 4 = n^2 - 5n + 38 < n^2 - 3n + 18 = M_1(B_{11}).$$

This completes the proof of this result.

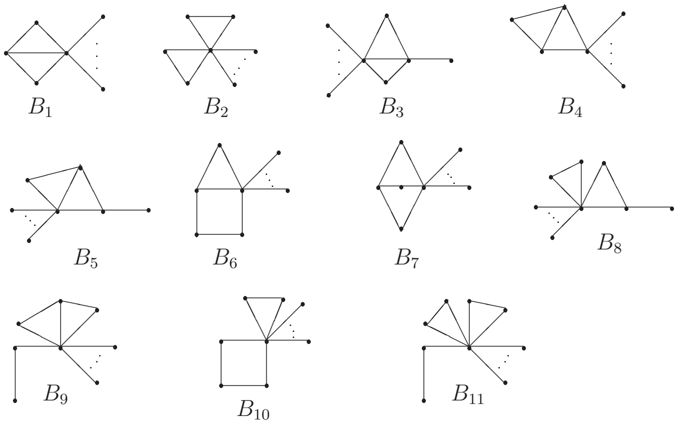

Fig. 3. The bicyclic graphs B_1,..., B_{11}.

Corollary 2.3 [9] *B_1 is the unique graph with the greatest Zagreb index among the class of connected bicyclic graphs of order n.*

Since the degree sequence $(2, .., 2, 1, 1)$ is minimal in the class of $\mathcal{T}(n)$ (i.e., in the order $\trianglelefteq$), the degree sequence $(2, 2, .., 2)$ is minimal in the class of $\mathbb{U}(n)$, and the degree sequence $(3, 3, 2, .., 2)$ is minimal in the class of $\mathbb{B}(n)$, by Theorem 2.1 we have

Theorem 2.7 [8, 9] (1) *If $T \in \mathcal{T}_n \setminus \{P_n\}$, then $M_1(T) > M_1(P_n)$;* (2) *If $G \in \mathbb{U}_n \setminus \{C_n\}$, then $M_1(G) > M_1(C_n)$;* (3) *Let $\mathcal{H}$ be the class of connected bicyclic graphs with $(3, 3, 2, ..., 2)$ as theirs degree sequences. If $G \in \mathbb{B}_n \setminus \{\mathcal{H}\}$, then $M_1(G) > M_1(H_1)$, where H_1 is a graph of $\mathcal{H}$.*

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