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Some properties of the first general Zagreb index*

Muhuo Liu[†] Bolian Liu[‡]

School of Mathematic Science
South China Normal University
Guangzhou 510631
P. R. China

Abstract

In this paper, the effects on the first general Zagreb index are observed when some operations, such as edge moving, edge separating and edge switching are applied to the graphs. Moreover, we obtain the majorization theorem to the first general Zagreb indices between two graphic sequences. Furthermore, we illustrate the application of these new properties, and obtain the largest or smallest first general Zagreb indices among some class of connected graphs.

1 Introduction

Throughout the paper, $G = (V, E)$ is a connected undirected simple graph with $|V| = n$ and $|E| = m$. If $m = n + c - 1$, then G is called a $c-$cyclic graph. In particular, if $c = 0$ or 1, then G is called a tree or a unicyclic graph, respectively. The symbol uv is used to denoted an edge whose endpoints are the vertices u and v. Let $N(u)$ be the first neighbor vertex set of u; then $d(u) = |N(u)|$ is called the degree of u. In particular, $\Delta = \Delta(G)$ is called the maximum degree of vertices of G, and a vertex of degree 1 is called a pendant vertex of G. Suppose the degree of vertex v_i equals d_i for $i = 1, 2, \ldots, n$; then $\pi(G) = (d_1, \ldots, d_n)$ is called the *graphic sequence* of G. Throughout this paper, we enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$. Sometimes we write $d_G(u)$ and $N_G(u)$ in place of $d(u)$ and $N(u)$, respectively, in order to indicate the dependence on G. As usual, $K_{1,n-1}$ and C_n denote a star and a cycle of order n, respectively.

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† Also at Department of Applied Mathematics, South China Agricultural University, Guangzhou 510642, P. R. China.

‡ E-mail address `liubl@scnu.edu.cn`

The Zagreb index was first introduced by Gutman and Trinajstić [4]; it is an important molecular descriptor and has been closely correlated with many chemical properties [4, 7]. Thus, it attracted more and more attention from chemists and mathematicians [1–3, 11, 15]. The *first Zagreb index* $M_1(G)$ is defined as [4]:

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

Recently, Li and Zheng [9] introduced the concept of the *first general Zagreb index* $M_1^\alpha(G)$ of G as follows:

$$M_1^\alpha(G) = \sum_{v \in V} d(v)^\alpha,$$

where α is an arbitrary real number, not 0 and 1. As one can easily see, $M_1^2(G)$ is just the first Zagreb index $M_1(G)$.

Li and Zhao [8] characterized all trees with the first three smallest and largest values of the first general Zegreb index when α is an integer or a fraction $\frac{1}{k}$ for a nonzero integer k. All unicyclic graphs with the first three smallest and largest values of the first general Zagreb index were identified in [13]. The notation of the first general Zagreb index is also referred to be the general zeroth-order Randić index [10, 13]. The molecular graphs with the smallest and largest values of the general zeroth-order Randić index were determined by Hu et al. in [6]. Moreover, all bicyclic graphs with the first three smallest and largest values of the first general Zagreb index were identified in [14].

In this paper, the effects on the first general Zagreb index are observed when some operations, such as edge moving, edge separating and edge switching are applied to the graphs. Moreover, the majorization theorem to the first general Zagreb indices between two graphic sequences is given. Furthermore, with the application of these new properties, we obtain the largest or smallest first general Zagreb indices among some classes of connected graphs.

2 Some properties for $M_1^\alpha(G)$

Let $G - u$ or $G - uv$ denote the graphs that are obtained from G by deleting the vertex $u \in V(G)$ or the edge $uv \in E(G)$, respectively. Similarly, $G + uv$ is a graph that is obtained from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$.

2.1 The majorization theorem

We recall the notation of *majorization* (see [5, 12]). Suppose $(x) = (x_1, x_2, \ldots, x_n)$ and $(y) = (y_1, y_2, \ldots, y_n)$ are two non-increasing sequences of real numbers. Then 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 $j = 1, 2, \ldots, n$. Furthermore, by $(x) \lhd (y)$ we mean that $(x) \trianglelefteq (y)$ and (x) is not the rearrangement of (y), i.e., $(x) \neq (y)$. It has been shown that

Lemma 2.1 [5] *Suppose* $(x) = (x_1, x_2, \ldots, x_n)$ *and* $(y) = (y_1, y_2, \ldots, y_n)$ *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 graphic sequence* $(a) = (d_1, d_2, \ldots, d_n)$ *and* G' *be a connected graph with graphic sequence* $(b) = (d_1', d_2', \ldots, d_n')$.

(1) *If* $(a) \trianglelefteq (b)$, $\alpha < 0$ *or* $\alpha > 1$*, then* $M_1^\alpha(G) \leq M_1^\alpha(G')$*, where equality holds if and only if* $(a) = (b)$.

(2) *If* $(a) \trianglelefteq (b)$, $0 < \alpha < 1$*, then* $M_1^\alpha(G) \geq M_1^\alpha(G')$*, where equality holds if and only if* $(a) = (b)$.

Proof. (1) Observe that for $\alpha \neq 0, 1$, and $x > 0$, x^α is a strictly convex function if $\alpha < 0$ or $\alpha > 1$. By Lemma 2.1 it follows that $M_1^\alpha(G) \leq M_1^\alpha(G')$. Once again, Lemma 2.1 implies that the equality holds if and only if $(a) = (b)$.

(ii) Observe that for $\alpha \neq 0, 1$, and $x > 0$, $-x^\alpha$ is a strictly convex function if $0 < \alpha < 1$. Using similar arguments as in the proof of (1), we may prove (2). □

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 $\mathcal{T}_n^s = \{T \in \mathcal{T}_n \mid \Delta(T) = s\}$.

Corollary 2.1 *Let* T *be a tree in* $\mathcal{T}_n^s$*, where* $s \geq \lceil \frac{n}{2} \rceil$.

(1) *If* $\alpha < 0$ *or* $\alpha > 1$*, then* $M_1^\alpha(T) \leq M_1^\alpha(S(n, s))$*, where equality holds if and only if* $T \cong S(n, s)$.

(2) *If* $0 < \alpha < 1$*, then* $M_1^\alpha(T) \geq M_1^\alpha(S(n, s))$*, where equality holds if and only if* $T \cong S(n, s)$.

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

2.2 Edge moving operation

Suppose v is a vertex of graph G. As shown in Fig. 1, let $G_{k,l}$ $(l \geq k \geq 1)$ be the graph obtained from G by attaching two new paths P: $v(= v_0)v_1v_2 \ldots v_k$ and Q:

$v(=u_0)u_1u_2\dots u_l$ of length k and l, respectively, at v, where $v_1, v_2, \dots, v_k$ and $u_1, u_2, \dots, u_l$ are distinct new vertices. Let $G_{k-1,l+1} = G_{k,l} - v_{k-1}v_k + u_lv_k$.

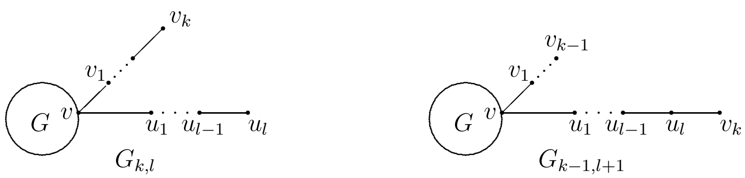

Fig. 1.

Theorem 2.2 *Suppose G is a connected graph on $n \geq 2$ vertices and $l \geq k \geq 1$.*

(1) *If $\alpha < 0$ or $\alpha > 1$, then $M_1^\alpha(G_{k,l}) \geq M_1^\alpha(G_{k-1,l+1})$, and the inequality is strict if and only if $k = 1$.*

(2) *If $0 < \alpha < 1$, then $M_1^\alpha(G_{k,l}) \leq M_1^\alpha(G_{k-1,l+1})$, and the inequality is strict if and only if $k = 1$.*

Proof. We consider the next two cases.

Case 1. $k \geq 2$. It is easy to see that

$$\begin{aligned} M_1^\alpha(G_{k,l}) - M_1^\alpha(G_{k-1,l+1}) &= d^\alpha_{G_{k,l}}(v_{k-1}) + d^\alpha_{G_{k,l}}(u_l) - (d^\alpha_{G_{k-1,l+1}}(v_{k-1}) + d^\alpha_{G_{k-1,l+1}}(u_l)) \\ &= 2^\alpha + 1^\alpha - (1^\alpha + 2^\alpha) \\ &= 0. \end{aligned}$$

Case 2. $k = 1$. It is easy to see that

$$M_1^\alpha(G_{k,l}) - M_1^\alpha(G_{k-1,l+1}) = d^\alpha_{G_{k,l}}(v) + d^\alpha_{G_{k,l}}(u_l) - (d^\alpha_{G_{k-1,l+1}}(v) + d^\alpha_{G_{k-1,l+1}}(u_l)). \quad (1)$$

Note that G is a connected graph on $n \geq 2$ vertices, so then $d_{G_{k,l}}(v) \geq 3$. Let $(x) = (d_{G_{k,l}}(v), d_{G_{k,l}}(u_l)) = (d_{G_{k,l}}(v), 1)$ and $(y) = (d_{G_{k-1,l+1}}(v), d_{G_{k-1,l+1}}(u_l)) = (d_{G_{k,l}}(v) - 1, 2)$. Thus, $(y) \lhd (x)$.

If $\alpha < 0$ or $\alpha > 1$, since x^α is a strictly convex function when $x > 0$. Thus, by Lemma 2.1 and equality (1) it follows that $M_1^\alpha(G_{k,l}) > M_1^\alpha(G_{k-1,l+1})$.

If $0 < \alpha < 1$, since $-x^\alpha$ is a strictly convex function when $x > 0$. Thus, by Lemma 2.1 and equality (1) it follows that $M_1^\alpha(G_{k,l}) < M_1^\alpha(G_{k-1,l+1})$.

This completes the proof of this result. □

Corollary 2.2 [9] *Suppose $T \in \mathcal{T}_n \setminus \{P_n\}$.*
(1) *If $\alpha < 0$ or $\alpha > 1$, then $M_1^\alpha(T) > M_1^\alpha(P_n)$.*
(2) *If $0 < \alpha < 1$, then $M_1^\alpha(T) < M_1^\alpha(P_n)$.*

2.3 Edge separating operation

Let $e = uv$ be a cut edge of G. If G' is obtained from G by contracting the edge e into a new vertex u_e, which becomes adjacent to all the former neighbors of u and of v, and adding a new pendent edge $u_e v_e$, where v_e is a new pendent vertex. We say that G' is obtained from G by separating an edge uv (see Fig. 2).

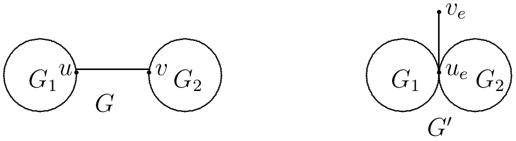

Fig. 2.

Theorem 2.3 *Suppose $e = uv$ is a cut edge of a connected graph G, where $d_G(v) \geq 2$ and $d_G(u) \geq 2$. Let G' be the graph obtained from G by separating the edge uv.*

(1) *If $\alpha < 0$ or $\alpha > 1$, then $M_1^\alpha(G) < M_1^\alpha(G')$.*

(2) *If $0 < \alpha < 1$, then $M_1^\alpha(G) > M_1^\alpha(G')$.*

Proof. It is easy to see that

$$M_1^\alpha(G') - M_1^\alpha(G) \ = \ d_{G'}^\alpha(u_e) + d_{G'}^\alpha(v_e) - (d_G^\alpha(u) + d_G^\alpha(v)). \tag{2}$$

Without loss of generality, suppose $d_G(u) \geq d_G(v)$. Let $(x) = (d_{G'}(u_e), d_{G'}(v_e)) = (d_G(u) + d_G(v) - 1, 1)$ and $(y) = (d_G(u), d_G(v))$. Clearly, $(y) \lhd (x)$. Observe that for $\alpha \neq 0, 1$, and $x > 0$, x^α is a strictly convex function if $\alpha < 0$ or $\alpha > 1$, and $-x^\alpha$ is a strictly convex function if $0 < \alpha < 1$. Thus, the conclusion follows from Lemma 2.1 and equality (2). $\square$

Corollary 2.3 [9] *Suppose $T \in \mathcal{T}_n \setminus \{K_{1,n-1}\}$.*

(1) *If $\alpha < 0$ or $\alpha > 1$, then $M_1^\alpha(T) < M_1^\alpha(K_{1,n-1})$.*

(2) *If $0 < \alpha < 1$, then $M_1^\alpha(T) > M_1^\alpha(K_{1,n-1})$.*

2.4 Edge switching operation

Theorem 2.4 *Let u, v be two vertices of a connected graph G with $d_G(v) \geq d_G(u)$. Suppose that $v_1, \ldots, v_s$ $(1 \leq s \leq d_G(u)-1)$ are some vertices of $N_G(u) \setminus \{N_G(v) \cup v\}$. Let G^* be a new graph obtained from G by deleting edges uv_i and adding edges vv_i for $i = 1, \ldots, s$.*

(1) *If $\alpha < 0$ or $\alpha > 1$, then $M_1^\alpha(G) < M_1^\alpha(G^*)$.*

(2) *If $0 < \alpha < 1$, then $M_1^\alpha(G) > M_1^\alpha(G^*)$.*

Proof. It is easy to see that

$$M_1^\alpha(G^*) - M_1^\alpha(G) \;=\; d_{G^*}^\alpha(u) + d_{G^*}^\alpha(v) - (d_G^\alpha(u) + d_G^\alpha(v)). \qquad (3)$$

Let $(x) = (d_{G^*}(v), d_{G^*}(u)) = (d_G(v)+s, d_G(u)-s)$ and $(y) = (d_G(v), d_G(u))$. Clearly, $(y) \lhd (x)$. Observe that for $\alpha \neq 0, 1$, and $x > 0$, x^α is a strictly convex function if $\alpha < 0$ or $\alpha > 1$, and $-x^\alpha$ is a strictly convex function if $0 < \alpha < 1$. Thus the conclusion follows from Lemma 2.1 and equality (3). □

3 Some applications

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. Let $\mathcal{S}_n(c, k)$ be the class of connected graphs on n vertices obtained by attaching c cycles (not necessary with equal length) 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 c-cyclic graphs with $(2c + k, \underbrace{2, 2, \ldots, 2}_{n-k-1}, \underbrace{1, 1, \ldots, 1}_{k})$ as their graphic 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. 3. By definition, $U_3, U_4 \in \mathcal{S}_n(1, n-4)$. If G',$G \in \mathcal{S}_n(c, k)$, since they share the same graphic sequences, we have

Proposition 3.1 *Let G' and G be the graphs in $\mathcal{S}_n(c, k)$, where $c \geq 0$ and $1 \leq k \leq n - 2c - 1$. Then $M_1^\alpha(G) = M_1^\alpha(G')$ holds for any α.*

Theorem 3.1 *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 $1 \leq k \leq n - 2c - 1$.*

(1) *If $\alpha < 0$ or $\alpha > 1$, then $M_1^\alpha(G) < M_1^\alpha(G')$.*

(2) *If $0 < \alpha < 1$, then $M_1^\alpha(G) > M_1^\alpha(G')$.*

Proof. Clearly, G', $G \in \mathcal{G}_n(c, k)$. Thus, there are exactly k elements 1 in their graphic sequences. Since $G' \in \mathcal{S}_n(c, k)$, we have

$$\pi(G') = (d_1', d_2', \ldots, d_{n-k}', \underbrace{1, 1, \ldots, 1}_{k}) \;=\; (2c + k, \underbrace{2, 2, \ldots, 2}_{n-k-1}, \underbrace{1, 1, \ldots, 1}_{k}).$$

Let $\pi(G) = (d_1, d_2, \ldots, d_{n-k}, \underbrace{1, 1, \ldots, 1}_{k})$, where $d_1 \geq d_2 \geq \cdots \geq d_{n-k} \geq 2$. Since $\sum_{i=1}^{n-k} d_i = 2(n + c - 1) - k$, $d_1 \leq 2c + k$. 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, $d_1 < 2c + k = d_1'$. Since $d_i \geq 2$ holds for $2 \leq i \leq n - k$, we have $\sum_{l=1}^{i} d_l = 2(n + c - 1) - k - d_{i+1} - d_{i+2} - \cdots - d_{n-k} \leq 2(n + c - 1) - k - 2(n - k - i) = \sum_{l=1}^{i} d_l'$ holds for $2 \leq i \leq n - k$. Thus, $\pi(G) \lhd \pi(G')$. Now by Theorem 2.1, the result follows. □

A pendant path is a path with one of its end vertices having degree one and all the internal vertices having degree two. A pendant edge is an edge with a pendant vertex as its endpoint. Obviously, a pendant path of length one is just a pendant edge.

Lemma 3.1 *Let G and G' be the graphs in $\mathcal{S}_n(c,k)$ and $\mathcal{S}_n(c,k+1)$, respectively, where $c \geq 0$ and $1 \leq k \leq n-2c-2$.*

(1) *If $\alpha < 0$ or $\alpha > 1$, then $M_1^\alpha(G) < M_1^\alpha(G')$.*

(2) *If $0 < \alpha < 1$, then $M_1^\alpha(G) > M_1^\alpha(G')$.*

Proof. Here we only need to prove (1), because (2) can be proved similarly. Since $G \in \mathcal{S}_n(c,k)$ and $1 \leq k \leq n-2c-2$, by Proposition 3.1 there exists one graph, say G_1, such that $M_1^\alpha(G) = M_1^\alpha(G_1)$ and G_1 has one pendant path with length being larger than 1. Let G_2 be the graph obtained from G_1 by separating an edge (not a pendant edge) in the pendant path of G_1. Then $G_2 \in \mathcal{G}_n(c,k+1)$. By Theorem 2.3, it follows that $M_1^\alpha(G_1) < M_1^\alpha(G_2)$. Thus, by Theorem 3.1 we can conclude that $M_1^\alpha(G) = M_1^\alpha(G_1) < M_1^\alpha(G_2) \leq M_1^\alpha(G')$. This completes the proof. □

By Lemma 3.1 and Theorem 3.1, the following immediately follows:

Theorem 3.2 (1) *Let G and G' be the graphs with the largest first general Zagreb indices in $\mathcal{G}_n(c,k)$ and $\mathcal{G}_n(c,k+1)$, respectively, where $c \geq 0$ and $1 \leq k \leq n-2c-2$. If $\alpha < 0$ or $\alpha > 1$, then $M_1^\alpha(G) < M_1^\alpha(G')$.*

(2) *Let G and G' be the graphs with the smallest first general Zagreb indices in $\mathcal{G}_n(c,k)$ and $\mathcal{G}_n(c,k+1)$, respectively, where $c \geq 0$ and $1 \leq k \leq n-2c-2$. If $0 < \alpha < 1$, then $M_1^\alpha(G) > M_1^\alpha(G')$.*

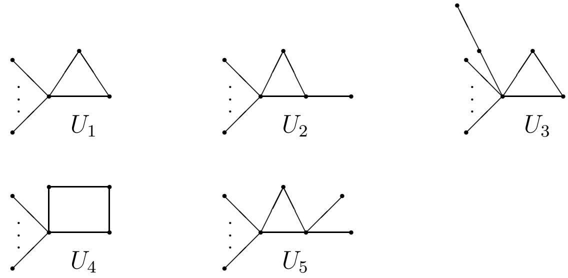

Fig. 3. The unicyclic graphs $U_1, \ldots, U_5$.

Let $\mathbb{U}(n)$ denote the class of connected unicyclic graphs of order n. Let U_1, U_2, U_3, U_4, U_5 be the unicyclic graphs as shown in Fig. 3.

Theorem 3.3 *Suppose $G \in \mathbb{U}(n)$ and $n \geq 6$.*

(1) *If $\alpha < 0$ or $\alpha > 1$, then*

(*i*) *$M_1^\alpha(G)$ attains the largest value if and only if $G \cong U_1$;*

(ii) $M_1^\alpha(G)$ *attains the second largest value if and only if* $G \cong U_2$*;*

(iii) $M_1^\alpha(G)$ *attains the third largest value if and only if*

$$M_1^\alpha(G) = \max\{M_1^\alpha(U_3), M_1^\alpha(U_5)\}.$$

(2) *If* $0 < \alpha < 1$*, then*

(i) $M_1^\alpha(G)$ *attains the smallest value if and only if* $G \cong U_1$*;*

(ii) $M_1^\alpha(G)$ *attains the second smallest value if and only if* $G \cong U_2$*;*

(iii) $M_1^\alpha(G)$ *attains the third smallest value if and only if*

$$M_1^\alpha(G) = \min\{M_1^\alpha(U_3), M_1^\alpha(U_5)\}.$$

Proof. Here we only prove (1), because (2) can be proved analogously with (1). By Theorem 2.1 and Proposition 3.1, we have $M_1^\alpha(U_3) = M_1^\alpha(U_4)$ and $M_1^\alpha(U_1) > M_1^\alpha(U_2) > \max\{M_1^\alpha(U_3), M_1^\alpha(U_5)\}$. Next we only need to prove that if $G \in \mathbb{U}(n) \setminus \{U_1, U_2, U_3, U_4, U_5\}$, then $\max\{M_1^\alpha(U_3), M_1^\alpha(U_5)\} > M_1^\alpha(G)$.

Note that U_1, U_2, U_3, U_4 are the all unicyclic graphs with $n-2 \le \Delta \le n-1$, since $G \in \mathbb{U}(n) \setminus \{U_1, U_2, U_3, U_4\}$, then $\Delta(G) \le n-3$. Clearly, there exists some k $(0 \le k \le n-3)$ such that $G \in \mathcal{G}_n(1, k)$. Three cases occur as follows.

Case 1. $k = n-3$. Suppose the graphic sequence of G is $(a) = (d_1, d_2, d_3, 1, \ldots, 1)$. Since $G \ncong U_1$, $G \ncong U_2$ and $G \ncong U_5$, we have $(a) \trianglelefteq (b)$, where $(b) = (n-3, 4, 2, 1, \ldots, 1)$. Note that U_5 is the unique graph with (b) as its graphic sequence. Thus, $(a) \triangleleft (b)$. This implies that $M_1^\alpha(G) < M_1^\alpha(U_5)$ by Theorem 2.1.

Case 2. $k = n-4$. Suppose the graphic sequence of G is $(c) = (d_1, d_2, d_3, d_4, 1, \ldots, 1)$. Since $G \ncong U_3$ and $G \ncong U_4$, then $(c) \trianglelefteq (d)$, where $(d) = (n-3, 3, 2, 2, 1, \ldots, 1)$. Thus, $M_1^\alpha(G) < M_1^\alpha(U_5)$ follows from Theorem 2.1 because $(d) \triangleleft (b)$.

Case 3. $0 \le k \le n-5$. Suppose the graphic sequence of G is $(e) = (d_1, d_2, \ldots, d_n)$. Since $G \ncong U_1$, $G \ncong U_2$, $G \ncong U_3$ and $G \ncong U_4$, then $(e) \trianglelefteq (f)$, where $(f) = (n-3, 2, 2, 2, 2, 1, \ldots, 1)$. By Theorem 2.1, it follows that $M_1^\alpha(G) < M_1^\alpha(U_5)$ because $(f) \triangleleft (b)$.

This completes the proof of this result. □

Remark. The results in Theorem 3.3 have been proved in [13]; here we just give another simple method to show this again.

Let $T_1 = K_{1,n-1}$, $T_2, T_3, \ldots, T_6$ be the trees on n vertices as shown in Fig. 4.

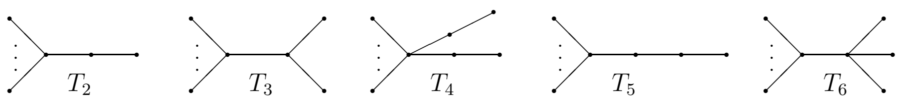

Fig. 4. The trees $T_2, \ldots, T_6$.

Theorem 3.4 *Suppose $T \in \mathcal{T}_n \setminus \{T_1, T_2, \dots, T_6\}$.*

(1) *If $\alpha < 0$ or $\alpha > 1$, then*

$$M_1^\alpha(T_1) > M_1^\alpha(T_2) > M_1^\alpha(T_3) > \max\{M_1^\alpha(T_4), M_1^\alpha(T_6)\} > M_1^\alpha(T).$$

(2) *If $0 < \alpha < 1$, then*

$$M_1^\alpha(T_1) < M_1^\alpha(T_2) < M_1^\alpha(T_3) < \min\{M_1^\alpha(T_4), M_1^\alpha(T_6)\} < M_1^\alpha(T).$$

Proof. Here we only prove (1), because (2) can be proved similarly to (1). 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 all the trees with $\Delta = n-3$. By Theorem 2.1 and Proposition 3.1 it follows that $M_1^\alpha(T_4) = M_1^\alpha(T_5)$ and $M_1^\alpha(T_1) > M_1^\alpha(T_2) > M_1^\alpha(T_3) > \max\{M_1^\alpha(T_4), M_1^\alpha(T_6)\}$. Next we only need to prove that if $G \in \mathbb{U}(n) \setminus \{T_1, T_2, T_3, T_4, T_5, T_6\}$, then $\max\{M_1^\alpha(T_4), M_1^\alpha(T_6)\} > M_1^\alpha(T)$.

Since $T \in \mathcal{T}_n \setminus \{T_1, T_2, \dots, T_6\}$, then $\Delta(T) \leq n-4$. Let $(a) = (d_1, d_2, \dots, d_n)$ be the graphic sequence of T. Noting that the graphic sequence of T_6 is $(b) = (n-4, 4, 1, \dots, 1)$, it is easy to see that $(a) \trianglelefteq (b)$. Note that T_6 is the unique tree with (b) as its graphic sequence, so that $(a) \triangleleft (b)$. Thus, the conclusion follows from Theorem 2.1 □

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