Research Article Sharp bounds on general multiplicative Zagreb indices of trees

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Abstract

The first and second general multiplicative Zagreb indices of a simple graph are defined as the product over all pairs of adjacent vertices a, b of the terms $[d(a) + d(b)]^{\alpha}$ and $[d(a) d(b)]^{\alpha}$, respectively, where d(a) denotes the degree of the vertex a, and α is a real number. In this paper, we obtain bounds on these indices for trees with fixed maximum degree, and characterize the extremal cases.

Keywords: Zagreb indices; general multiplicative Zagreb indices; degree (of vertex); tree.

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1. Introduction

Let G be an undirected simple connected graph whose vertex and edge sets are V(G) and E(G), respectively. For $a \in V(G)$, the open neighborhood of a is the set $N(a) = \{b \in V(G) \mid ab \in E(G)\}$. The degree of a vertex a in G is the cardinality of N(a), and will be denoted by d(a) (or, where necessary, by $d_G(a)$). The maximum degree of G is denoted by $\Delta(G) = \Delta$. The distance between the vertices $a, b \in V(G)$, d(a, b), is the length of a shortest (a, b)-path in G.

The first Zagreb index [11, 14] and the second Zagreb index [6, 13] are the oldest members of the nowadays rich family of vertex-degree-based indices, and are respectively defined as

$$M_1(G) = \sum_{ab \in E(G)} [d(a) + d(b)]$$
 and $M_2(G) = \sum_{ab \in E(G)} d(a) d(b)$

For comprehensive and transparent information on these indices, we refer the reader to [2,5,12]. Research on these indices is still intensively ongoing; the papers [16, 17, 21, 24, 25] may serve as examples of the latest developments in the theory of these indices.

Iranmanesh et al. [10, 15] defined the multiplicative versions of the Zagreb indices. The first and second multiplicative Zagreb indices are defined, respectively, as

$$\mathcal{M}_1(G) = \prod_{ab \in E(G)} \left[d(a) + d(b) \right] \tag{1}$$

and

$$\mathcal{M}_2(G) = \prod_{ab \in E(G)} d(a) \, d(b) \,. \tag{2}$$

Eventually, these degree-based graph invariants attracted much attention and were studied by several researchers. See, for example, [34] for extremal problems in the classes of trees, unicyclic graphs, and bicyclic graphs; [9] for the trees with the first fourteen smallest multiplicative Zagreb indices; and [4] for a study of these indices on graph transformations. For more details, see [3, 7, 19, 22, 23, 26, 29–33, 35].

Recently, Kulli et al. [20] defined the general versions of the multiplicative Zagreb indices as

$$\mathcal{M}_1^{\alpha}(G) = \prod_{ab \in E(G)} \left[d(a) + d(b) \right]^{\alpha} \tag{3}$$

and

$$\mathcal{M}_2^{\alpha}(G) = \prod_{ab \in E(G)} \left[d(a) \, d(b) \right]^{\alpha},\tag{4}$$

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where α is a real number, $\alpha \neq 0$. We can see that $\mathcal{M}_1^{\alpha}(G) = (\mathcal{M}_1(G))^{\alpha}$ and $\mathcal{M}_2^{\alpha}(G) = (\mathcal{M}_2(G))^{\alpha}$. Various extremal problems on the general multiplicative Zagreb indices were examined by both mathematicians and chemists. See, for example, [1] for their investigation over graphs with a small number of cycles; [27] for a study over trees; and [28] for an investigation over graphs with a given clique number. For some recent works on general multiplicative Zagreb indices, see [8, 18, 27]. Needless to say, for $\alpha = 1$, the general multiplicative Zagreb indices (3) and (4) reduce to their ordinary values, Eqs. (1) and (2). Therefore, the results stated in the subsequent section also directly apply to the ordinary multiplicative Zagreb indices.

In this paper, we obtain bounds on the first and second general multiplicative Zagreb indices of trees with a fixed maximum vertex degree and characterize the respective extremal trees.

2. Main results

A *rooted tree* is a tree together with a special vertex chosen as the *root* of the tree. A vertex of a tree of degree one is said to be a *leaf*. A *branching vertex* of a tree is any vertex of degree greater than two.

A tree with exactly one branching vertex is called a *spider*. The branching vertex of a spider T is its *center*. A *leg* of a spider is a path from its center to a leaf. A star is a spider whose all legs have length one. Also a path can be considered to be a spider with one or two legs.

In this section, T denotes a rooted tree with root a where $d(a) = \Delta$ and $N(a) = \{a_1, a_2, \ldots, a_{\Delta}\}$. For positive integers n and Δ , let $\mathcal{T}_{n,\Delta}$ be the set of all trees with n vertices and maximum degree Δ .

Lemma 2.1. Let $T \in \mathcal{T}_{n,\Delta}$. Let b be a branching vertex of T with maximum distance to a. If such a vertex does exist, then there is a tree $T' \in \mathcal{T}_{n,\Delta}$ such that $\mathcal{M}_i^{\alpha}(T') > \mathcal{M}_i^{\alpha}(T)$ when $\alpha < 0$ and $\mathcal{M}_i^{\alpha}(T') < \mathcal{M}_i^{\alpha}(T)$ when $\alpha > 0$, where i = 1, 2.

Proof. Let $b \neq a$ be a vertex of T with $d(b) = \beta \ge 3$ and let $N(b) = \{b_1, b_2, \dots, b_{\beta-1}, b_\beta\}$ where b_β lies on the (a, b)-path of T. By our assumption, we have $d(b_i) \in \{1, 2\}$ for $1 \le i \le \beta - 1$. We distinguish the following cases.

Case 1. *b* is adjacent to at least two leaves.

We can assume that b_1 and b_2 are leaves. Let $T' = (T - \{bb_1\}) \cup \{b_1b_2\}$. Then

$$\begin{aligned} \frac{\mathcal{M}_{1}^{\alpha}(T)}{\mathcal{M}_{1}^{\alpha}(T')} &= \frac{(d(b_{1}) + d(b))^{\alpha}(d(b_{2}) + d(b))^{\alpha} \prod_{i=3}^{\beta} (d(b_{i}) + d(b))^{\alpha}}{(d_{T'}(b_{1}) + d_{T'}(b_{2}))^{\alpha}(d_{T'}(b_{2}) + d_{T'}(b))^{\alpha} \prod_{i=3}^{\beta} (d_{T'}(b_{i}) + d_{T'}(b))^{\alpha}} \\ &= \frac{(\beta + 1)^{\alpha}(\beta + 1)^{\alpha} \prod_{i=3}^{\beta} (d(b_{i}) + \beta)^{\alpha}}{3^{\alpha}(\beta + 1)^{\alpha} \prod_{i=3}^{\beta} (d(b_{i}) + \beta - 1)^{\alpha}} = \left(\frac{\beta + 1}{3}\right)^{\alpha} \prod_{i=3}^{\beta} \left(\frac{d(b_{i}) + \beta}{d(b_{i}) + \beta - 1}\right)^{\alpha} \end{aligned}$$

Since $\beta \geq 3$, then $\frac{\beta+1}{3} > 1$. Also $\frac{d(b_i)+\beta}{d(b_i)+\beta-1} > 1$ for $3 \leq i \leq \beta$. Therefore, if $\alpha > 0$, then $\mathcal{M}_1^{\alpha}(T) > \mathcal{M}_1^{\alpha}(T')$ and if $\alpha < 0$, then $\mathcal{M}_1^{\alpha}(T) < \mathcal{M}_1^{\alpha}(T')$.

$$\frac{\mathcal{M}_{2}^{\alpha}(T)}{\mathcal{M}_{2}^{\alpha}(T')} = \frac{(d(b_{1})d(b))^{\alpha}(d(b_{2})d(b))^{\alpha}\prod_{i=3}^{\beta}(d(b_{i})d(b))^{\alpha}}{(d_{T'}(b_{1})d_{T'}(b_{2}))^{\alpha}(d_{T'}(b_{2})d_{T'}(b))^{\alpha}\prod_{i=3}^{\beta}(d_{T'}(b_{i})d_{T'}(b))^{\alpha}} \\
= \frac{\beta^{\alpha}\beta^{\alpha}\prod_{i=3}^{\beta}(\beta d(b_{i}))^{\alpha}}{2^{\alpha}(2\beta-2)^{\alpha}\prod_{i=3}^{\beta}((\beta-1)d(b_{i}))^{\alpha}} \\
= \frac{\beta^{\alpha\beta}}{4^{\alpha}(\beta-1)^{\alpha(\beta-1)}} = \left(\frac{\beta^{\beta}}{4(\beta-1)^{\beta-1}}\right)^{\alpha}.$$

If $\beta \geq 4$, then

$$\frac{\beta^{\beta}}{4(\beta-1)^{\beta-1}} = \frac{\beta}{4} (\frac{\beta}{\beta-1})^{\beta-1} > 1.$$

Now, let $\beta = 3$. Then

$$\frac{\beta^{\beta}}{4(\beta-1)^{\beta-1}}=\frac{27}{16}>1.$$

Therefore, if $\alpha > 0$, then $\mathcal{M}_2^{\alpha}(T) > \mathcal{M}_2^{\alpha}(T')$ and if $\alpha < 0$, then $\mathcal{M}_2^{\alpha}(T) < \mathcal{M}_2^{\alpha}(T')$.

Case 2. *b* is adjacent to exactly one leaf.

Assume that b_1 is the unique leaf and $bc_1c_2 \dots c_\ell$ is a path in T for $\ell \ge 2$ and $b_2 = c_1$. Let $T' = (T - \{bb_1\}) \cup \{b_1c_\ell\}$. Then

$$\frac{\mathcal{M}_{1}^{\alpha}(T)}{\mathcal{M}_{1}^{\alpha}(T')} = \frac{(d(b_{1}) + d(b))^{\alpha}(d(c_{\ell}) + d(c_{\ell-1}))^{\alpha} \prod_{i=2}^{\beta} (d(b_{i}) + d(b))^{\alpha}}{(d_{T'}(b_{1}) + d_{T'}(c_{\ell}))^{\alpha}(d_{T'}(c_{\ell}) + d_{T'}(c_{\ell-1}))^{\alpha} \prod_{i=2}^{\beta} (d_{T'}(b_{i}) + d_{T'}(b))^{\alpha}}$$
$$= \frac{(\beta + 1)^{\alpha} 3^{\alpha} \prod_{i=2}^{\beta} (d(b_{i}) + \beta)^{\alpha}}{3^{\alpha} 4^{\alpha} \prod_{i=2}^{\beta} (d(b_{i}) + \beta - 1)^{\alpha}} = \left(\frac{\beta + 1}{4}\right)^{\alpha} \prod_{i=2}^{\beta} \left(\frac{d(b_{i}) + \beta}{d(b_{i}) + \beta - 1}\right)^{\alpha}.$$

Since $\beta \geq 3$, then $\frac{\beta+1}{4} \geq 1$. Also $\frac{d(b_i)+\beta}{d(b_i)+\beta-1} > 1$ for $2 \leq i \leq \beta$. Therefore, if $\alpha > 0$, then $\mathcal{M}_1^{\alpha}(T) > \mathcal{M}_1^{\alpha}(T')$ and if $\alpha < 0$, then $\mathcal{M}_1^{\alpha}(T) < \mathcal{M}_1^{\alpha}(T')$.

$$\frac{\mathcal{M}_{2}^{\alpha}(T)}{\mathcal{M}_{2}^{\alpha}(T')} = \frac{(d(b_{1})d(b))^{\alpha}(d(c_{\ell})d(c_{\ell-1}))^{\alpha}\prod_{i=2}^{\beta}(d(b_{i})d(b))^{\alpha}}{(d_{T'}(b_{1})d_{T'}(c_{\ell}))^{\alpha}(d_{T'}(c_{\ell})d_{T'}(c_{\ell-1}))^{\alpha}\prod_{i=2}^{\beta}(d_{T'}(b_{i})d_{T'}(b))^{\alpha}}$$

$$=\frac{\beta^{\alpha}2^{\alpha}\prod_{i=2}^{\beta}(\beta d(b_i))^{\alpha}}{2^{\alpha}4^{\alpha}\prod_{i=2}^{\beta}((\beta-1)d(b_i))^{\alpha}}=\frac{\beta^{\alpha\beta}}{4^{\alpha}(\beta-1)^{\alpha(\beta-1)}}=\left(\frac{\beta^{\beta}}{4(\beta-1)^{\beta-1}}\right)^{\alpha}.$$

In the same way as in Case 1, if $\alpha > 0$, then $\mathcal{M}_2^{\alpha}(T) > \mathcal{M}_2^{\alpha}(T')$ and if $\alpha < 0$, then $\mathcal{M}_2^{\alpha}(T) < \mathcal{M}_2^{\alpha}(T')$.

Case 3. All vertices adjacent to b, except b_{β} , have degree two.

Let $bc_1c_2 \dots c_t$, $bd_1d_2 \dots d_\ell$ be two paths in T, such that $\ell, t \ge 2$, $b_1 = c_1$ and $b_2 = d_1$. Let T' be the tree constructed from $T - \{c_1, c_2, \dots, c_t\}$ by attaching the path $d_\ell c_1 c_2 \dots c_t$. Then $\mathcal{M}_1^{\alpha}(T)/\mathcal{M}_1^{\alpha}(T')$ is equal to

$$\frac{(d(b_1) + d(b))^{\alpha}(d(b_2) + d(b))^{\alpha}(d(d_{\ell}) + d(d_{\ell-1}))^{\alpha} \prod_{i=3}^{\beta} (d(b_i) + d(b))^{\alpha}}{(d_{T'}(b_2) + d_{T'}(b))^{\alpha}(d_{T'}(b_1) + d_{T'}(d_{\ell}))^{\alpha}(d_{T'}(d_{\ell}) + d_{T'}(d_{\ell-1}))^{\alpha} \prod_{i=3}^{\beta} (d_{T'}(b_i) + d_{T'}(b))^{\alpha}} = \frac{(\beta + 2)^{\alpha} 3^{\alpha}(\beta + 2)^{\alpha} \prod_{i=3}^{\beta} (d(b_i) + \beta)^{\alpha}}{4^{\alpha} 4^{\alpha}(\beta + 1)^{\alpha} \prod_{i=3}^{\beta} (d(b_i) + \beta - 1)^{\alpha}} = \left(\frac{3(\beta + 2)^2}{16(\beta + 1)}\right)^{\alpha} \prod_{i=3}^{\beta} \left(\frac{d(b_i) + \beta}{d(b_i) + \beta - 1}\right)^{\alpha}.$$

Since $\beta \geq 3$, then $\frac{3(\beta+2)^2}{16(\beta+1)} \geq 1$. Also $\frac{d(b_i)+\beta}{d(b_i)+\beta-1} > 1$ for $3 \leq i \leq \beta$. Therefore, if $\alpha > 0$, then $\mathcal{M}_1^{\alpha}(T) > \mathcal{M}_1^{\alpha}(T')$ and if $\alpha < 0$, then $\mathcal{M}_1^{\alpha}(T) < \mathcal{M}_1^{\alpha}(T')$.

$$\frac{\mathcal{M}_{2}^{\alpha}(T)}{\mathcal{M}_{2}^{\alpha}(T')} = \frac{(d(b_{1})d(b))^{\alpha}(d(d_{\ell})d(d_{\ell-1}))^{\alpha}\prod_{i=2}^{\beta}(d(b_{i})d(b))^{\alpha}}{(d_{T'}(b_{1})d_{T'}(d_{\ell}))^{\alpha}(d_{T'}(d_{\ell})d_{T'}(d_{\ell-1}))^{\alpha}\prod_{i=2}^{\beta}(d(b_{i})d(b))^{\alpha}} \\
= \frac{(2\beta)^{\alpha}2^{\alpha}\prod_{i=2}^{\beta}(\beta d(b_{i}))^{\alpha}}{4^{\alpha}4^{\alpha}\prod_{i=2}^{\beta}((\beta-1)d(b_{i}))^{\alpha}} = \frac{\beta^{\alpha\beta}}{4^{\alpha}(\beta-1)^{\alpha(\beta-1)}} = \left(\frac{\beta^{\beta}}{4(\beta-1)^{\beta-1}}\right)^{\alpha}.$$

By the same way in the Case 1, if $\alpha > 0$, then $\mathcal{M}_2^{\alpha}(T) > \mathcal{M}_2^{\alpha}(T')$ and if $\alpha < 0$, then $\mathcal{M}_2^{\alpha}(T) < \mathcal{M}_2^{\alpha}(T')$.

Lemma 2.2. Let $T \in \mathcal{T}_{n,\Delta}$ be a spider with $\Delta \geq 3$, having at least one leg of length one and one leg of length greater than two. Then there exists a spider $T' \in \mathcal{T}_{n,\Delta}$, such that $\mathcal{M}_1^{\alpha}(T') > \mathcal{M}_1^{\alpha}(T)$ when $\alpha < 0$ and $\mathcal{M}_1^{\alpha}(T') < \mathcal{M}_1^{\alpha}(T)$ when $\alpha > 0$.

Proof. Let $d(a) = \Delta$ and $N(a) = \{a_1, a_2, \dots, a_{\Delta}\}$. Assume that $aa_1, ac_1c_2 \dots c_{\ell-1}c_\ell$ be two legs, such that $\ell \ge 3$ and $c_1 = a_2$. Let T' be the tree constructed from $T - \{c_\ell c_{\ell-1}\}$ by attaching the path $c_\ell a_1$. Then

$$\frac{\mathcal{M}_{1}^{\alpha}(T)}{\mathcal{M}_{1}^{\alpha}(T')} = \frac{(d(a_{1}) + d(a))^{\alpha}(d(c_{\ell}) + d(c_{\ell-1}))^{\alpha}(d(c_{\ell-1}) + d(c_{\ell-2}))^{\alpha}}{(d_{T'}(a_{1}) + d_{T'}(a))^{\alpha}(d_{T'}(a_{1}) + d_{T'}(c_{\ell}))^{\alpha}(d_{T'}(c_{\ell-1}) + d_{T'}(c_{\ell-2}))^{\alpha}} \\
= \frac{(\Delta + 1)^{\alpha} \, 3^{\alpha} \, 4^{\alpha}}{(\Delta + 2)^{\alpha} \, 3^{\alpha} \, 3^{\alpha}} = \left(\frac{4(\Delta + 1)}{3(\Delta + 2)}\right)^{\alpha}.$$

Since $\Delta \geq 3$, then $\frac{4(\Delta+1)}{3(\Delta+2)} > 1$. Therefore, if $\alpha > 0$, then $\mathcal{M}_1^{\alpha}(T) > \mathcal{M}_1^{\alpha}(T')$ and if $\alpha < 0$, then $\mathcal{M}_1^{\alpha}(T) < \mathcal{M}_1^{\alpha}(T')$. Lemma 2.3. Let $T \in \mathcal{T}_{n,\Delta}$ be a spider. Then

$$\mathcal{M}_2^{\alpha}(T) = \Delta^{\Delta \alpha} \, 4^{(n-\Delta-1)\alpha}$$

Proof. Let $d(a) = \Delta$ and $N(a) = \{a_1, a_2, \dots, a_{\Delta}\}$. Also, let $d(a_1) = \dots = d(a_k) = 1$ and $d(a_{k+1}) = \dots = d(a_{\Delta}) = 2$. Then $\mathcal{M}_2^{\alpha}(T) = \prod_{xy \in E(G)} \left[d(x) \, d(y) \right]^{\alpha} = \Delta^{k\alpha} \left(2\Delta \right)^{(\Delta - k)\alpha} 2^{(\Delta - k)\alpha} \, 4^{(n-2\Delta + k-1)\alpha} = \Delta^{\Delta\alpha} \, 4^{(n-\Delta - 1)\alpha}.$

Theorem 2.1. For $T \in \mathcal{T}_{n,\Delta}$,

$$\mathcal{M}_{1}^{\alpha}(T) \leqslant \begin{cases} (3\Delta+6)^{\alpha\Delta} 4^{\alpha(n-2\Delta-1)} & \text{if } \Delta \leq \frac{n-1}{2} \\ \\ (\Delta+1)^{\alpha(2\Delta-n+1)} (3\Delta+6)^{\alpha(n-\Delta-1)} & \text{if } \Delta > \frac{n-1}{2} \end{cases}$$

when $\alpha < 0$, and

$$\mathcal{M}_{1}^{\alpha}(T) \geqslant \begin{cases} (3\Delta+6)^{\alpha\Delta} 4^{\alpha(n-2\Delta-1)} & \text{if } \Delta \leq \frac{n-1}{2} \\ (\Delta+1)^{\alpha(2\Delta-n+1)} (3\Delta+6)^{\alpha(n-\Delta-1)} & \text{if } \Delta > \frac{n-1}{2} \end{cases}$$

when $\alpha > 0$. Equality holds if and only if T is a spider whose all legs have length at most two or all legs have length at least two.

Proof. Let $\alpha < 0$ (respectively, $\alpha > 0$) and $T_1 \in \mathcal{T}_{n,\Delta}$ such that $\mathcal{M}_1^{\alpha}(T_1) \leq \mathcal{M}_1^{\alpha}(T)$ (respectively, $\mathcal{M}_1^{\alpha}(T_1) \geq \mathcal{M}_1^{\alpha}(T)$) for all $T \in \mathcal{T}_{n,\Delta}$. If $\Delta = 2$, then T is a path of order n and $\mathcal{M}_1^{\alpha}(P_n) = 9^{\alpha}4^{\alpha(n-3)}$. Let $\Delta \geq 3$. By the choice of T_1 , we conclude from Lemma 2.1, that T_1 is a spider with center a. It follows from Lemma 2.2 and the choice of T_1 that all legs of T_1 either have length at most two or have length at least two. First let all legs of T_1 have length at least two. Then clearly $\Delta \leq \frac{n-1}{2}$ and

$$\mathcal{M}_1^{\alpha}(T_1) = (3\Delta + 6)^{\alpha \Delta} 4^{\alpha(n-2\Delta-1)}$$

as desired. Now let all legs of T_1 have length at most two. Considering the above case, we may assume that T_1 has a leg of length 1. If T_1 is a star, then the result is immediate. Assume that T_1 is not a star. Then the number of leaves adjacent to a is $2\Delta + 1 - n$ and hence

$$\mathcal{M}_{1}^{\alpha}(T_{1}) = (\Delta + 1)^{\alpha(2\Delta - n + 1)} (3\Delta + 6)^{\alpha(n - \Delta - 1)}.$$

This completes the proof.

Theorem 2.2. For $T \in \mathcal{T}_{n,\Delta}$,

 $\mathcal{M}_2^{\alpha}(T) \le \Delta^{\Delta \alpha} \, 4^{(n-\Delta-1)\alpha},$

when $\alpha < 0$, and

$$\mathcal{M}_{2}^{\alpha}(T) > \Delta^{\Delta \alpha} \, 4^{(n-\Delta-1)\alpha}.$$

when $\alpha > 0$. Equality holds if and only if T is a spider.

Proof. Let $\alpha < 0$ (respectively, $\alpha > 0$) and $T_1 \in \mathcal{T}_{n,\Delta}$ such that $\mathcal{M}_2^{\alpha}(T_1) \leq \mathcal{M}_2^{\alpha}(T)$ (respectively, $\mathcal{M}_2^{\alpha}(T_1) \geq \mathcal{M}_2^{\alpha}(T)$). By the choice of T_1 , we conclude from Lemma 2.1, that T_1 is a spider with center a. It follows from Lemma 2.3,

$$\mathcal{M}_2^{\alpha}(T_1) = \Delta^{\Delta \alpha} \, 4^{(n-\Delta-1)\alpha}.$$

Therefore, $\mathcal{M}_{2}^{\alpha}(T) \leq \Delta^{\Delta \alpha} 4^{(n-\Delta-1)\alpha}$ when $\alpha < 0$, and $\mathcal{M}_{2}^{\alpha}(T) \geq \Delta^{\Delta \alpha} 4^{(n-\Delta-1)\alpha}$ when $\alpha > 0$

By Theorem 2.1, we have the next corollary.

Corollary 2.1. Let T be a molecular tree of order n and maximum degree Δ , $3 \le \Delta \le 4$. If $\Delta = 3$ and $n \ge 7$, then

$$\mathcal{M}_1^{\alpha}(T) \le 15^{3\alpha} \, 4^{\alpha(n-7)}$$

when $\alpha < 0$, and

when $\alpha > 0$. Also, if $\Delta = 4$ and $n \ge 9$, then

 $\mathcal{M}_1^{\alpha}(T) \le 18^{4\alpha} \, 4^{\alpha(n-9)},$

 $\mathcal{M}_1^{\alpha}(T) \ge 15^{3\alpha} \, 4^{\alpha(n-7)},$

when $\alpha < 0$, and

$$\mathcal{M}_1^{\alpha}(T) \ge 18^{4\alpha} \, 4^{\alpha(n-9)}.$$

when $\alpha > 0$. Equality holds if and only if T is a spider whose all legs have length at least two.

By Theorem 2.2, we have the next corollary.

Corollary 2.2. Let T be a molecular tree of order n and maximum degree Δ , $3 \le \Delta \le 4$. If $\Delta = 3$, then

$$\mathcal{M}_2^{\alpha}(T) < 3^{3\alpha} \, 4^{(n-3)\alpha}$$

when $\alpha < 0$, and

$$\mathcal{M}_2^{\alpha}(T) \ge 3^{3\alpha} \, 4^{(n-4)\alpha}$$

when $\alpha > 0$. Also, if $\Delta = 4$, then

$$\mathcal{M}_2^{\alpha}(T) \le 4^{(n-1)\alpha}$$

when $\alpha < 0$, and

$$\mathcal{M}_2^{\alpha}(T) \ge 4^{(n-1)\alpha},$$

when $\alpha > 0$. Equality holds if and only if T is a spider.

The following observation is immediately achieved from the definitions of \mathcal{M}_1^{α} and \mathcal{M}_2^{α} indices.

Observation 2.1. Let G be a graph and $e \notin E(G)$. Then $\mathcal{M}_1^{\alpha}(G+e) > \mathcal{M}_1^{\alpha}(G)$, $\mathcal{M}_2^{\alpha}(G+e) > \mathcal{M}_2^{\alpha}(G)$ when $\alpha > 0$ and $\mathcal{M}_1^{\alpha}(G+e) < \mathcal{M}_1^{\alpha}(G)$, $\mathcal{M}_2^{\alpha}(G+e) < \mathcal{M}_2^{\alpha}(G)$ when $\alpha < 0$.

Applications of Theorems 2.1, 2.2, and Observation 2.1 provide the next result.

Theorem 2.3. If G is a graph of order n with maximum degree Δ , then

$$\mathcal{M}_{1}^{\alpha}(G) \leqslant \begin{cases} (3\Delta+6)^{\alpha\Delta} 4^{\alpha(n-2\Delta-1)} & \text{if } \Delta \leq \frac{n-1}{2} \\ (\Delta+1)^{\alpha(2\Delta-n+1)} (3\Delta+6)^{\alpha(n-\Delta-1)} & \text{if } \Delta > \frac{n-1}{2}, \end{cases}$$

when $\alpha < 0$, and

$$\mathcal{M}_{1}^{\alpha}(G) \geqslant \begin{cases} (3\Delta+6)^{\alpha\Delta} 4^{\alpha(n-2\Delta-1)} & \text{if } \Delta \leq \frac{n-1}{2} \\ (\Delta+1)^{\alpha(2\Delta-n+1)} (3\Delta+6)^{\alpha(n-\Delta-1)} & \text{if } \Delta > \frac{n-1}{2}, \end{cases}$$

when $\alpha > 0$. Equality holds if and only if G is a spider whose all legs have length at most two or all legs have length at least two.

Theorem 2.4. If G be a graph of order n with maximum degree Δ , then

$$\mathcal{M}_2^{\alpha}(G) \le \Delta^{\Delta \alpha} \, 4^{(n-\Delta-1)\alpha}$$

when $\alpha < 0$, and

$$\mathcal{M}_{2}^{\alpha}(G) > \Delta^{\Delta \alpha} \, 4^{(n-\Delta-1)\alpha},$$

when $\alpha > 0$. Equality holds if and only if G is a spider.

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