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On Extremal Modified Zagreb Indices of Trees

Chang Liu, Jianping Li*, Yingui Pan

College of Liberal Arts and Sciences, National University of Defense Technology
Changsha, Hunan, 410073, P. R. China

clnudt19@126.com, lijianping65@nudt.edu.cn, panygui@163.com

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Abstract

For a molecular graph, the modified first Zagreb (${}^mM_1$) index is equal to the sum of the reciprocal of the squares of the vertex degrees, and the modified second Zagreb (${}^mM_2$) index is equal to the sum of the reciprocal of the products of degrees of pairs of adjacent vertices. In this paper, lower and upper bounds on ${}^mM_1$ index of trees are presented and the extremal trees are characterized. In addition, a lower bound on ${}^mM_2$ index of trees is determined and the extremal trees are also characterized. Finally, lower and upper bounds for the ${}^mM_1$ index of trees with a given domination number are determined and the extremal trees are characterized as well.

1 Introduction

First and second Zagreb indices [6], which were introduced in the 1970s and originated from chemical researches on total π-electron energy of conjugated molecules, are two important vertex-degree-based graph invariants. Over the past four decades, Zagreb indices have been extensively studied, and lots of their mathematical properties have been investigated, see [1, 4, 9, 11, 16, 24, 27]. Nowadays, these indices and their variants are widely used to study molecular complexity [14, 21, 22], ZE-isomerism [10], and chirality [8].

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, let d_v denote the degree of the vertex v. The (original) first and second Zagreb indices are defined as below:

$$M_1(G) = \sum_{v \in V(G)} (d_v)^2,$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

However, Zagreb indices have a problem that their contributing parts give larger weights to inner (interior) vertices and edges and smaller weights to outer (terminal) vertices and edges of a graph. Since the outer vertices and bonds are related to a larger part of the molecular surface, it is possible to describe the physical, chemical and biological properties of molecules better. In order to make up for the shortcomings of Zagreb indices, researchers tried to consider the modified first (${}^mM_1$) and second (${}^mM_2$) Zagreb indices, which are defined as below [20]:

$${}^mM_1(G) = \sum_{v \in V(G)} \frac{1}{(d_v)^2},$$

and

$${}^mM_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

It is worth noting that there is an analogy between the method of creating a modified Zagreb index based on the (original) Zagreb index, and the method of creating a Harary index [15, 23] from the Wiener index [25]. So far, there have been many published bibliography and papers summarized the Zagreb indices and its various modifications [7, 18, 19, 28]. In 2011, Hao [13] discussed the relations between the Zagreb indices and the modified Zagreb indices, and presented some mathematical properties of them.

Meanwhile, the extremal graphs of topological indices and the connection between these indices and domination number have also attracted a lot of interest [3, 12, 17]. In 2016, Borovićanin and Furtula [2] gave the strict upper bounds for Zagreb indices of trees in terms of domination number and a lower bound for the first Zagreb index (M_1) of trees in terms of domination number and characterized the corresponding extremal graphs. Two years later, Wang et al. [26] determined upper and lower bounds of first and second multiplicative Zagreb index on trees with a given domination number.

Motivated by [2] and [26], we aim to consider the similar issues regarding modified first (${}^mM_1$) and second (${}^mM_2$) Zagreb indices in this paper. Let T be a tree with vertex set $V(T)$ and edge set $E(T)$. Given a vertex $v \in V(T)$, the set of neighbors of v is $N(v) = \{u \in V(T) | \ uv \in E(T)\}$. The maximum vertex degree in T is denoted by Δ. A vertex $v \in V(T)$ with $d_v = 1$ is called a pendent vertex. The diameter of a tree is the longest path between two pendent vertices. The domination set of a graph G, denoted by D, is a subset of $V(G)$ such that each vertex of $V(G)\backslash D$ is adjacent to at least one vertex of D. Domination number $\gamma(G)$ of the graph G is the minimum cardinality among any dominating set D of the graph G.

Based on the above considerations, the rest of this paper is organized as below. In Section 2, lower and upper bounds on ${}^mM_1$ index of trees are presented and the extremal trees are characterized. In addition, a lower bound on ${}^mM_2$ index of trees is determined and the extremal trees are also characterized. In Section 3, lower and upper bounds for the ${}^mM_1$ index of trees in terms of the domination number are determined and the extremal trees are characterized as well.

2 Bounds for modified Zagreb indices of trees

To obtain bounds for modified first Zagreb indices, we now consider a graph transformation: let T and T' be n-vertices trees as depicted in Figure 1, where T' is obtained by moving a pendent vertex $v_4 \in V(T)$ such that it is adjacent another pendent vertex $v_2 \in V(T)$. Obviously, one can see that $d(v_1') = d(v_1)$, $d(v_2') = 2$, $d(v_3') = d(v_3) - 1$ and $d(v_4') = d(v_4) = 1$.

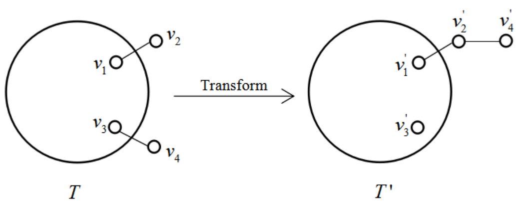

Figure 1. Graph transform $T \to T'$.

Lemma 1. *Let T and T' be n-vertex trees as depicted in Figure 1 with $d_{v_2} = d_{v_4} = 1$ and*

$d_{v_3} \geq 2$. *Then*

$$^{m}M_1(T) \geq ^{m} M_1(T')\,,$$

with equality holding if and only if $d_{v_3} = 2$.

Proof. It's easy to calculate that

$$^{m}M_1(T) - ^{m}M_1(T') = \frac{1}{(d_{v_3})^2} - \frac{1}{(d_{v_3}-1)^2} + \frac{3}{4} \geq \frac{1}{4} - 1 + \frac{3}{4} = 0$$

with equality holding if and only if $d_{v_3} = 2$. ∎

By Lemma 1, we can get bounds for $^{m}M_1$ and characterize their extremal trees as below.

Theorem 2. *Let T be a tree with n vertices. Then*

(i) $^{m}M_1(T) \geq \dfrac{n+6}{4}$, *with equality holding if and only if* $T \cong P_n$,

(ii) $^{m}M_1(T) \leq n - 1 + (\dfrac{1}{n-1})^2$, *with equality holding if and only if* $T \cong S_n$.

Proof. By continuing the above transformation $T \to T'$, we can move all vertices of T until the desired path P_n is generated, which will always reduce the $^{m}M_1$-value. In addition, for a n-vertices tree, the star S_n has the largest $^{m}M_1$-value (see [13]). ∎

Next we give the lower bound of the modified second Zagreb index by induction hypothesis. The upper bound of the $^{m}M_2$ cannot be obtained through a simple discussion. But by analogy and simple verification, we propose a conjecture in the following.

Theorem 3. *Let T be a tree with n vertices. Then $^{m}M_2(T) \geq 1$, with equality holding if and only if $T \cong S_n$.*

Proof. For $T \cong S_3$ ($T \cong P_3$), $T \cong P_4$ and $T \cong S_4$, we have $^{m}M_2(S_3) = 1$, $^{m}M_2(P_4) = \frac{5}{4} > 1$, and $^{m}M_2(S_4) = 1$. Suppose that results hold for any trees with $n-1$ vertices. If $|V(T)| = n$, we take a diameter $v_1 v_2 \cdots v_l$ ($l \geq 4$) in T. Let $T_1 = T - \{v_1\}$, then we obtain

$$\begin{aligned} ^{m}M_2(T) &= ^{m}M_2(T_1) - (\frac{1}{d_{v_2}-1} - \frac{1}{d_{v_2}})(d_{v_2} - 2 + \frac{1}{d_{v_3}}) + \frac{1}{d_{v_2}} \\ &\geq 1 - (\frac{1}{d_{v_2}-1} - \frac{1}{d_{v_2}})(d_{v_2} - 2 + \frac{1}{2}) + \frac{1}{d_{v_2}} \qquad (1) \\ &= 1 + \frac{1}{2}(\frac{1}{d_{v_2}-1} - \frac{1}{d_{v_2}}) > 1\,. \end{aligned}$$

Equality holds in (1) if and only if $^{m}M_2(T_1) = 1$ and $d_{v_3} = 1$, which implies that $T \cong S_n$. ∎

Definition 1. Let $\mathcal{F}$ be a set of trees. The path P_n all belong to $\mathcal{F}$, and then we construct new graphs in the set on following way. If $T' \in \mathcal{F}$ satisfies that there exists $v \in V(T')$ such that $N\{u_1, u_2, \cdots, u_{d_v}\}$, $d_{u_1} = d_{u_2} = \cdots = d_{u_{d_v}} = 2$, and we take any path $P_t = w_1 w_2 \cdots w_t$ with $t \geq 2$, then the tree T such that $V(T) = V(T') \cup V(P_t)$ and $E(T) = E(T') \cup E(P_t) \cup \{vw_1\}$, belongs to $\mathcal{F}$.

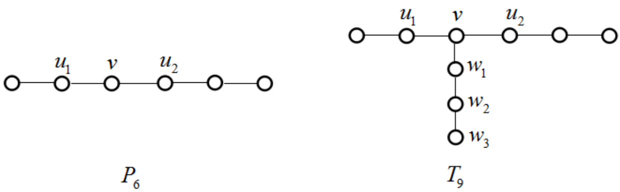

Figure 2. Two trees from the set $\mathcal{F}$.

Conjecture 2.1. Let T be a tree on n vertices. Then ${}^mM_2(T) \leq \dfrac{n+1}{4}$, with equality holding if and only if $T \in \mathcal{F}$.

3 Bounds for the modified first Zagreb index of trees with a given domination number

In this section, we will discuss sharp bounds for the modified first Zagreb index (${}^mM_1$) of trees in terms of domination number and characterize their extremal graphs. First we consider the lower bound of ${}^mM_1$.

Note that $1 \leq \gamma(T) \leq \frac{n}{2}$ for any n-vertices trees, and $\gamma(T) = 1$ if and only if $T \cong S_n$. By Theorem 2, one can see that ${}^mM_1(T)$ attain its lower bound when $T \cong P_n$, and in this case, $\gamma = \lceil \frac{n}{3} \rceil$. Based on the above statement, it's not difficult to find that the structure of extremal trees of ${}^mM_1(T)$ may differ for $1 \leq \gamma \leq \frac{n}{3}$ and $\frac{n}{3} < \gamma \leq \frac{n}{2}$.

Assume that D is a minimum dominating set of the n-vertices tree T. The domination number is denoted by γ, where $\gamma = \gamma(T) = |D|$. Let $\overline{D} = V(T) \backslash D$, and then $E_1(T) = \left\{uv \in E(T) |\ u \in D,\ v \in \overline{D}\right\}$, $E_2(T) = \{uv \in E(T) |\ u \in D,\ v \in D\}$, $E_3(T) = \left\{uv \in E(T) |\ u \in \overline{D},\ v \in \overline{D}\right\}$. The number of edges in $E_1(T)$, $E_2(T)$, $E_3(T)$ are written by m_1, m_2, and m_3, respectively. Obviously, the following equations always hold for a tree T.

$$\begin{cases} m_1+m_2+m_3=n-1, \\ \sum\limits_{v\in D} d_v = m_1+2m_2, \\ \sum\limits_{\overline{v}\in \overline{D}} d_{\overline{v}} = m_1+2m_3. \end{cases} \tag{2}$$

Combining with (2) and the definition of ${}^mM_1$, we get

$${}^mM_1(T) = \sum_{v\in D}\left(\frac{1}{d_v}\right)^2 + \sum_{\overline{v}\in\overline{D}}\left(\frac{1}{d_{\overline{v}}}\right)^2. \tag{3}$$

The formula shown in (3) attains the minimum if $d_v \in \left\{\lfloor\frac{m_1+2m_2}{\gamma}\rfloor, \lceil\frac{m_1+2m_2}{\gamma}\rceil\right\}$ for each $v\in D$ while $d_{\overline{v}} \in \left\{\lfloor\frac{m_1+2m_3}{n-\gamma}\rfloor, \lceil\frac{m_1+2m_3}{n-\gamma}\rceil\right\}$ for each $\overline{v}\in\overline{D}$. Moreover, each vertex in $\overline{D}$ is adjacent to at least one vertex of D, then $m_1 \geq n-\gamma$. From (2), it's easy to get that $m_2+m_3 \leq \gamma-1$, implying

$$|m_2-m_3| \leq \gamma-1\ . \tag{4}$$

Let $m_1+2m_2 = k_1\gamma + r_1$ and $m_1+2m_3 = k_2(n-\gamma)+r_2$, where $k_1 = \lfloor\frac{m_1+2m_2}{\gamma}\rfloor$, $r_1 = m_1+2m_2-\gamma\lfloor\frac{m_1+2m_2}{\gamma}\rfloor$, $k_2 = \lfloor\frac{m_1+2m_3}{n-\gamma}\rfloor$, and $r_2 = m_1+2m_3-(n-\gamma)\lfloor\frac{m_1+2m_3}{n-\gamma}\rfloor$. Based on previous considerations, one can see that the formula shown in (3) will attain the minimum if r_1 vertices in D have degree k_1+1, $\gamma-r_1$ vertices in D have degree k_1, r_2 vertices in $\overline{D}$ have degree k_2+1 and $(n-\gamma)-r_2$ vertices in $\overline{D}$ have degree k_2.

Thus,

$$\begin{aligned}\sum_{v\in D}\left(\frac{1}{d_v}\right)^2 &\geq r_1\left(\frac{1}{k_1+1}\right)^2 + (\gamma-r_1)\left(\frac{1}{k_1}\right)^2 \\ &= \left[(n-1+m_2-m_3) - \gamma\left\lfloor\frac{n-1+m_2-m_3}{\gamma}\right\rfloor\right] \\ &\times\left[\left(\frac{1}{\left\lfloor\frac{n-1+m_2-m_3}{\gamma}\right\rfloor+1}\right)^2 - \left(\frac{1}{\left\lfloor\frac{n-1+m_2-m_3}{\gamma}\right\rfloor}\right)^2\right] \\ &+\gamma\left(\left\lfloor\frac{n-1+m_2-m_3}{\gamma}\right\rfloor\right)^2,\end{aligned} \tag{5}$$

and

$$\sum_{\overline{v}\in\overline{D}}\left(\frac{1}{d_{\overline{v}}}\right)^2 \geq r_2\left(\frac{1}{k_2+1}\right)^2+(n-\gamma-r_2)\left(\frac{1}{k_2}\right)^2$$
$$=\left[(n-1+m_3-m_2)-(n-\gamma)\left\lfloor\frac{n-1+m_3-m_2}{n-\gamma}\right\rfloor\right]$$
$$\times\left[\left(\frac{1}{\left\lfloor\frac{n-1+m_3-m_2}{n-\gamma}\right\rfloor+1}\right)^2-\left(\frac{1}{\left\lfloor\frac{n-1+m_3-m_2}{n-\gamma}\right\rfloor}\right)^2\right] \tag{6}$$
$$+(n-\gamma)\left(\left\lfloor\frac{n-1+m_3-m_2}{n-\gamma}\right\rfloor\right)^2 .$$

Combining with (5) and (6), we have

$$\begin{aligned} {}^mM_1(T) \geq & \left[(n-1+m_2-m_3)-\gamma\left\lfloor\frac{n-1+m_2-m_3}{\gamma}\right\rfloor\right] \\ & \times\left[\left(\frac{1}{\left\lfloor\frac{n-1+m_2-m_3}{\gamma}\right\rfloor+1}\right)^2-\left(\frac{1}{\left\lfloor\frac{n-1+m_2-m_3}{\gamma}\right\rfloor}\right)^2\right] \\ & +\left[(n-1+m_3-m_2)-(n-\gamma)\left\lfloor\frac{n-1+m_3-m_2}{n-\gamma}\right\rfloor\right] \\ & \times\left[\left(\frac{1}{\left\lfloor\frac{n-1+m_3-m_2}{n-\gamma}\right\rfloor+1}\right)^2-\left(\frac{1}{\left\lfloor\frac{n-1+m_3-m_2}{n-\gamma}\right\rfloor}\right)^2\right]+\gamma\left(\left\lfloor\frac{n-1+m_2-m_3}{\gamma}\right\rfloor\right)^2 \\ & +(n-\gamma)\left(\left\lfloor\frac{n-1+m_3-m_2}{n-\gamma}\right\rfloor\right)^2 . \end{aligned} \tag{7}$$

In fact, the lower bound for the modified first Zagreb index can be determined by a function $g(m_2-m_3)$, and its domain of definition is given by (4). From (7), we get ${}^mM_1(T)\geq g(m_2-m_3)$. Next, we discuss the lower bound of ${}^mM_1$ in two categories.

Definition 2. Let $\mathcal{G}_1(n,\gamma)$ be a set of trees T with n vertices and domination number γ. For each $T\in\mathcal{G}_1(n,\gamma)$, T consists of the stars of orders $\lfloor\frac{n-\gamma}{\gamma}\rfloor$ and $\lceil\frac{n-\gamma}{\gamma}\rceil$ with exactly $\gamma-1$ pairs of adjacent pendent vertices in neighboring stars.

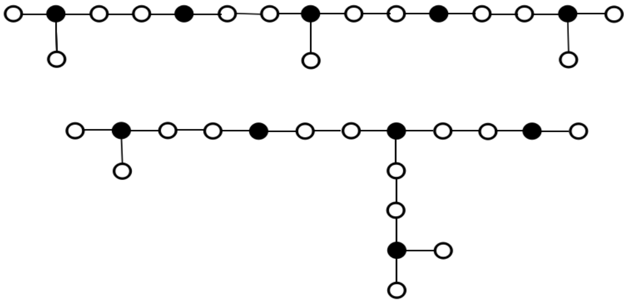

Figure 3. Two non-isomorphic trees from $\mathcal{G}_1(n,\gamma)$ with 18 vertices and 5 domination number.

Theorem 4. *Let T be a tree on n vertices with domination number γ, where $1 \le \gamma \le \frac{n}{3}$. Then we have*

$$
\begin{aligned}
{}^mM_1(T) \ge \left(n-\gamma\left\lfloor\frac{n-1}{\gamma}\right\rfloor\right)\left[\left(\frac{1}{\left\lfloor\frac{n-1}{\gamma}\right\rfloor}\right)^2-\left(\frac{1}{\left\lfloor\frac{n-1}{\gamma}\right\rfloor-1}\right)^2\right] \\
+\gamma\left(\frac{1}{\left\lfloor\frac{n-1}{\gamma}\right\rfloor-1}\right)^2+\left(n-\frac{5}{2}\gamma+\frac{3}{2}\right)\ .
\end{aligned}
\tag{8}
$$

Equality holds if and only if $T \in \mathcal{G}_1(n,\gamma)$.

Proof. For $T \cong P_3$, we have $\gamma = 1$ and ${}^mM_1(P_3) = (3-2)(\dfrac{1}{4}-1)+1+(3-\dfrac{5}{2}+\dfrac{3}{2}) = \dfrac{9}{4}$. Then we can suppose that $n > 3$. Note that $1 < \gamma \le \frac{n}{3}$, then we obtain $n-\gamma \ge \frac{2n}{3}$, and $\frac{\gamma-1}{n-\gamma} \le \frac{n-3}{2n} < \frac{1}{2}$. From (4), one can see that

$$1 = \frac{n-1+(1-\gamma)}{n-\gamma} \le \frac{n-1+(m_3-m_2)}{n-\gamma} \le \frac{n-1+(\gamma-1)}{n-\gamma} = 1+2\frac{\gamma-1}{n-\gamma} < 2,$$

consequently,

$$k_2 = \left\lfloor\frac{n-1+m_3-m_2}{n-\gamma}\right\rfloor = 1\ .$$

Furthermore, $\frac{n-1+(m_2-m_3)}{\gamma} \ge \frac{n-1+(1-\gamma)}{\gamma} = \frac{n-\gamma}{\gamma} \ge \frac{2n}{n} = 2$, implying $k_1 = \lfloor\frac{n-1+m_2-m_3}{\gamma}\rfloor$ ≥ 2. Based on the previous discussion, we can get the simplified formula of $g(m_2-m_3)$, that is

$$
\begin{aligned}
g(m_2-m_3) = &\left[\left(\frac{1}{k_1+1}\right)^2-\left(\frac{1}{k_1}\right)^2+\frac{3}{4}\right](m_2-m_3)+(n-\gamma k_1-1) \\
&\times\left[\left(\frac{1}{k_1+1}\right)^2-\left(\frac{1}{k_1}\right)^2\right]+\gamma\left(\frac{1}{k_1}\right)^2+\left(n-\frac{7}{4}\gamma+\frac{3}{4}\right).
\end{aligned}
\tag{9}
$$

Next, we need to consider two cases.

Case 1. $0 \leq m_2 - m_3 \leq \gamma - 1$.

In this case, we have $\frac{n-1}{\gamma-1} \leq \frac{n-1+m_2-m_3}{\gamma} \leq \frac{n-1}{\gamma} + \frac{\gamma-1}{\gamma} < \frac{n-1}{\gamma} + 1$. The following equations are easily to obtained.

$$k_1 = \lfloor \frac{n-1+m_2-m_3}{\gamma} \rfloor = \lfloor \frac{n-1}{\gamma} \rfloor, \qquad \text{for } 0 \leq m_2 - m_3 \leq \gamma \lfloor \frac{n-1}{\gamma} \rfloor + \gamma - n, \tag{10}$$

$$k_1 = \lfloor \frac{n-1+m_2-m_3}{\gamma} \rfloor = \lfloor \frac{n-1}{\gamma} \rfloor + 1, \quad \text{for } \gamma \lfloor \frac{n-1}{\gamma} \rfloor + \gamma - n + 1 \leq m_2 - m_3 \leq \gamma - 1. \tag{11}$$

Combining with (9), (10) and (11), one can see that the function $g(m_2 - m_3)$ increases for $\left[0, \gamma \lfloor \frac{n-1}{\gamma} \rfloor + \gamma - n\right]$ and $\left[\gamma \lfloor \frac{n-1}{\gamma} \rfloor + \gamma - n + 1, \gamma - 1\right]$. Therefore, the function $g(m_2 - m_3)$ may attain its minimum if $m_2 - m_3 = 0$ or $m_2 - m_3 = \gamma \lfloor \frac{n-1}{\gamma} \rfloor + \gamma - n + 1$. We have to calculate the following equation:

$$\begin{aligned} g(\gamma \lfloor \frac{n-1}{\gamma} \rfloor + \gamma - n + 1) - g(0) = & \left[\gamma \left\lfloor \frac{n-1}{\gamma} \right\rfloor + \gamma - (n-1)\right] \\ & \left[\left(\frac{1}{\left\lfloor \frac{n-1}{\gamma} \right\rfloor + 1}\right)^2 - \left(\frac{1}{\left\lfloor \frac{n-1}{\gamma} \right\rfloor}\right)^2 + \frac{3}{4}\right]. \end{aligned} \tag{12}$$

Note that $\frac{n-1}{\gamma} \geq \frac{3(n-1)}{n} \geq 2 + \frac{n-3}{n}$, implying $\lfloor \frac{n-1}{\gamma} \rfloor \geq 2$, then

$$\left[\left(\frac{1}{\left\lfloor \frac{n-1}{\gamma} \right\rfloor + 1}\right)^2 - \left(\frac{1}{\left\lfloor \frac{n-1}{\gamma} \right\rfloor}\right)^2 + \frac{3}{4}\right] \geq \left(\frac{1}{9} - \frac{1}{4} + \frac{3}{4}\right) = \frac{11}{18} > 0\ . \tag{13}$$

From (12) and (13), we have $g(0) < g(\gamma \lfloor \frac{n-1}{\gamma} \rfloor + \gamma - n + 1)$, then

$$g(0) = (n - \gamma \lfloor \frac{n-1}{\gamma} \rfloor - 1) \left[\left(\frac{1}{\lfloor \frac{n-1}{\gamma} \rfloor + 1}\right)^2 - \left(\frac{1}{\lfloor \frac{n-1}{\gamma} \rfloor}\right)^2\right] + \gamma \left(\frac{1}{\lfloor \frac{n-1}{\gamma} \rfloor}\right)^2 + \left(n - \frac{7}{4}\gamma + \frac{3}{4}\right).$$

Case 2. $-\gamma + 1 \leq m_2 - m_3 \leq 0$.

In this case, $\frac{n-1}{\gamma} - 1 \leq \frac{n-\gamma}{\gamma} \leq \frac{n-1+m_2-m_3}{\gamma} \leq \frac{n-1}{\gamma}$. Then by (4), we have

$$k_1 = \lfloor \frac{n-1+m_2-m_3}{\gamma} \rfloor = \lfloor \frac{n-1}{\gamma} \rfloor, \qquad \text{for } \gamma \lfloor \frac{n-1}{\gamma} \rfloor - n + 1 \leq m_2 - m_3 \leq 0, \tag{14}$$

$$k_1 = \lfloor \frac{n-1+m_2-m_3}{\gamma} \rfloor = \lfloor \frac{n-1}{\gamma} \rfloor - 1, \quad \text{for } 1 - \gamma \leq m_2 - m_3 \leq \gamma \lfloor \frac{n-1}{\gamma} \rfloor - n. \tag{15}$$

Similarly, combining with (9), (14) and (15), we conclude that the function $g(m_2 - m_3)$ attains its minimum if $m_2 - m_3 = \gamma \lfloor \frac{n-1}{\gamma} \rfloor - n + 1$ or $m_2 - m_3 = 1 - \gamma$. Thus, we let

$$g\left(\gamma\left\lfloor\frac{n-1}{\gamma}\right\rfloor-n+1\right)-g(1-\gamma)=-\left[(n-\gamma)-\gamma\lfloor\frac{n-1}{\gamma}\rfloor\right]$$
$$\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor-1}\right)^2+\frac{3}{4}\right].$$

Analogously, we have

$$\left[(n-\gamma)-\gamma\lfloor\frac{n-1}{\gamma}\rfloor\right]\leq 0,\quad \text{for } \gamma\geq 2, \tag{16}$$

and

$$\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor-1}\right)^2+\frac{3}{4}\right]\geq 0,\quad \text{for } \lfloor\frac{n-1}{\gamma}\rfloor\geq 2. \tag{17}$$

Briefly, $g(\gamma\lfloor\frac{n-1}{\gamma}\rfloor-n+1)-g(1-\gamma)\geq 0$, i.e., $g(1-\gamma)\leq g(\gamma\lfloor\frac{n-1}{\gamma}\rfloor-n+1)$. If the equality holds in (16), we get $\frac{n-\gamma}{\gamma}=\lfloor\frac{n-1}{\gamma}\rfloor$, which implies that only the relation (14) holds. In addition, the equality holds in (17) if and only if $\lfloor\frac{n-1}{\gamma}\rfloor=2$, i.e., $2\gamma+1\leq n<3\gamma+1$. Based on previous assumptions, we have $n=3\gamma$, then the corresponding tree T is consists of γ stars of order 3 (S_3) with exactly $\gamma-1$ pairs of adjacent pendent vertices in neighbouring stars. One can easily check that $T\in\mathcal{G}_1(n,\gamma)$. Therefore, we just need to consider the following formula:

$$g(1-\gamma)=\left(n-\gamma\left\lfloor\frac{n-1}{\gamma}\right\rfloor\right)\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor-1}\right)^2\right]$$
$$+\gamma\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor-1}\right)^2+\left(n-\frac{5}{2}\gamma+\frac{3}{2}\right).$$

Finally, in order to find the feasible minimum value of the function $g(m_2-m_3)$, we have to calculate the difference between $g(0)$ and $g(1-\gamma)$. The formula of $g(0)-g(1-\gamma)$ is given by

$$\begin{aligned}g(0)-g(1-\gamma)=&\left(n-\gamma\left\lfloor\frac{n-1}{\gamma}\right\rfloor\right)\\&\times\left\{\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor+1}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2\right]-\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor-1}\right)^2\right]\right\}\\&-\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor+1}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2\right]+\gamma\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor-1}\right)^2\right]\\&+\frac{3}{4}(\gamma-1)\ .\end{aligned}$$

Obviously,

$$\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor+1}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2\right]>\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor-1}\right)^2\right],$$

then we get

$$\begin{aligned} g(0)-g(1-\gamma) > & \left(n-\gamma\left\lfloor\frac{n-1}{\gamma}\right\rfloor\right) \\ & \times\left\{\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor+1}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2\right]-\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor-1}\right)^2\right]\right\} \\ & +(\gamma-1)\left[\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor}\right)^2-\left(\frac{1}{\lfloor\frac{n-1}{\gamma}\rfloor-1}\right)^2+\frac{3}{4}\right]>0. \end{aligned}$$

This inequality is strict.

In brief, the equality holds in (8) if and only if $m_2-m_3=1-\gamma$. Note that m_1, m_2, and m_3 are all non-negative, then by system (2) and (3), we can obtain $m_2=0$, $m_3=\gamma-1$, and $m_1=n-\gamma$. It's not difficult to find that the corresponding extremal trees all belong to $\mathcal{G}_1(n,\gamma)$. ■

Definition 3. Let $\mathcal{G}_2(n,\gamma)$ be a set of n-vertices trees T with domination number γ. If $T\in\mathcal{G}_2(n,\gamma)$, then each vertex in $V(T)$ has at most one pendent neighbor and T satisfies one of the following conditions.

(i) There exists a minimum dominating set D of T has $3\gamma-n-2$ vertices with degree 3 and $2(n-2\gamma)$ vertices with degree 2, while $\overline{D}$ has $n-2\gamma+2$ vertices with degree 2 and $3\gamma-n$ pendent vertices.

(ii) There exists a minimum dominating set D of T has $n-2\gamma$ vertices with degree 2 and $3\gamma-n$ pendent vertices, while $\overline{D}$ has $2(n-2\gamma+1)$ vertices with degree 2, $3\gamma-n-2$ with degree 3, and each vertex in $\overline{D}$ has only one neighbor in domination set D.

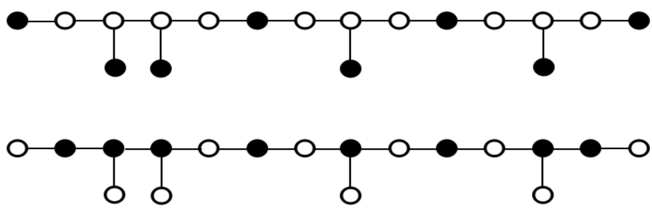

Figure 4. A tree from $\mathcal{G}_2(n,\gamma)$ with 18 vertices and 8 domination number.

Theorem 5. *Let T be a tree on n vertices with domination number γ, where $\frac{n}{3} \leq \gamma \leq \frac{n}{2}$. Then we have*

$$^{m}M_1(T) \geq \begin{cases} \frac{n+6}{4}, & \text{for } \gamma = \lceil \frac{n}{3} \rceil \\ \frac{11}{6}\gamma - \frac{13}{36}n + \frac{5}{18}, & \text{for } \frac{n+3}{3} < \gamma \leq \frac{n}{2} \end{cases}. \tag{18}$$

Equality holds if and only if $T \in \mathcal{G}_2(n, \gamma)$.

Proof. By Theorem 2, one can see that the path P_n attains the $^{m}M_1$-value of trees with $\gamma = \lceil \frac{n}{3} \rceil$. Thus, we can suppose that $\gamma \geq \frac{n+3}{3}$. Due to $2n \leq \gamma \leq 3\gamma - 3$, trees which we consider in the subsequence have to satisfy $\gamma \geq 3$ and $n \geq 6$.

Note that

$$1 = \frac{n-\gamma}{n-\gamma} \leq \frac{n-1+m_3-m_2}{n-\gamma} \leq \frac{n-1+\gamma-1}{n-\gamma} = 1 + 2\frac{\gamma-1}{n-\gamma} < 3,$$

implying $k_2 = \lfloor \frac{n-1+m_3-m_2}{n-\gamma} \rfloor = 1$ or $k_2 = \lfloor \frac{n-1+m_3-m_2}{n-\gamma} \rfloor = 2$. Therefore, we consider the following two cases.

Case 1. $k_2 = \lfloor \frac{n-1+m_3-m_2}{n-\gamma} \rfloor = 1$.

It is obvious that $1 \leq \frac{n-1+m_3-m_2}{n-\gamma} < 2$, implying $m_2 - m_3 \geq 2\gamma - n$. Since $\gamma \leq \frac{n}{2}$, then $2\gamma - n \leq 0$. Next, we must discuss further.

Case 1.1. $2\gamma - n \leq -1$.

Then we have $2 \leq \frac{n-1}{\gamma} \leq \frac{n-1}{(n/3)+1} < 3$, implying $\lfloor \frac{n-1}{\gamma} \rfloor = 2$. If $2\gamma - n \leq m_2 - m_3 \leq 0$, we get

$$k_1 = \lfloor \frac{n-1+m_2-m_3}{\gamma} \rfloor = \lfloor \frac{n-1}{\gamma} \rfloor = 2, \qquad \text{for } 2\gamma - n + 1 \leq m_2 - m_3 \leq 0,$$
$$k_1 = \lfloor \frac{n-1+m_2-m_3}{\gamma} \rfloor = \lfloor \frac{n-1}{\gamma} \rfloor - 1 = 1, \quad \text{for } m_2 - m_3 = 2\gamma - n.$$

Since $\gamma \geq \frac{n+3}{3}$, combining with (7), then the formula of $g(m_2 - m_3)$ can be given by

$$g(m_2 - m_3) = \frac{11}{18}(m_2 - m_3) + \frac{31}{36}n - \frac{11}{9}\gamma + \frac{8}{9}, \quad \text{for } 2\gamma - n + 1 \leq m_2 - m_3 \leq 0. \tag{19}$$

Analogously, suppose that $0 \leq m_2 - m_3 \leq \gamma - 1$, then we have

$$k_1 = \lfloor \frac{n-1+m_2-m_3}{\gamma} \rfloor = \lfloor \frac{n-1}{\gamma} \rfloor = 2, \qquad \text{for } 0 \leq m_2 - m_3 \leq 3\gamma - n,$$
$$k_1 = \lfloor \frac{n-1+m_2-m_3}{\gamma} \rfloor = \lfloor \frac{n-1}{\gamma} \rfloor + 1 = 3, \quad \text{for } 3\gamma - n + 1 \leq m_2 - m_3 \leq \gamma - 1,$$

which implies that

$$g(m_2 - m_3) = \frac{11}{18}(m_2 - m_3) + \frac{31}{36}n - \frac{11}{9}\gamma + \frac{8}{9}, \quad \text{for } 0 \leq m_2 - m_3 \leq 3\gamma - n, \tag{20}$$

and

$$g(m_2-m_3)=\frac{101}{144}(m_2-m_3)+\frac{137}{144}n-\frac{215}{144}\gamma+\frac{115}{144},\quad \text{for } 3\gamma-n+1\le m_2-m_3\le\gamma-1.$$

From (19) and (20), we get

$$g(m_2-m_3)=\frac{11}{18}(m_2-m_3)+\frac{31}{36}n-\frac{11}{9}\gamma+\frac{8}{9},\quad \text{for } 2\gamma-n+1\le m_2-m_3\le 3\gamma-n, \tag{21}$$

Due to $g(3\gamma-n+1)-g(3\gamma-n)=\frac{11}{18}>0$, we just need to consider the relation (21).

In order to determine the minimum value of m_2-m_3, we have to continue the discussion. For an arbitrary minimum dominating set D of T, the number of vertices with degree 2, and 3 are denoted by n_2 and n_3, respectively, while for the set $\overline{D}$, the number of vertices with degree 1, and 2 are denoted by $\overline{n}_1$ and $\overline{n}_2$.

Easily, we get

$$\begin{cases} n(T)=n_2+n_3+\overline{n}_1+\overline{n}_2,\\ n_2+n_3=\gamma,\\ \overline{n}_1+\overline{n}_2=n-\gamma. \end{cases} \tag{22}$$

Moreover,

$$\sum_{v\in V(T)} d_v=2(n-1)=2(n_2+n_3+\overline{n}_1+\overline{n}_2-1)=\overline{n}_1+2(n_2+\overline{n}_2)+3n_3,$$

implying $n_3=\overline{n}_1-2$. By system (22), we get $n_2-\overline{n}_2=2\gamma-n+2$, then

$$\begin{cases} n-1+m_2-m_3=2n_2+3\overline{n}_1-6,\\ n-1+m_3-m_2=\overline{n}_1+2\overline{n}_2. \end{cases} \tag{23}$$

Combining with (7) and system (23), the function $g(m_2-m_3)$ can be given as below.

$$g(\overline{n}_1)=\frac{11}{18}\overline{n}_1+\frac{1}{4}n+\frac{5}{18},\quad \text{for } 2\le\overline{n}_1\le\gamma+1.$$

Case 1.2. $2\gamma-n=0$, and $\gamma=\frac{n}{2}$ if n is even.

Then we get $1\le\frac{n-1}{\gamma}=1+\frac{\gamma-1}{\gamma}<2$, implying $\lfloor\frac{n-1}{\gamma}\rfloor=1$.

Analogously, we can deduce the following relations.

$$k_1=\lfloor\frac{n-1+m_2-m_3}{\gamma}\rfloor=\lfloor\frac{n-1}{\gamma}\rfloor=1,\qquad \text{for } m_2-m_3=0,$$
$$k_1=\lfloor\frac{n-1+m_2-m_3}{\gamma}\rfloor=\lfloor\frac{n-1}{\gamma}\rfloor+1=2,\quad \text{for } 1\le m_2-m_3\le\frac{n}{2}-1.$$

Through the same derivation process, the function $g(m_2-m_3)$ can be given by

$$g(\overline{n}_1)=\frac{11}{18}\overline{n}_1+\frac{1}{4}n+\frac{5}{18},\quad \text{for } 2\le\overline{n}_1\le\frac{n}{2}.$$

In 2016, Borovićanin and Furtula [2] have proved that $\overline{n}_1 \geq 3\gamma - n$ for any trees, and $\overline{n}_1 > 3\gamma - n$ always holds if there exists a vertex in $V(T)$ have two pendent neighbors. Hence, we can get the feasible minimum value of the function $g(m_2 - m_3)$, that is

$$g(3\gamma - n) = \frac{11}{6}\gamma - \frac{13}{36}n + \frac{5}{18}. \tag{24}$$

The lower bound of ${}^{m}M_1$ of trees given in (24) will be achieved if $\overline{n}_1 = 3\gamma - n$, i.e., $m_2 - m_3 = 5\gamma - 2n + 1$. In this case, extremal trees which make all equalities hold in (18) belong to $\mathcal{G}_2(n,\gamma)$ (Definition 3 (i)).

Case 2. $k_2 = \lfloor \frac{n-1+m_3-m_2}{n-\gamma} \rfloor = 2$.

Since $2 \leq \frac{n-1+m_3-m_2}{n-\gamma} < 3$, we get $m_2 - m_3 \leq 2\gamma - n + 1$. The following relation:

$$1 \leq \frac{n-\gamma}{\gamma} \leq \frac{n-1+m_2-m_3}{\gamma} \leq \frac{2(\gamma-1)}{\gamma} < 2,$$

implies that $k_1 = \lfloor \frac{n-1+m_2-m_3}{\gamma} \rfloor = 1$.

If $m_3 - m_2 = n - 2\gamma + 1$, then $\frac{n-1+m_3-m_2}{n-\gamma} = 2$, which implies that all vertices in $\overline{D}$ has degrees 2, where D is an arbitrary dominating set. One can easily check that all vertices in D have degree 1 or 2, implying $T \cong P_n$, a contradiction, since $\gamma \geq \frac{n+3}{3}$. We suppose that $m_3 - m_2 \geq n - 2\gamma + 2$, i.e., $m_2 - m_3 \leq 2\gamma - n - 2$.

From (7), then

$$g(m_2 - m_3) = -\frac{11}{18}(m_2 - m_3) - \frac{13}{36}n + \frac{11}{9}\gamma + \frac{8}{9}, \quad \text{for } 1 - \gamma \leq m_2 - m_3 \leq 2\gamma - n - 2.$$

Similarly, we need to find the feasible minimum value of $m_2 - m_3$. For an arbitrary minimum dominating set D of T, the number of vertices with degree 1, and 2 are denoted by n_1 and n_2, respectively, while for the set $\overline{D}$, the number of vertices with degree 2, and 3 are denoted by $\overline{n}_2$ and $\overline{n}_3$.

Obviously, from relations $n_2 - \overline{n}_2 = 2\gamma - n - 2$ and $m_2 - m_3 = 2\gamma - n - n_1 + 1$, we get

$$g(n_1) = \frac{11}{18}n_1 + \frac{1}{4}n + \frac{15}{18}, \quad \text{for } 3 \leq n_1 \leq 3\gamma - n.$$

According to previous consideration, we can determine the only possible value of n_1, that is $3\gamma - n$, implying $m_2 - m_3 = 1 - \gamma$. Thus, the feasible minimum value of the function $g(m_2 - m_3)$ can be given by

$$g(3\gamma - n) = \frac{11}{6}\gamma - \frac{13}{36}n + \frac{5}{18}.$$

Then, we will infer that the extremal trees which meets all conditions discussed above, where $\frac{n+3}{3} < \gamma \leq \frac{n}{2}$, satisfy that their all vertices in an arbitrary minimum dominating set D have degrees 1 and 2, while all vertices in $\overline{D}$ have degrees 2 and 3.

On the whole, $\frac{11}{6}\gamma - \frac{13}{36}n + \frac{5}{18}$ is the minimum of ${}^{m}M_1(T)$ for $\frac{n+3}{3} < \gamma \leq \frac{n}{2}$. At this time, we can get $m_2 - m_3 = 1 - \gamma$, $m_1 = n - \gamma$, $m_2 = 0$, and $m_3 = \gamma - 1$. One can easily check that the corresponding extremal trees belong to the set $\mathcal{G}_2(n, \gamma)$ (Definition 3 (ii)).

This completes the proofs. ■

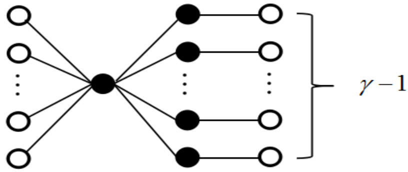

Figure 5. The trees $T(n, \gamma)$

Finally, we derive the upper bound for the modified first Zagreb index of trees with a given domination number. So, we have the following theorem.

Theorem 6. *Let T be a tree on n vertices with domination number γ. Then*

$$ {}^{m}M_1(T) \leq (n - \gamma) + \left(\frac{1}{n - \gamma}\right)^2 + \frac{1}{4}(\gamma - 1). \tag{25} $$

Equality holds if and only if $T \cong T(n, \gamma)$.

Proof. For $\Delta = 2$, it's obvious that $T \cong T(2, 1)$, $T \cong T(3, 1)$, and $T \cong T(4, 2)$. If $n \geq 5$, then $\gamma = \lceil \frac{n}{3} \rceil$, the inequality in (25) is strict.

For $\Delta \geq 3$, we take a diameter path $v_1 v_2 \cdots v_l$ $(l \geq 4)$. Based on the definition of domination number, we have $\Delta \leq n - \gamma$, then we can suppose that the inequality shown in (25) holds for $|V(T)| = n - 1$. If $|V(T)| = n$, according to the discussion above, we let $T_1 = T - \{v_1\}$ and consider the following two cases.

Case 1. $\gamma(T_1) = \gamma(T)$.

By induction hypothesis, we have

$$\begin{aligned}
{}^{m}M_1(T) &= {}^{m}M_1(T_1) - \left(\frac{1}{d_{v_2}-1}\right)^2 + \left(\frac{1}{d_{v_2}}\right)^2 + 1 \\
&\le (n-\gamma-1) + \left(\frac{1}{n-\gamma-1}\right)^2 + \frac{1}{4}(\gamma-1) - \left(\frac{1}{d_{v_2}-1}\right)^2 + \left(\frac{1}{d_{v_2}}\right)^2 + 1 \\
&= (n-\gamma) + \left(\frac{1}{n-\gamma}\right)^2 + \frac{1}{4}(\gamma-1) + \left[\left(\frac{1}{n-\gamma-1}\right)^2 - \left(\frac{1}{n-\gamma}\right)^2\right] \\
&- \left[\left(\frac{1}{d_{v_2}-1}\right)^2 - \left(\frac{1}{d_{v_2}}\right)^2\right] \le (n-\gamma) + \left(\frac{1}{n-\gamma}\right)^2 + \frac{1}{4}(\gamma-1).
\end{aligned}$$

All equalities hold if and only if $d_{v_2} = n-\gamma$, i.e., $T = T(n,\gamma)$.

Case 2. $\gamma(T_1) = \gamma(T) - 1$.

According to the definition of dominating set, one can see that $d_{v_2} = 2$. Then

$$\begin{aligned}
{}^{m}M_1(T) &= {}^{m}M_1(T_1) - \left(\frac{1}{d_{v_2}-1}\right)^2 + \left(\frac{1}{d_{v_2}}\right)^2 + 1 \\
&\le (n-\gamma) + \left(\frac{1}{n-\gamma}\right)^2 + \frac{1}{4}(\gamma-1) - \frac{1}{4} - \left(\frac{1}{d_{v_2}-1}\right)^2 + \left(\frac{1}{d_{v_2}}\right)^2 + 1 \\
&= (n-\gamma) + \left(\frac{1}{n-\gamma}\right)^2 + \frac{1}{4}(\gamma-1).
\end{aligned}$$

Equality holds if and only if $T_1 = T(n-1,\gamma-1)$. Hence, $T = T(n,\gamma)$.

This completes the proof. ■

Nevertheless, we cannot determine the lower bound for ${}^{m}M_2$ of trees in terms of domination number γ and characterize its extremal trees by similar methods of listing cases. For this reason, we propose the following conjecture. Meanwhile, we believe that the formula of upper bound for ${}^{m}M_2$ of trees in terms of domination number γ is regardless of γ. We hope these problems can be solved in our next work.

Conjecture 3.1. Let T be a tree on n vertices with domination number γ. Then

$${}^{m}M_2(T) \ge -\frac{\gamma-1}{2(n-\gamma)} + \frac{\gamma+1}{2},$$

with equality holding if and only if $T \cong T(n,\gamma)$.

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