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Extremal values on Zagreb indices of trees with given distance k-domination number

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Abstract

Let $G = (V(G), E(G))$ be a graph. A set $D \subseteq V(G)$ is a distance k-dominating set of G if for every vertex $u \in V(G) \setminus D$, $d_G(u,v) \leq k$ for some vertex $v \in D$, where k is a positive integer. The distance k-domination number $\gamma_k(G)$ of G is the minimum cardinality among all distance k-dominating sets of G. The first Zagreb index of G is defined as $M_1 = \sum_{u\in V(G)} d^2(u)$ and the second Zagreb index of G is $M_2 = \sum_{uv\in E(G)} d(u)d(v)$. In this paper, we obtain the upper bounds for the Zagreb indices of n-vertex trees with given distance k-domination number and characterize the extremal trees, which generalize the results of Borovićanin and Furtula (Appl. Math. Comput. 276:208–218, 2016). What is worth mentioning, for an n-vertex tree T, is that a sharp upper bound on the distance k-domination number $\gamma_k(T)$ is determined.

MSC: 05C35; 05C69

Keywords: first Zagreb index; second Zagreb index; trees; distance k-domination number

1 Introduction

Throughout this paper, all graphs considered are simple, undirected and connected. Let $G = (V, E)$ be a simple and connected graph, where $V = V(G)$ is the vertex set and $E = E(G)$ is the edge set of G. The *eccentricity* of v is defined as $\varepsilon_G(v) = \max\{d_G(u,v) \mid u \in V(G)\}$. The *diameter* of G is $\mathrm{diam}(G) = \max\{\varepsilon_G(v) \mid v \in V(G)\}$. A path P is called a *diameter path* of G if the length of P is $\mathrm{diam}(G)$. Denote by $N_G^i(v)$ the set of vertices with distance i from v in G, that is, $N_G^i(v) = \{u \in V(G) \mid d(u,v) = i\}$. In particular, $N_G^0(v) = \{v\}$ and $N_G^1(v) = N_G(v)$. A vertex $v \in V(G)$ is called a *private k-neighbor* of u with respect to D if $\bigcup_{i=0}^k N_G^i(v) \cap D = \{u\}$. That is, $d_G(v,u) \leq k$ and $d_G(v,x) \geq k+1$ for any vertex $x \in D \setminus \{u\}$. The *pendent* vertex is the vertex of degree 1.

A chemical molecule can be viewed as a graph. In a molecular graph, the vertices represent the atoms of the molecule and the edges are chemical bonds. A topological index of a molecular graph is a mathematical parameter which is used for studying various properties of this molecule. The distance-based topological indices, such as the Wiener index [2, 3] and the Balaban index [4], have been extensively researched for many decades. Meanwhile the spectrum-based indices developed rapidly, such as the Estrada index [5], the Kirchhoff index [6] and matching energy [7]. The eccentricity-based topological indices, such as the eccentric distance sum [8], the connective eccentricity index [9] and the adjacent eccentric distance sum [10], were proposed and studied recently. The degree-based topological indices, such as the Randić index [11–13], the general sum-connectivity index [14, 15], the Zagreb indices [16], the multiplicative Zagreb indices [17, 18] and the augmented Zagreb index [19], where the Zagreb indices include the *first Zagreb index* $M_1 = \sum_{u\in V(G)} d^2(u)$ and the *second Zagreb index* $M_2 = \sum_{uv\in E(G)} d(u)d(v)$, represent one kind of the most famous topological indices. In this paper, we continue the work on Zagreb indices. Further study about the Zagreb indices can be found in [20–25]. Many researchers are interested in establishing the bounds for the Zagreb indices of graphs and characterizing the extremal graphs [1, 26–40].

A set $D \subseteq V(G)$ is a *dominating set* of G if, for any vertex $u \in V(G) \setminus D$, $N_G(u) \cap D \neq \emptyset$. The *domination number* $\gamma(G)$ of G is the minimum cardinality of dominating sets of G. For $k \in N^+$, a set $D \subseteq V(G)$ is a *distance k-dominating set* of G if, for every vertex $u \in V(G)\setminus D$, $d_G(u,v) \le k$ for some vertex $v \in D$. The *distance k-domination number* $\gamma_k(G)$ of G is the minimum cardinality among all distance k-dominating sets of G [41, 42]. Every vertex in a minimum distance k-dominating set has a private k-neighbor. The domination number is the special case of the distance k-domination number for $k = 1$. Two famous books [43, 44] written by Haynes *et al.* show us a comprehensive study of domination. The topological indices of graphs with given domination number or domination variations have attracted much attention of researchers [1, 45–47].

Borovićanin [1] showed the sharp upper bounds on the Zagreb indices of n-vertex trees with domination number γ and characterized the extremal trees. Motivated by [1], we describe the upper bounds for the Zagreb indices of n-vertex trees with given distance k-domination number and find the extremal trees. Furthermore, a sharp upper bound, in terms of n, k and Δ, on the distance k-domination number $\gamma_k(T)$ for an n-vertex tree T is obtained in this paper.

2 Lemmas

In this section, we give some lemmas which are helpful to our results.

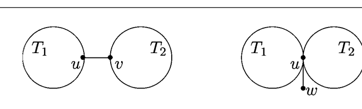
Lemma 2.1 ([24, 48]) *If T is an n-vertex tree, different from the star S_n, then $M_i(T) < M_i(S_n)$ for $i = 1, 2$.*

In what follows, we present two graph transformations that increase the Zagreb indices.

Transformation I ([49]) Let T be an n-vertex tree ($n > 3$) and $e = uv \in E(T)$ be a non-pendent edge. Assume that $T - uv = T_1 \cup T_2$ with vertex $u \in V(T_1)$ and $v \in V(T_2)$. Let T' be the tree obtained by identifying the vertex u of T_1 with vertex v of T_2 and attaching a pendent vertex w to the u (= v) (see Figure 1). For the sake of convenience, we denote $T' = \tau(T, uv)$.

Lemma 2.2 *Let T be a tree of order n (≥ 3) and $T' = \tau(T, uv)$. Then $M_i(T') > M_i(T)$, $i = 1, 2$.*

Figure 1 ***T* and *T′* in Transformation I.**



Proof It is obvious that $d_{T'}(u) = d_T(u) + d_T(v) - 1$ and

$$\begin{aligned} M_1(T') - M_1(T) &= (d_T(u) + d_T(v) - 1)^2 + 1 - d_T^2(u) - d_T^2(v) \\ &= 2(d_T(u) - 1)(d_T(v) - 1) \\ &> 0. \end{aligned}$$

Let $x \in V(T)$ be a vertex different from u and v. Then

$$\begin{aligned} M_2(T') - M_2(T) &= (d_T(u) + d_T(v) - 1)\Big(\sum_{xu \in E(T_1)} d_T(x) + \sum_{xv \in E(T_2)} d_T(x) + 1\Big) \\ &\quad - d_T(u) \sum_{xu \in E(T_1)} d_T(x) - d_T(v) \sum_{xv \in E(T_2)} d_T(x) - d_T(u)d_T(v) \\ &= (d_T(v) - 1) \sum_{xu \in E(T_1)} d_T(x) + (d_T(u) - 1) \sum_{xv \in E(T_2)} d_T(x) \\ &\quad + d_T(u) + d_T(v) - 1 - d_T(u)d_T(v) \\ &\geq 2(d_T(v) - 1)(d_T(u) - 1) + d_T(u) + d_T(v) - 1 - d_T(u)d_T(v) \\ &= (d_T(v) - 1)(d_T(u) - 1) \\ &> 0. \end{aligned}$$

This completes the proof. □

Lemma 2.3 ([50]) *Let u and v be two distinct vertices in G. $u_1, u_2, \ldots, u_r$ are the pendent vertices adjacent to u and $v_1, v_2, \ldots, v_t$ are the pendent vertices adjacent to v. Define $G' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$ and $G'' = G - \{uu_1, uu_2, \ldots, uu_r\} + \{vu_1, vu_2, \ldots, vu_r\}$, as shown in Figure 2. Then either $M_i(G') > M_i(G)$ or $M_i(G'') > M_i(G)$, $i = 1, 2$.*

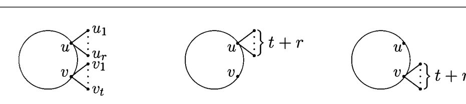
Lemma 2.4 ([51]) *For a connected graph G of order n with $n \geq k + 1$, $\gamma_k(G) \leq \lfloor \frac{n}{k+1} \rfloor$.*

Let G be a connected graph of order n. If $\gamma_k(G) \geq 2$, then $n \geq k + 1$. Otherwise, $\gamma_k(G) = 1$, a contradiction. Hence, by Lemma 2.4, we have $\gamma_k(G) \leq \lfloor \frac{n}{k+1} \rfloor$ and $n \geq (k + 1)\gamma_k$ for any connected graph G of order n if $\gamma_k(G) \geq 2$.

Lemma 2.5 *Let T be an n-vertex tree with distance k-domination number $\gamma_k \geq 2$. Then $\triangle \leq n - k\gamma_k$.*

Proof Suppose that $\triangle \geq n - k\gamma_k + 1$. Let $v \in V(T)$ be the vertex such that $d(v) = \triangle$ and $N(v) = \{v_1, \ldots, v_\triangle\}$. Denote by T^i the component of $T - v$ containing the vertex v_i, $i =$

Figure 2 ***G*, *G′* and *G″* in Lemma 2.3.**



$1, \ldots, \triangle$. Let D be a minimum distance k-dominating set of T,

$$S_1 = \{i \mid i \in \{1, 2, \ldots, \triangle\}, 0 \le \varepsilon_{T^i}(v_i) \le k - 1\}$$

and

$$S_2 = \{i \mid i \in \{1, 2, \ldots, \triangle\}, \varepsilon_{T^i}(v_i) \ge k\}.$$

Clearly, $|S_2| \ge 1$. If not, $\{v\}$ is a distance k-dominating set of T, which contradicts $\gamma_k \ge 2$. If $|S_1| = 0$, then $\varepsilon_{T^i}(v_i) \ge k$ for $i = 1, \ldots, \triangle$, so $|V(T^i) \cap D| \ge 1$. Therefore, $\gamma_k \ge \triangle \ge n - k\gamma_k + 1$, which implies that $\gamma_k \ge \frac{n+1}{k+1}$. Since $\gamma_k \ge 2$, $\gamma_k \le \lfloor \frac{n}{k+1} \rfloor$ by Lemma 2.4, a contradiction. Thus, $|S_1| \ge 1$. Let $i_1 \in S_1$ and

$$\varepsilon_{T^{i_1}}(v_{i_1}) = \max\{\varepsilon_{T^i}(v_i) \mid i \in S_1\} = \lambda.$$

Then $0 \le \lambda \le k - 1$, so $|S_2| \le \lfloor \frac{n-\triangle-1-\lambda}{k} \rfloor \le \lfloor \frac{k\gamma_k - 2}{k} \rfloor \le \gamma_k - 1$.

If $V(T^i) \cap D = D_1 \ne \emptyset$ for some $i \in S_1$, then $D - D_1 + \{v\}$ is a distance k-dominating set according to the definition of S_1. Thus, we assume that $V(T^i) \cap D = \emptyset$ for each $i \in S_1$. Similarly, suppose that $D' \cap V(T^{i_1}) = \emptyset$ where D' is a minimum distance k-dominating set of the tree $T' = T - \bigcup_{i \in S_1 \setminus \{i_1\}} V(T^i)$.

We claim that D' is a distance k-dominating set of T. Let $y \in V(T^{i_1})$ be the vertex such that $d(v_{i_1}, y) = \lambda$ and $y' \in D'_1 = \bigcup_{i=0}^{k} N^i_{T'}(y) \cap D'$. Then $y' \in V(T') \setminus V(T^{i_1})$ and $d(y, y') = d(y, v) + d(v, y') \le k$, so, for $x \in \bigcup_{i \in S_1 \setminus \{i_1\}} V(T^i)$, we have $d(x, y') = d(x, v) + d(v, y') \le d(y, v) + d(v, y') \le k$. Hence, all the vertices in $\bigcup_{i \in S_1 \setminus \{i_1\}} V(T^i)$ can be dominated by $y' \in D'$. Therefore, D' is a distance k-dominating set of T, so the claim is true.

In view of

$$k + 1 < (k+1)|S_2| + \lambda + 2 \le |V(T')| \le n - |S_1| + 1 = n - \triangle + |S_2| + 1,$$

one has

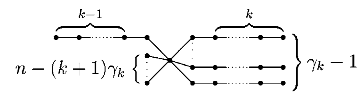
$$\begin{aligned} \gamma_k &\le |D'| \\ &\le \left\lfloor \frac{n - \triangle + |S_2| + 1}{k+1} \right\rfloor \quad \text{(by Lemma 2.4)} \\ &\le \left\lfloor \frac{(k+1)\gamma_k - 1}{k+1} \right\rfloor \quad (\text{since } \triangle \ge n - k\gamma_k + 1, |S_2| \le \gamma_k - 1) \\ &< \gamma_k, \end{aligned}$$

a contradiction as desired. □

Determining the bound on the distance k-domination number of a connected graph is an attractive problem. In Lemma 2.5, an upper bound for the distance k-domination number of a tree is characterized. Namely, if T is an n-vertex tree with distance k-domination number $\gamma_k \ge 2$, then $\gamma_k(T) \le \frac{n-\Delta(T)}{k}$.

Let $\mathcal{T}_{n,k,\gamma_k}$ be the set of all n-vertex trees with distance k-domination number γ_k and $S_{n-k\gamma_k+1}$ be the star of order $n - k\gamma_k + 1$ with pendent vertices $v_1, v_2, \ldots, v_{n-k\gamma_k}$. Denote by T_{n,k,γ_k} the tree formed from $S_{n-k\gamma_k}$ by attaching a path P_{k-1} to v_1 and attaching a path

Figure 3 T_{n,k,γ_k}.



P_k to v_i for each $i \in \{2,\dots,\gamma_k\}$, as shown in Figure 3. Then $T_{n,k,\gamma_k} \in \mathcal{T}_{n,k,\gamma_k}$. Even more noteworthy is the notion that $\gamma_k(T_{n,k,\gamma_k}) = \gamma_k = \frac{n-\Delta(T_{n,k,\gamma_k})}{k}$. It implies that the upper bound on the distance k-domination number mentioned in the above paragraph is sharp.

The Zagreb indices of T_{n,k,γ_k} are computed as

$$M_1(T_{n,k,\gamma_k}) = (n-k\gamma_k)(n-k\gamma_k+1) + 4(k\gamma_k-1)$$

and

$$M_2(T_{n,k,\gamma_k}) = \begin{cases} (n-k\gamma_k)[n-(k-1)\gamma_k] + (4k-2)\gamma_k - 4 & \text{if } k \geq 2, \\ 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1) & \text{if } k = 1. \end{cases}$$

For $k = 1$, the distance k-domination number $\gamma_1(G)$ is the domination number $\gamma(G)$. Furthermore, the upper bounds on the Zagreb indices of an n-vertex tree with domination number were studied in [1], so we only consider $k \geq 2$ in the following.

Lemma 2.6 ([52]) *T be a tree on $(k+1)n$ vertices. Then $\gamma_k(T) = n$ if and only if at least one of the following conditions holds*:

(1) *T is any tree on $k+1$ vertices*;
(2) *$T = R \circ k$ for some tree R on $n \geq 1$ vertices, where $R \circ k$ is the graph obtained by taking one copy of R and $|V(R)|$ copies of the path P_{k-1} of length $k-1$ and then joining the ith vertex of R to exactly one end vertex in the ith copy of P_{k-1}.*

Lemma 2.7 *Let T be an n-vertex tree with distance k-domination number $\gamma_k(T) \geq 3$. If $n = (k+1)\gamma_k$, then*

$$M_1(T) \leq \gamma_k(\gamma_k+1) + 4(k\gamma_k-1)$$

and

$$M_2(T) \leq 2\gamma_k^2 + (4k-2)\gamma_k - 4,$$

with equality if and only if $T \cong T_{n,k,\gamma_k}$.

Proof When $n = (k+1)\gamma_k$, $T = R \circ k$ for some tree R on γ_k vertices by Lemma 2.6. Assume that $V(R) = \{v_1,\dots,v_{\gamma_k}\}$. Then $d_R(v_i) = d_T(v_i) - 1$. It is well known that $\sum_{i=1}^{n} d(u_i) = 2(n-1)$ for any n-vertex tree with vertex set $\{u_1,\dots,u_n\}$. Hence, $\sum_{i=1}^{\gamma_k} d_R(v_i) = 2(\gamma_k - 1)$. By the definition of the first Zagreb index, we have

$$\begin{aligned} M_1(T) &= \sum_{i=1}^{\gamma_k} d_T^2(v_i) + \sum_{x \in V(T)\setminus V(R)} d_T^2(x) \\ &= \sum_{i=1}^{\gamma_k} \bigl(d_T(v_i)-1\bigr)^2 + \sum_{x \in V(T)\setminus V(R)} d_T^2(x) + 2\sum_{i=1}^{\gamma_k} \bigl(d_T(v_i)-1\bigr) + \gamma_k \end{aligned}$$

$$\begin{aligned}
&= M_1(R) + 4(k-1)\gamma_k + \gamma_k + 2\sum_{i=1}^{\gamma_k} d_R(v_i) + \gamma_k \\
&\leq M_1(S_{\gamma_k}) + 4(k-1)\gamma_k + 2\gamma_k + 4(\gamma_k - 1) \\
&= \gamma_k(\gamma_k + 1) + 4(k\gamma_k - 1).
\end{aligned}$$

The equality holds if and only if $R \cong S_{\gamma_k}$, that is, $T \cong T_{n,k,\gamma_k}$. We have

$$\begin{aligned}
M_2(T) &= \sum_{xy\in E(R)} d_T(x)d_T(y) + \sum_{xy\in E(T)\setminus E(R)} d_T(x)d_T(y) \\
&= \sum_{xy\in E(R)} \bigl(d_T(x)-1\bigr)\bigl(d_T(y)-1\bigr) + \sum_{xy\in E(R)} \bigl(d_T(x)+d_T(y)-1\bigr) \\
&\quad + \sum_{xy\in E(T)\setminus E(R)} d_T(x)d_T(y) \\
&= M_2(R) + \sum_{x\in V(R)} d_T(x)\bigl(d_T(x)-1\bigr) - (\gamma_k - 1) \\
&\quad + \sum_{x\in V(R)} 2d_T(x) + 4(k-2)\gamma_k + 2\gamma_k \\
&= M_2(R) + \sum_{x\in V(R)} \bigl(d_T(x)-1\bigr)^2 + 3\sum_{x\in V(R)} \bigl(d_T(x)-1\bigr) + 4k\gamma_k - 5\gamma_k - 1 \\
&= M_2(R) + M_1(R) + 6(\gamma_k - 1) + 4k\gamma_k - 5\gamma_k + 1 \\
&\leq M_2(S_{\gamma_k}) + M_1(S_{\gamma_k}) + 4k\gamma_k + \gamma_k - 5 \\
&= 2\gamma_k^2 + (4k-2)\gamma_k - 4.
\end{aligned}$$

The equality holds if and only if $R \cong S_{\gamma_k}$. As a consequence, $T \cong T_{n,k,\gamma_k}$. □

Lemma 2.8 *Let G be a graph which has a maximum value of the Zagreb indices among all n-vertex connected graphs with distance k-domination number and $S_G = \{v \in V(G) \mid d_G(v) = 1, \gamma_k(G - v) = \gamma_k(G)\}$. If $S_G \neq \emptyset$, then $|N_G(S_G)| = 1$.*

Proof Suppose that $|N_G(S_G)| \geq 2$ and u and v are two distinct vertices in $N_G(S_G)$. $x_1, x_2, \ldots, x_r$ are the pendent vertices adjacent to u and $y_1, y_2, \ldots, y_t$ are the pendent vertices adjacent to v, where $r \geq 1$ and $t \geq 1$. Let D be a minimum distance k-dominating set of G. If $x_i \in D$ for some $i \in \{1, \ldots, r\}$, then $D - x_i + u$ is a distance k-dominating set of T. Hence, we assume that $x_i \notin D$, $i = 1, \ldots, r$. Similarly, $y_i \notin D$ for $1 \leq i \leq t$. Define $G_1 = G - \{vy_1\} + \{uy_1\}$ and $G_2 = G - \{ux_1\} + \{vx_1\}$. Then $\gamma_k(G_1) = \gamma_k(G_2) = \gamma_k(G)$. In addition, we have either $M_i(G_1) > M_i(G)$ or $M_i(G_2) > M_i(G)$, $i = 1, 2$, by a similar proof of Lemma 2.3 and thus omitted here (for reference, see the Appendix). It follows a contradiction, as desired. □

3 Main results

In this section, we give upper bounds on the Zagreb indices of a tree with given order n and distance k-domination number γ_k. If $P = v_0v_1 \cdots v_d$ is a diameter path of an n-vertex tree T, then denote by T_i the component of $T - \{v_{i-1}v_i, v_iv_{i+1}\}$ containing v_i, $i = 1, 2, \ldots, d-1$. By Lemma 2.1, we obtain Theorem 3.1 directly.

Theorem 3.1 *Let T be an n-vertex tree and $\gamma_k(T) = 1$. Then $M_1(T) \leq n(n-1)$ and $M_2(T) \leq (n-1)^2$. The equality holds if and only if $T \cong S_n$.*

Let $T^i_{n,k,2}$ be the tree obtained from the path $P_{2k+2} = v_0 \cdots v_{2k+1}$ by joining $n - 2(k+1)$ pendent vertices to v_i, where $i \in \{1, \dots, 2k\}$.

Theorem 3.2 *If T is an n-vertex tree with distance k-domination number $\gamma_k(T) = 2$, then*

$$M_1(T) \leq (n-2k)(n-2k+1) + 4(2k-1),$$

with equality if and only if $T \cong T^i_{n,k,2}$, where $i \in \{1, \dots, k\}$. Also,

$$M_2(T) \leq (n-2k)(n-2k+2) + 8k - 8,$$

with equality if and only if $T \cong T^i_{n,k,2}$, where $i \in \{2, \dots, k\}$.

Proof Assume that $T \in \mathcal{T}_{n,k,2}$ is the tree that maximizes the Zagreb indices and $P = v_0 v_1 \cdots v_d$ is a diameter path of T. If $d \leq 2k$, then $\{v_{\lfloor \frac{d}{2} \rfloor}\}$ is a distance k-dominating set of T, a contradiction to $\gamma_k(T) = 2$. If $d \geq 2k+2$, define $T' = \tau(T, v_i v_{i+1})$, where $i \in \{1, \dots, d-2\}$. Then $T' \in \mathcal{T}_{n,k,2}$. By Lemma 2.2, we have $M_i(T') > M_i(T)$, $i = 1, 2$, a contradiction. Hence, $d = 2k + 1$.

If T_i is not a star for some $i \in \{1, 2, \dots, d-1\}$, then there exists an n-vertex tree T' in $\mathcal{T}_{n,k,2}$ such that $M_i(T') > M_i(T)$ for $i = 1, 2$ by Lemma 2.2, a contradiction. Besides, $T \cong T^i_{n,k,2}$ for some $i \in \{1, \dots, d-1\}$ by Lemma 2.3.

Since $M_1(T^i_{n,k,2}) = M_1(T^j_{n,k,2})$ for $1 \leq i \neq j \leq d-1$ and $T^i_{n,k,2} \cong T^{d-i}_{n,k,2}$ for $k+1 \leq i \leq d-1$, we get $T \cong T^i_{n,k,2}$, $i \in \{1, \dots, k\}$. By direct computation, one has $M_1(T) = M_1(T^i_{n,k,2}) = (n-2k)(n-2k+1) + 4(2k-1)$, $i \in \{1, \dots, k\}$. In addition, $M_2(T^1_{n,k,2}) = M_2(T^{d-1}_{n,k,2}) < M_2(T^2_{n,k,2}) = \cdots = M_2(T^{d-2}_{n,k,2})$ and $T^i_{n,k,2} \cong T^{d-i}_{n,k,2}$ for $i \in \{k+1, \dots, d-2\}$. Hence, $T \cong T^i_{n,k,2}$, where $i \in \{2, \dots, k\}$. Moreover, $M_2(T) = M_2(T^i_{n,k,2}) = (n-2k)(n-2k+2) + 8k - 8$. This completes the proof. □

Lemma 3.3 *Let tree $T \in \mathcal{T}_{n,k,3}$. Then*

$$M_1(T) \leq (n-3k)(n-3k+1) + 4(3k-1)$$

and

$$M_2(T) \leq (n-3k)(n-3k+3) + 12k - 10,$$

with equality if and only if $T \cong T_{n,k,3}$.

Proof Assume that $T \in \mathcal{T}_{n,k,3}$. We complete the proof by induction on n. By Lemma 2.4, we have $n \geq (k+1)\gamma_k$. This lemma is true for $n = (k+1)\gamma_k$ by Lemma 2.7. Suppose that $n > 3(k+1)$ and the statement holds for $n-1$ in the following.

Let D be a minimum distance k-dominating set of T and $P = v_0 v_1 \cdots v_d$ be a diameter path of T. Then $d \geq 2k+2$. Otherwise, $\{v_k, v_{k+1}\}$ is a distance k-dominating set, a contradiction. Note that $\bigcup_{i=0}^{k} N^i_T(v_0) \cap D \neq \emptyset$ and $\bigcup_{i=0}^{k} N^i_T(v_0) \subseteq (\bigcup_{i=0}^{k-1} V(T_i) \cup \{v_k\})$. Hence,

$(\bigcup_{i=0}^{k-1} V(T_i) \cup \{v_k\}) \cap D \neq \emptyset$. However, $\bigcup_{i=0}^{k} N_T^i(x) \subseteq \bigcup_{i=0}^{k} N_T^i(v_k)$ for $x \in \bigcup_{i=0}^{k} V(T_i) \setminus \{v_k\}$, so we assume that $v_k \in D$ and $(\bigcup_{i=0}^{k} V(T_i) \setminus \{v_k\}) \cap D = \emptyset$. Similarly, $v_{d-k} \in D$ and $(\bigcup_{i=d-k}^{d} V(T_i) \setminus \{v_{d-k}\}) \cap D = \emptyset$. Suppose that $v_0 = u_1, v_d = u_2, \dots, u_m$ are the pendent vertices of T and $S_T = \{u_i \mid 1 \leq i \leq m, \gamma_k(T - u_i) = \gamma_k(T)\}$. We have the following claim.

Claim 1 $S_T \neq \emptyset$.

Proof Assume that $S_T = \emptyset$. Namely, $\gamma_k(T - u_i) = \gamma_k(T) - 1$ for each $i \in \{1, \dots, m\}$. If $D \setminus \{w_i\}$ is a minimum distance k-dominating set of the tree $T - u_i$, where $w_i \in D$, then $w_i \neq w_j$ for $1 \leq i \neq j \leq m$. Otherwise, $\gamma_k(T - u_i) = \gamma_k(T)$ or $\gamma_k(T - u_j) = \gamma_k(T)$, a contradiction. It follows that $m \leq \gamma_k$.

If $d_T(v_i) \geq 3$ for some $i \in \{2, \dots, k, d-k, \dots, d-1\}$, then $V(T_i) \cap \{u_3, \dots, u_m\} \neq \emptyset$. In view of $\{v_k, v_{d-k}\} \subseteq D$, we have $\gamma_k(T - x) = \gamma_k(T)$ for $x \in V(T_i) \cap \{u_3, \dots, u_m\}$, a contradiction. Hence, $d_T(v_i) = 2$ for $i \in \{2, \dots, k, d-k, \dots, d-1\}$.

Since $\gamma_k(T - v_0) = \gamma_k(T) - 1$, v_1 must be dominated by the vertices in $D \setminus \{v_k\}$. Bearing in mind that $(\bigcup_{i=0}^{k} V(T_i) \setminus \{v_k\}) \cap D = \emptyset$, one has $v_{k+1} \in D$. The same applies to v_{d-k-1}. Hence, $\{v_k, v_{k+1}, v_{d-k-1}, v_{d-k}\} \subseteq D$. If $d > 2k + 2$, then the vertices v_k, v_{k+1}, v_{d-k-1} and v_{d-k} are different from each other, a contradiction to $\gamma_k(T) = 3$. As a consequence, $d = 2k + 2$ and thus $D = \{v_k, v_{k+1}, v_{d-k}\}$.

If $d_T(v_{k+1}) = 2$, then $T \cong P_{2k+3}$ and $\{v_k, v_{d-k}\}$ is a distance k-dominating set, a contradiction. It follows that $d_T(v_{k+1}) \geq 3$. Hence, $m \geq 3 = \gamma_k$. Recalling that $m \leq \gamma_k = 3$, we have $m = 3$, which implies that T_{k+1} is a path with end vertices v_{k+1} and u_3. If $d(v_{k+1}, u_3) > k$, then u_3 cannot be dominated by the vertices in D. If $d(v_{k+1}, u_3) < k$, then $D \setminus \{v_{k+1}\}$ is a distance k-dominating set, a contradiction. Therefore, $d(v_{k+1}, u_3) = k$. We conclude that $|V(T)| = 3(k + 1)$, which contradicts $n > 3(k + 1)$, so Claim 1 is true. □

Considering $S_T \neq \emptyset$ for $T \in \mathcal{T}_{n,k,3}$, the tree among $\mathcal{T}_{n,k,3}$ that maximizes the Zagreb indices must be in the set $\{T^* \in \mathcal{T}_{n,k,3} \mid |N_{T^*}(S_{T^*})| = 1\}$ by Lemma 2.8. To determine the extremal trees among $\mathcal{T}_{n,k,3}$, we assume that $T \in \{T^* \in \mathcal{T}_{n,k,3} \mid |N_{T^*}(S_{T^*})| = 1\}$ in what follows.

Let u_i be a pendent vertex such that $\gamma_k(T - u_i) = \gamma_k(T)$ and s be the unique vertex adjacent to u_i. By Lemma 2.5, $d_T(s) \leq \triangle \leq n - k\gamma_k$. Define $A = \{x \in V(T) \mid d_T(x) = 1, xs \notin E(T)\}$ and $B = \{x \in V(T) \mid d_T(x) \geq 2, xs \notin E(T)\}$. Then $\gamma_k(T - x) = \gamma_k(T) - 1$ for all $x \in A$. As a consequence, $|A| \leq \gamma_k$ from the proof of Claim 1. By the induction hypothesis,

$$\begin{aligned} M_1(T) &= M_1(T - u_i) + 2d(s) \\ &\leq (n - 1 - k\gamma_k)(n - 1 - k\gamma_k + 1) + 4(k\gamma_k - 1) + 2(n - k\gamma_k) \\ &= (n - k\gamma_k)(n - k\gamma_k + 1) + 4(k\gamma_k - 1). \end{aligned}$$

The equality holds if and only if $T - u_i \cong T_{n-1,k,\gamma_k}$ and $d_T(s) = \triangle = n - k\gamma_k$, *i.e.*, $T \cong T_{n,k,\gamma_k}$.

Note that $|A| + |B| = n - 1 - d_T(s)$ and $|A| \leq \gamma_k$. Therefore, $|B| = n - 1 - d_T(s) - |A| \geq n - 1 - d_T(s) - \gamma_k$ and

$$\sum_{xs \notin E(T)} d(x) \geq |A| + 2|B| = \bigl(|A| + |B|\bigr) + |B| \geq 2\bigl(n - 1 - d_T(s)\bigr) - \gamma_k.$$

By the above inequality and the definition of M_2, we have

$$\begin{aligned} M_2(T) &= M_2(T-u_i) + \sum_{v\in V(T)} d_T(v) - \sum_{xs\notin E(T)} d_T(x) - 1 \\ &\le M_2(T-u_i) + 2(n-1) - 2\big(n-1-d_T(s)\big) + \gamma_k - 1 \qquad (1) \\ &\le (n-1-k\gamma_k)\big[n-1-(k-1)\gamma_k\big] + (4k-2)\gamma_k - 4 \\ &\quad + 2(n-k\gamma_k) + \gamma_k - 1 \quad \big(\text{since } d_T(s) \le \triangle \le n-k\gamma_k\big) \qquad (2) \\ &= (n-k\gamma_k)\big[n-(k-1)\gamma_k\big] + (4k-2)\gamma_k - 4. \end{aligned}$$

The equality (1) holds if and only if $|A| = \gamma_k$, $|B| = n-1-d_T(s)-\gamma_k$ and $d_T(x) = 2$ for $x \in B$. The equality (2) holds if and only if $T - u_i \cong T_{n-1,k,\gamma_k}$ and $d_T(s) = \triangle = n-k\gamma_k$. Hence, $M_2(T) \le (n-k\gamma_k)[n-(k-1)\gamma_k] + (4k-2)\gamma_k - 4$ with equality if and only if $T \cong T_{n,k,\gamma_k}$. □

Theorem 3.4 *Let T be a tree of order n with distance k-domination number γ_k (≥ 3). Then*

$$M_1(T) \le (n-k\gamma_k)(n-k\gamma_k+1) + 4(k\gamma_k - 1)$$

and

$$M_2(T) \le (n-k\gamma_k)\big[n-(k-1)\gamma_k\big] + (4k-2)\gamma_k - 4,$$

with equality if and only if $T \cong T_{n,k,\gamma_k}$.

Proof Let $T \in \mathcal{T}_{n,k,\gamma_k}$ and $P = v_0v_1\cdots v_d$ be a diameter path of T. Define $S_T = \{u \in V(T) \mid d_T(u) = 1, \gamma_k(T-u) = \gamma_k(T)\}$. If $S_T = \emptyset$, then $\gamma_k(T-v_i) = \gamma_k(T) - 1$ for $i = 0, d$. If $S_T \ne \emptyset$, then we suppose that $T \in \{T^* \in \mathcal{T}_{n,k,\gamma_k} \mid |N_{T^*}(S_{T^*})| = 1\}$ by Lemma 2.8 for establishing the maximum Zagreb indices of trees among $\mathcal{T}_{n,k,\gamma_k}$. If $v_d \in S_T \ne \emptyset$, then $\gamma_k(T-v_0) = \gamma_k(T) - 1$, which implies that $\gamma_k(T-v_0) = \gamma_k(T) - 1$ or $\gamma_k(T-v_d) = \gamma_k(T) - 1$. Assume that $\gamma_k(T - v_0) = \gamma_k(T) - 1$. Then there is a minimum distance k-dominating set D of T such that $\{v_k, v_{k+1}, v_{d-k}\} \subseteq D$ from the proof of Lemma 3.3.

Let T' be the tree obtained from T by applying Transformation I on T_i repeatedly for $i = 1, \ldots, k$ such that $T_i' \cong S_{|V(T_i')|}$, where T_i' is the component of $T' - \{v_{i-1}v_i, v_iv_{i+1}\}$ containing v_i, $i = 1, \ldots, k$ (see Figure 4). Then $T' \in \mathcal{T}_{n,k,\gamma_k}$. By Lemma 2.2, we have $M_i(T) \le M_i(T')$, $i = 1, 2$, with equality if and only if $T \cong T'$.

By Lemma 2.3, for some $i_0, i_1 \in \{1, \ldots, k\}$, define

$$\begin{aligned} T'' = T' &- \bigcup_{i\in\{1,\ldots,k\}\setminus\{i_0\}} \big\{v_ix \mid x \in N_{T'}(v_i) \setminus \{v_{i-1}, v_{i+1}\}\big\} \\ &+ \bigcup_{i\in\{1,\ldots,k\}\setminus\{i_0\}} \big\{v_{i_0}x \mid x \in N_{T'}(v_i) \setminus \{v_{i-1}, v_{i+1}\}\big\} \end{aligned}$$

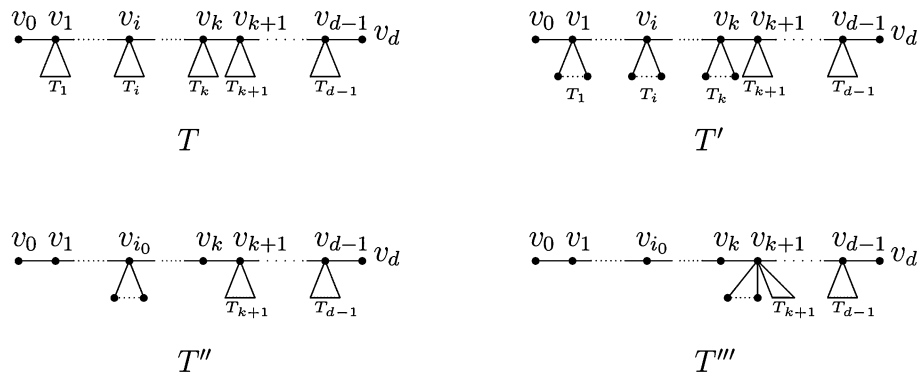


Figure 4 ***T*, *T′*, *T″* and *T‴*.**

and

$$\begin{aligned}\widetilde{T}'' = T' &- \bigcup_{i\in\{1,\ldots,k\}\setminus\{i_1\}} \bigl\{v_i x \mid x \in N_{T'}(v_i) \setminus \{v_{i-1}, v_{i+1}\}\bigr\} \\ &+ \bigcup_{i\in\{1,\ldots,k\}\setminus\{i_1\}} \bigl\{v_{i_1} x \mid x \in N_{T'}(v_i) \setminus \{v_{i-1}, v_{i+1}\}\bigr\}.\end{aligned}$$

Then one has $M_1(T') \le M_1(T'')$ with equality if and only if $T' \cong T''$ and $M_2(T') \le M_2(\widetilde{T}'')$ with equality if and only if $T' \cong \widetilde{T}''$.

Suppose that $|N_{T''}(v_{i_0}) \setminus \{v_{i_0-1}, v_{i_0+1}\}| = |N_{\widetilde{T}''} \setminus \{v_{i_1-1}, v_{i_1+1}\}| = m$, $m \ge 0$. Let

$$\begin{aligned}T''' &= T'' - \bigl\{v_{i_0} x \mid x \in N_{T''}(v_{i_0}) \setminus \{v_{i_0-1}, v_{i_0+1}\}\bigr\} \\ &\quad + \bigl\{v_{k+1} x \mid x \in N_{T''}(v_{i_0}) \setminus \{v_{i_0-1}, v_{i_0+1}\}\bigr\} \\ &= \widetilde{T}'' - \bigl\{v_{i_1} x \mid x \in N_{\widetilde{T}''}(v_{i_1}) \setminus \{v_{i_1-1}, v_{i_1+1}\}\bigr\} \\ &\quad + \bigl\{v_{k+1} x \mid x \in N_{\widetilde{T}''}(v_{i_1}) \setminus \{v_{i_1-1}, v_{i_1+1}\}\bigr\}.\end{aligned}$$

Then D is a minimum distance k-dominating set of T''' and $d_{T'''}(v_i) = 2$ for $i = 1, \ldots, k$. Assume that $PN_{k,D}(x)$ is the set of all private k-neighbors of x with respect to D in T'''. It is clear that the vertices in $\bigcup_{i=0}^{k} N^i_{T'''}(v_k) \setminus \{v_0, \ldots, v_k\}$ can be dominated by $v_{k+1} \in D$. Thus, $D \setminus \{v_k\}$ is a distance k-dominating set of tree $T''' - \{v_0, \ldots, v_k\}$. In addition, $PN_{k,D}(v_{k+1}) \subseteq V(T''') \setminus \{v_0, \ldots, v_k\}$, which means that $D \setminus \{v_k\}$ is a minimum distance k-dominating set of $T''' - \{v_0, \ldots, v_k\}$. So $\gamma_k(T''' - \{v_0, \ldots, v_k\}) = \gamma_k - 1$. Analogously, $\gamma_k(T''' - \{v_0, \ldots, v_{k-1}\}) = \gamma_k - 1$.

By the definition of the first Zagreb index, we get

$$\begin{aligned}M_1(T''') - M_1(T'') &= 4 + \bigl(d_{T''}(v_{k+1}) + m\bigr)^2 - (2+m)^2 - d^2_{T''}(v_{k+1}) \\ &= 2m\bigl(d_{T''}(v_{k+1}) - 2\bigr) \\ &\ge 0,\end{aligned}$$

so $M_1(T''') - M_1(T'') = 0$ if and only if at least one of the following conditions holds:

(1) $m = 0$, which implies that $T'' \cong T'''$;

(2) $d_{T''}(v_{k+1}) = 2$.

If $i_1 = 1$, then

$$\begin{aligned} M_2(T''') - M_2(\widetilde{T}'') &= 6 + \bigl(d_{\widetilde{T}''}(v_{k+1}) + m\bigr)\Bigl(m + \sum_{x\in N_{\widetilde{T}''}(v_{k+1})} d_{\widetilde{T}''}(x)\Bigr) \\ &\quad - (m+2)(m+3) - d_{\widetilde{T}''}(v_{k+1}) \sum_{x\in N_{\widetilde{T}''}(v_{k+1})} d_{\widetilde{T}''}(x) \\ &= m\Bigl[d_{\widetilde{T}''}(v_{k+1}) + \sum_{x\in N_{\widetilde{T}''}(v_{k+1})} d_{\widetilde{T}''}(x) - 5\Bigr] \\ &\geq 0, \end{aligned}$$

with equality if and only if $m = 0$, that is, $\widetilde{T}'' \cong T'''$. If $i_1 \neq 1$ and $i_1 \neq k$, then

$$\begin{aligned} M_2(T''') - M_2(\widetilde{T}'') &= 8 + \bigl(d_{\widetilde{T}''}(v_{k+1}) + m\bigr)\Bigl(m + \sum_{x\in N_{\widetilde{T}''}(v_{k+1})} d_{\widetilde{T}''}(x)\Bigr) \\ &\quad - (m+2)(m+4) - d_{\widetilde{T}''}(v_{k+1}) \sum_{x\in N_{\widetilde{T}''}(v_{k+1})} d_{\widetilde{T}''}(x) \\ &= m\Bigl[d_{\widetilde{T}''}(v_{k+1}) + \sum_{x\in N_{\widetilde{T}''}(v_{k+1})} d_{\widetilde{T}''}(x) - 6\Bigr] \\ &\geq 0. \end{aligned}$$

Also, $M_2(T''') - M_2(\widetilde{T}'') = 0$ if and only if at least one of the following conditions holds:
(1) $m = 0$, namely, $\widetilde{T}'' \cong T'''$;
(2) $d_{\widetilde{T}''}(v_k) = d_{\widetilde{T}''}(v_{k+1}) = d_{\widetilde{T}''}(v_{k+2}) = 2$.
If $i_1 \neq 1$ and $i_1 = k$, then

$$\begin{aligned} M_2(T''') - M_2(\widetilde{T}'') &= 4 + \bigl(d_{\widetilde{T}''}(v_{k+1}) + m\bigr)\Bigl(m + 2 + \sum_{x\in N_{\widetilde{T}''}(v_{k+1})\setminus\{v_k\}} d_{\widetilde{T}''}(x)\Bigr) \\ &\quad - (m+2)(m+2) - d_{\widetilde{T}''}(v_{k+1})\Bigl(\sum_{x\in N_{\widetilde{T}''}(v_{k+1})\setminus\{v_k\}} d_{\widetilde{T}''}(x) + m + 2\Bigr) \\ &= m\Bigl(\sum_{x\in N_{\widetilde{T}''}(v_{k+1})\setminus\{v_k\}} d_{\widetilde{T}''}(x) - 2\Bigr) \\ &\geq 0. \end{aligned}$$

As a result, $M_2(T''') - M_2(\widetilde{T}'') = 0$ if and only if at least one of the following conditions holds:
(1) $m = 0$, which implies that $\widetilde{T}'' \cong T'''$;
(2) $d_{\widetilde{T}''}(v_{k+1}) = d_{\widetilde{T}''}(v_{k+2}) = 2$.

In what follows, we prove $M_1(T''') \leq (n - k\gamma_k)(n - k\gamma_k + 1) + 4(k\gamma_k - 1)$ and $M_2(T''') \leq (n - k\gamma_k)[n - (k-1)\gamma_k] + (4k-2)\gamma_k - 4$ with equality if and only if $T''' \cong T_{n,k,\gamma_k}$ by induction on γ_k. The statement is true for $\gamma_k = 3$ and $n \geq (k+1)\gamma_k$ by Lemma 3.3. Assume that $\gamma_k \geq 4$, the statement holds for $\gamma_k - 1$ and all the $n \geq (k+1)(\gamma_k - 1)$.

In view of $\gamma_k(T''' - \{v_0, v_1, \ldots, v_k\}) = \gamma_k - 1$ and $|V(T''' - \{v_0, v_1, \ldots, v_k\})| = n - k - 1 \geq (k+1)(\gamma_k - 1)$, by the induction hypothesis, we get

$$\begin{aligned} M_1(T''') &= M_1(T''' - \{v_0, v_1, \ldots, v_k\}) + 2d_{T'''}(v_{k+1}) - 1 + \sum_{i=0}^{k} d_{T'''}^2(v_i) \\ &\leq M_1(T_{n-k-1,k,\gamma_k-1}) + 2(n - k\gamma_k) + 4k \\ &= (n - k\gamma_k)(n - k\gamma_k + 1) + 4(k\gamma_k - 1). \end{aligned}$$

The equality holds if and only if $T''' - \{v_0, v_1, \ldots, v_k\} \cong T_{n-k-1,k,\gamma_k-1}$ and $d_{T'''}(v_{k+1}) = \triangle = n - k\gamma_k$. Recalling that $d_{T'''}(v_i) = 2$ for $i = 1, \ldots, k$, we have $M_1(T''') = (n - k\gamma_k)(n - k\gamma_k + 1) + 4(k\gamma_k - 1)$ if and only if $T''' \cong T_{n,k,\gamma_k}$.

Thus, $M_1(T) \leq M_1(T') \leq M_1(T'') \leq M_1(T''') \leq (n - k\gamma_k)(n - k\gamma_k + 1) + 4(k\gamma_k - 1)$ and $M_1(T) = (n - k\gamma_k)(n - k\gamma_k + 1) + 4(k\gamma_k - 1)$ if and only if at least one of the following conditions holds:

(1) $T \cong T' \cong T'' \cong T''' \cong T_{n,k,\gamma_k}$;

(2) $T \cong T' \cong T''$, where $d_{T''}(v_{k+1}) = 2$. Besides, $T''' \cong T_{n,k,\gamma_k}$.

However, the second condition is impossible. If $T''' \cong T_{n,k,\gamma_k}$, then $d_{T'''}(v_{k+1}) = n - k\gamma_k$ and the number of the pendent vertices in $N_{T'''}(v_{k+1})$ is $n - (k+1)\gamma_k$. By the definition of T''', we have

$$n - (k+1)\gamma_k \geq \left|N_{T''}(v_{i_0}) \setminus \{v_{i_0-1}, v_{i_0+1}\}\right|.$$

Hence,

$$\begin{aligned} d_{T''}(v_{k+1}) &= d_{T'''}(v_{k+1}) - |N_{T''}(v_{i_0}) \setminus \{v_{i_0-1}, v_{i_0+1}\}| \\ &\geq d_{T'''}(v_{k+1}) - \bigl[n - (k+1)\gamma_k\bigr] \\ &= \gamma_k \geq 3, \end{aligned}$$

a contradiction to $d_{T''}(v_{k+1}) = 2$. Therefore,

$$M_1(T) \leq (n - k\gamma_k)(n - k\gamma_k + 1) + 4(k\gamma_k - 1)$$

with equality if and only if $T \cong T_{n,k,\gamma_k}$.

Note that $\gamma_k(T''' - \{v_0, \ldots, v_{k-1}\}) = \gamma_k - 1$ and $|V(T''' - \{v_0, \ldots, v_{k-1}\})| > (k+1)(\gamma_k - 1)$. Then

$$\begin{aligned} M_2(T''') &= M_2(T''' - \{v_0, v_1, \ldots, v_{k-1}\}) + d_{T'''}(v_{k+1}) + 4(k-1) + 2 \\ &\leq M_2(T_{n-k,k,\gamma_k-1}) + n - k\gamma_k + 4(k-1) + 2 \\ &= (n - k\gamma_k)\bigl[n - (k-1)\gamma_k\bigr] + (4k-2)\gamma_k - 4. \end{aligned}$$

The equality holds if and only if $T''' - \{v_0, \ldots, v_{k-1}\} \cong T_{n-k,k,\gamma_k-1}$ and $d_{T'''}(v_{k+1}) = \triangle = n - k\gamma_k$. In consideration of $d_{T'''}(v_i) = 2$ for $i = 1, \ldots, k$, the equality holds if and only if $T''' \cong T_{n,k,\gamma_k}$.

Hence, if $i_1 \neq 1$, then $M_2(T) \leq M_2(T') \leq M_2(\widetilde{T}'') \leq M_2(T''') \leq (n - k\gamma_k)[n - (k-1)\gamma_k] + (4k-2)\gamma_k - 4$, with equality if and only if at least one of the following conditions holds:

(1) $T \cong T' \cong \widetilde{T}'' \cong T''' \cong T_{n,k,\gamma_k}$;
(2) $T \cong T' \cong \widetilde{T}''$, where $d_{\widetilde{T}''}(v_k) = d_{\widetilde{T}''}(v_{k+1}) = d_{\widetilde{T}''}(v_{k+2}) = 2$ and $\widetilde{T}''' \cong T_{n,k,\gamma_k}$.

Analogous to the analysis of the first Zagreb index, the second condition above is impossible. Thus,

$$M_2(T) \leq (n - k\gamma_k)\big[n - (k-1)\gamma_k\big] + (4k-2)\gamma_k - 4$$

and the equality holds if and only if $T \cong T_{n,k,\gamma_k}$.

Besides, if $i = 1$, then $M_2(T) \leq (n - k\gamma_k)[n - (k-1)\gamma_k] + (4k-2)\gamma_k - 4$ with equality if and only if $T \cong T_{n,k,\gamma_k}$ immediately. This completes the proof. □

Remark 3.5 Borovićanin and Furtula [1] proved

$$M_1(T) \leq (n-\gamma)(n-\gamma+1) + 4(\gamma-1)$$

and

$$M_2(T) \leq 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1),$$

with equality if and only if $T \cong T_{n,\gamma}$, where $T_{n,\gamma}$ is the tree obtained from the star $K_{1,n-\gamma}$ by attaching a pendent edge to its $\gamma - 1$ pendent vertices. In this paper, we determine the extremal values on the Zagreb indices of trees with distance k-domination number for $k \geq 2$. Note that the domination number is the special case of the distance k-domination number for $k = 1$ and $T_{n,k,\gamma_k} \cong T_{n,\gamma}$, $T^i_{n,k,2} \cong T_{n,\gamma}$, $i \in \{1,\dots,k\}$, when $k = 1$. Let T be an n-vertex tree with distance k-domination number γ_k. Then, by using Theorems 3.1, 3.2 and 3.4 and the results in [1], we have

$$M_1(T) \leq \begin{cases} n(n-1) & \text{if } \gamma_k = 1, \\ (n-k\gamma_k)(n-k\gamma_k+1) + 4(k\gamma_k - 1) & \text{if } \gamma_k \geq 2, \end{cases}$$

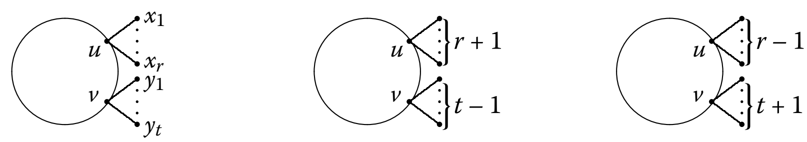
with equality if and only if $T \cong S_n$ when $\gamma_k = 1$, $T \cong T^i_{n,k,2}$, $i \in \{1,\dots,k\}$, when $\gamma_k = 2$, or $T \cong T_{n,k,\gamma_k}$ when $\gamma_k \geq 3$. Moreover,

$$M_2(T) \leq \begin{cases} 2(n-\gamma_k+1)(\gamma_k-1) + (n-\gamma_k)(n-2\gamma_k+1) & \text{if } k = 1, \\ (n-1)^2 & \text{if } k \geq 2, \gamma_k = 1, \\ (n-k\gamma_k)[n-(k-1)\gamma_k] + (4k-2)\gamma_k - 4 & \text{if } k \geq 2, \gamma_k \geq 2, \end{cases}$$

with equality if and only if $T \cong S_n$ when $k \geq 2$ and $\gamma_k = 1$, $T \cong T^i_{n,k,2}$, $i \in \{2,\dots,k\}$, when $k \geq 2$ and $\gamma_k = 2$, or $T \cong T_{n,k,\gamma_k}$ otherwise.

Appendix

Proof Either $M_i(G_1) > M_i(G)$ or $M_i(G_2) > M_i(G)$, $i = 1,2$, in Lemma 2.8, where $G_1 = G - \{vy_1\} + \{uy_1\}$ and $G_2 = G - \{ux_1\} + \{vx_1\}$, as shown in the following figure.



G G_1 G_2

Let $G^* = G - \{x_1, \dots, x_r, y_1, \dots, y_t\}$, $d_{G^*}(u) = a$ and $d_{G^*}(v) = b$. Then

$$\begin{aligned} M_1(G_1) - M_1(G) &= (a+r+1)^2 + (b+t-1)^2 - (a+r)^2 - (b+t)^2 \\ &= 2(a+r-b-t+1) \end{aligned}$$

and

$$\begin{aligned} M_1(G_2) - M_1(G) &= (a+r-1)^2 + (b+t+1)^2 - (a+r)^2 - (b+t)^2 \\ &= 2(b+t-a-r+1) \end{aligned}$$

by the definition of the first Zagreb index. Suppose that $M_1(G_1) - M_1(G) \leq 0$. Then $a + r \leq b + t - 1$. It follows that $M_1(G_2) - M_1(G) > 0$.

If $u \notin N_G(v)$, then

$$\begin{aligned} M_2(G_1) - M_2(G) &= (a+r+1)\Big(\sum_{x \in N_{G^*}(u)} d_G(x) + r + 1\Big) \\ &\quad + (b+t-1)\Big(\sum_{x \in N_{G^*}(v)} d_G(x) + t - 1\Big) \\ &\quad - (a+r)\Big(\sum_{x \in N_{G^*}(u)} d_G(x) + r\Big) - (b+t)\Big(\sum_{x \in N_{G^*}(v)} d_G(x) + t\Big) \\ &= \sum_{x \in N_{G^*}(u)} d_G(x) - \sum_{x \in N_{G^*}(v)} d_G(x) + 2r - 2t + a - b + 2 \end{aligned}$$

and

$$\begin{aligned} M_2(G_2) - M_2(G) &= (a+r-1)\Big(\sum_{x \in N_{G^*}(u)} d_G(x) + r - 1\Big) \\ &\quad + (b+t+1)\Big(\sum_{x \in N_{G^*}(v)} d_G(x) + t + 1\Big) \\ &\quad - (a+r)\Big(\sum_{x \in N_{G^*}(u)} d_G(x) + r\Big) - (b+t)\Big(\sum_{x \in N_{G^*}(v)} d_G(x) + t\Big) \\ &= \sum_{x \in N_{G^*}(v)} d_G(x) - \sum_{x \in N_{G^*}(u)} d_G(x) + 2t - 2r + b - a + 2. \end{aligned}$$

If $M_2(G_1) - M_2(G) \leq 0$, then $M_2(G_2) - M_2(G) > 0$.

If $u \in N_G(v)$, then

$$\begin{aligned}
&M_2(G_1) - M_2(G) \\
&\quad = (a+r+1)\Bigl(\sum_{x\in N_{G^*}(u)\setminus\{v\}} d_G(x) + r + 1\Bigr) + (b+t-1)\Bigl(\sum_{x\in N_{G^*}(u)\setminus\{v\}} d_G(x) + t - 1\Bigr) \\
&\qquad + (a+r+1)(b+t-1) - (a+r)\Bigl(\sum_{x\in N_{G^*}(u)\setminus\{v\}} d_G(x) + r\Bigr) \\
&\qquad - (b+t)\Bigl(\sum_{x\in N_{G^*}(u)\setminus\{v\}} d_G(x) + t\Bigr) - (a+r)(b+t) \\
&\quad = \sum_{x\in N_{G^*}(u)\setminus\{v\}} d_G(x) - \sum_{x\in N_{G^*}(v)\setminus\{u\}} d_G(x) + r - t + 1
\end{aligned}$$

and

$$\begin{aligned}
&M_2(G_2) - M_2(G) \\
&\quad = (a+r-1)\Bigl(\sum_{x\in N_{G^*}(u)\setminus\{v\}} d_G(x) + r - 1\Bigr) + (b+t+1)\Bigl(\sum_{x\in N_{G^*}(u)\setminus\{v\}} d_G(x) + t + 1\Bigr) \\
&\qquad + (a+r-1)(b+t+1) - (a+r)\Bigl(\sum_{x\in N_{G^*}(u)\setminus\{v\}} d_G(x) + r\Bigr) \\
&\qquad - (b+t)\Bigl(\sum_{x\in N_{G^*}(u)\setminus\{v\}} d_G(x) + t\Bigr) - (a+r)(b+t) \\
&\quad = \sum_{x\in N_{G^*}(v)\setminus\{u\}} d_G(x) - \sum_{x\in N_{G^*}(u)\setminus\{v\}} d_G(x) + t - r + 1.
\end{aligned}$$

Assume that $M_2(G_1) - M_2(G) \le 0$. Then $M_2(G_2) - M_2(G) > 0$. Therefore, either $M_i(G_1) > M_i(G)$ or $M_i(G_2) > M_i(G)$, $i = 1, 2$. □

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Competing interests
The authors declare that they have no competing interests.

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