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

Lidan Pei and Xiangfeng Pan

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

\[
M_1 = \sum_{u \in V(G)} d^2(u) \quad \text{and} \quad M_2 = \sum_{v \in V(G)} d(v)d(v).
\]

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 Borovičanin 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

\[
e_{G}(v) = \max\{d_G(u, v) \mid u \in V(G)\}.
\]

The diameter of \( G \) is \( \text{diam}(G) = \max\{e_G(v) \mid v \in V(G)\} \). A path \( P \) is called a diameter path of \( G \) if the length of \( P \) is \( \text{diam}(G) \). Denote by \( N^i_G(v) \) the set of vertices with distance \( i \) from \( v \) in \( G \), that is, \( N^i_G(v) = \{u \in V(G) \mid d(u, v) = i\} \). In particular, \( N^0_G(v) = \{v\} \) and \( N^1_G(v) = N_G(v) \). A vertex \( v \in V(G) \) is called a private \( k \)-neighbor of \( u \) with respect to \( D \) if \( \bigcup_{i=0}^{k-1} N^i_G(u) \cap D = \{u\} \). 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 pendant 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 $u \in V(G) \setminus D$, $d_G(u, v) \leq k$ 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 $\gamma$ 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 $\Delta$, 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 pendant 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 $n$ ($\geq 3$) and $T' = \tau(T, uv)$. Then $M_i(T') > M_i(T)$, $i = 1, 2$.

![Figure 1 T and T' in Transformation I.](image)
Lemma 2.4 (150) It is obvious that \(d_T(u) = d_T(u) + d_T(v) - 1\) and

\[
M_1(T') - M_1(T) = (d_T(u) + d_T(v) - 1)^2 + 1 - d_T^2(u) - d_T^2(v)
\]

\[
= 2(d_T(u) - 1)(d_T(v) - 1) > 0.
\]

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

\[
M_2(T') - M_2(T) = (d_T(u) + d_T(v) - 1)\left(\sum_{x \in E(T_1)} d_T(x) + \sum_{x \in E(T_2)} d_T(x) + 1\right)
\]

\[
- d_T(u) \sum_{x \in E(T_1)} d_T(x) - d_T(v) \sum_{x \in E(T_2)} d_T(x) - d_T(u)d_T(v)
\]

\[
= (d_T(v) - 1) \sum_{x \in E(T_1)} d_T(x) + (d_T(u) - 1) \sum_{x \in E(T_2)} d_T(x)
\]

\[
+ d_T(u) + d_T(v) - 1 - d_T(u)d_T(v)
\]

\[
\geq 2(d_T(v) - 1)(d_T(u) - 1) + d_T(u) + d_T(v) - 1 - d_T(u)d_T(v)
\]

\[
= (d_T(v) - 1)(d_T(u) - 1)
\]

\[
> 0.
\]

This completes the proof. \(\square\)

Lemma 2.3 (150) 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 \(G' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{u_1, u_2, \ldots, u_r\}\) and \(G'' = G - \{uu_1, uu_2, \ldots, uu_r\} + \{vv_1, vv_2, \ldots, vv_t\}\), 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 (151) 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 \(\Delta \leq n - k\gamma_k\).

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

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

and

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

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 \( i = 1, \ldots, \Delta \), so \(|V(T^i) \cap D| \ge 1\). Therefore, \( \gamma_k \ge \Delta \ge n - k\gamma_k + 1 \), which implies that \( \gamma_k \ge \frac{n+1}{k+1} \). Since \( \gamma_k \ge 2 \), \( \gamma_k \le \frac{n}{k+1} \) by Lemma 2.4, a contradiction. Thus, \(|S_1| \ge 1\). Let \( i_l \in S_1 \) and

\[
\varepsilon_{T^{i_l}}(v_{i_l}) = \max \{ \varepsilon_{T^{i}}(v_i) \mid i \in S_1 \} = \lambda.
\]

Then \( 0 \le \lambda \le k - 1 \), so \(|S_2| \le \lfloor \frac{n-\lambda-1}{k} \rfloor \le \lfloor \frac{2k-3}{k} \rfloor \le \gamma_k - 1\).

If \( V(T^i) \cap D = D_i \) for some \( i \in S_1 \), then \( D - D_i + |v| \) 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 \( D' \cap V(T^{i_l}) = \emptyset \) where \( D' \) is a minimum distance \( k \)-dominating set of the tree \( T' = T - \bigcup_{i \in S_1} V(T^i) \).

We claim that \( D' \) is a distance \( k \)-dominating set of \( T \). Let \( y \in V(T^{i_l}) \) be the vertex such that \( d(v_{i_l}, y) = \lambda \) and \( y' \in D_i' = \bigcup_{y \in D} N_{T^i}(y) \cap D' \). Then \( y' \in V(T') \setminus V(T^{i_l}) \) and \( d(y, y') = d(y, v) + d(v, y') \le k \), so, for \( x \in \bigcup_{i \in S_1} V(T^i) \), 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 \( \bigcup_{i \in S_1} V(T^i) \) 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

\[
k + 1 < (k + 1)|S_2| + \lambda + 2 \le |V(T^i)| \le n - |S_1| + 1 = n - \Delta + |S_2| + 1,
\]

one has

\[
\gamma_k \le |D'|
\le \left\lfloor \frac{n - \Delta + |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} \Delta \ge n - k\gamma_k + 1, |S_2| \le \gamma_k - 1\) \text{)}
\le \gamma_k,
\]

a contradiction as desired. \( \square \)

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 \( T_{n,k,\gamma_k} \) be the set of all \( n \)-vertex trees with distance \( k \)-domination number \( \gamma_k \) 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 \( T_{n,k,\gamma_k} \) the tree formed from \( S_{n-k\gamma_k} \) by attaching a path \( P_{k-1} \) to \( v_1 \) and attaching a path
For some tree $R$ on $k$ vertices by Lemma 2.6. Assume that $V(R) = \{v_1, \ldots, v_k\}$. Then $d_R(v_i) = d'_T(v_i) - 1$. It is well known that $\sum_{i=1}^{k} d(u_i) = 2(n-1)$ for any $n$-vertex tree with vertex set $\{u_1, \ldots, u_n\}$. Hence, $\sum_{i=1}^{k} d_R(v_i) = 2(\gamma_k - 1)$. By the definition of the first Zagreb index, we have

$$M_1(T) = \frac{\gamma_k}{k} \sum_{i=1}^{k} d^2_T(v_i) + \sum_{x \in V(T) \setminus V(R)} d^2_T(x)$$

$$= \sum_{i=1}^{k} (d_T(v_i) - 1)^2 + \sum_{x \in V(T) \setminus V(R)} d^2_T(x) + 2 \sum_{i=1}^{k} (d_T(v_i) - 1) + \gamma_k$$
\[ M_1(R) + 4(k - 1)\gamma_k + \gamma_k + 2 \sum_{i=1}^{\gamma_k} d_R(v_i) + \gamma_k \]
\[ \leq M_1(S_{\gamma_k}) + 4(k - 1)\gamma_k + 2\gamma_k + 4(\gamma_k - 1) \]
\[ = \gamma_k(\gamma_k + 1) + 4(k\gamma_k - 1). \]

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

\[ M_2(T) = \sum_{x \in E(R)} d_T(x)d_T(y) + \sum_{y \in E(T)} d_T(x)d_T(y) \]
\[ = \sum_{x \in E(R)} (d_T(x) - 1)(d_T(y) - 1) + \sum_{x \in E(R)} (d_T(x) + d_T(y) - 1) \]
\[ + \sum_{x \in E(T)} d_T(x)d_T(y) \]
\[ = M_2(R) + \sum_{x \in V(R)} d_T(x)(d_T(x) - 1) - (\gamma_k - 1) \]
\[ + \sum_{x \in V(R)} 2d_T(x) + 4(k - 2)\gamma_k + 2\gamma_k \]
\[ = M_2(R) + \sum_{x \in V(R)} (d_T(x) - 1)^2 + 3 \sum_{x \in V(R)} (d_T(x) - 1) + 4k\gamma_k - 5\gamma_k - 1 \]
\[ = M_2(S_{\gamma_k}) + M_1(S_{\gamma_k}) + 4k\gamma_k + \gamma_k - 5 \]
\[ = 2\gamma_k^2 + (4k - 2)\gamma_k - 4. \]

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

**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 pendant vertices adjacent to \( u \) and \( y_1, y_2, \ldots, y_t \) are the pendant 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 \( G_1 = G - \{ y_t \} + \{ u y_t \} \) and \( G_2 = G - \{ x_t \} + \{ v x_t \} \). 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. \( \square \)

### 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 \( \gamma_k \). 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 \( T - \{ v_{i-1}, v_{i}, v_{i+1} \} \) 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 $\gamma(T) = 1$. 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 $T_{n,k,2}^i$ be the tree obtained from the path $P_{2k+2} = v_0 \cdots v_{2k+1}$ by joining $n - 2(k + 1)$ pendant vertices to $v_i$, where $i \in \{1, \ldots, 2k\}$.

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 $T \cong T_{n,k,2}^i$, where $i \in \{1, \ldots, k\}$. Also,

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

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

Proof Assume that $T \in T_{n,k,2}$ is the tree that maximizes the Zagreb indices and $P = v_0v_1 \cdots v_d$ is a diameter path of $T$. If $d \leq 2k$, then $\{v_{i, d}\}$ is a distance $k$-dominating set of $T$, a contradiction to $\gamma_k(T) = 2$. If $d \geq 2k + 2$, define $T' = \tau(T, v_i \cup v_{i+1})$, where $i \in \{1, \ldots, d - 2\}$. Then $T' \in T_{n,k,2}$. By Lemma 2.2, we have $M_1(T') > M_i(T)$, $i = 1, 2$, a contradiction. Hence, $d = 2k + 1$.

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

Since $M_1(T_{n,k,2}^i) = M_2(T_{n,k,2}^i)$ for $1 \leq i \neq j \leq d - 1$ and $T_{n,k,2}^i \cong T_{n,k,2}^j$ for $k + 1 \leq i \leq d - 1$, we get $T \cong T_{n,k,2}^i$, $i \in \{1, \ldots, k\}$. By direct computation, one has $M_1(T) = M_1(T_{n,k,2}^i) = (n - 2k)(n - 2k + 1) + 4(2k - 1)$, $i \in \{1, \ldots, k\}$, $j \in \{1, \ldots, k\}$. In addition, $M_2(T_{n,k,2}^i) = M_2(T_{n,k,2}^j) = M_2(T_{n,k,2}^k) = M_3(T_{n,k,2}^k) = \cdots = M_3(T_{n,k,2}^{k-1})$ and $T_{n,k,2}^i \cong T_{n,k,2}^j$ for $i \in \{k + 1, \ldots, d - 2\}$. Hence, $T \cong T_{n,k,2}^i$, where $i \in \{2, \ldots, k\}$. Moreover, $M_2(T) = M_2(T_{n,k,2}^i) = (n - 2k)(n - 2k + 2) + 8k - 8$. This completes the proof.

Lemma 3.3 Let tree $T \in T_{n,k,3}$. 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 $T \in T_{n,k,3}$. 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 $n > (k + 1)\gamma_k$ and the statement holds for $n - 1$ in the following.

Let $D$ be a minimum distance $k$-dominating set of $T$ and $P = v_0v_1 \cdots v_d$ 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 $\bigcup_{i=0}^k N_i^D(v_0) \cap D \neq \emptyset$ and $\bigcup_{i=0}^k N_i^D(v_0) \subseteq \left( \bigcup_{i=0}^{k-1} V(T_i) \cup \{v_k\} \right)$. Hence,
\((\bigcup_{i=0}^{k} V(T_i) \cup \{v_k\}) \cap D \neq \emptyset\). However, \(\bigcup_{i=0}^{k} N_{T_i}^2(x) \subseteq \bigcup_{i=0}^{k} N_{T_i}^2(v_k)\) 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 \(\bigcup_{i=0}^{k} V(T_i) \setminus \{v_{d-k}\} \cap D = \emptyset\). Suppose that \(v_0 = u_1, v_d = u_2, \ldots, u_m\) are the pendant 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 \(i \in \{1, \ldots, m\}\). If \(D \setminus \{w_i\}\) is a minimum distance \(k\)-dominating set of the tree \(T - w_i\), 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 \(\gamma_k(T - u_i) = \gamma_k(T)\), a contradiction. It follows that \(m \leq \gamma_k\).

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

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, \(\{v_k, v_{k+1} \cap \{v_{d-k-1}, v_{d-k}\} \subseteq D\). 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. \(\square\)

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 \(u_i\) 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, \(d_T(s) \leq \Delta \leq n - k\gamma_k\). 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,

\[
M_1(T) = M_1(T - u_i) + 2d(s)
\]

\[
\leq (n - 1 - k\gamma_k)(n - 1 - k\gamma_k + 1) + 4(k\gamma_k - 1) + 2(n - k\gamma_k)
\]

\[
= (n - k\gamma_k)(n - k\gamma_k + 1) + 4(k\gamma_k - 1).
\]

The equality holds if and only if \(T - u_i \cong T_{n-1,k,\gamma_k}\) and \(d_T(s) = \Delta = n - k\gamma_k\), 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

\[
\sum_{x \notin E(T)} d(x) \geq |A| + |B| = (|A| + |B|) + |B| \geq 2(n - 1 - d_T(s)) - \gamma_k.
\]
By the above inequality and the definition of $M_2$, we have

$$M_2(T) = M_2(T - u_i) + \sum_{v \in V(T)} d_T(v) - \sum_{x \in E(T)} d_T(x) - 1$$

$$\leq M_2(T - u_i) + 2(n - 1) - 2(n - 1 - d_T(s)) + y_k - 1$$

$$\leq (n - 1 - ky_k)[n - (k - 1)y_k] + (4k - 2)y_k - 4$$

$$+ 2(n - ky_k) + y_k - 1 \quad \text{(since } d_T(s) \leq \Delta \leq n - ky_k)$$

$$= (n - ky_k)[n - (k - 1)y_k] + (4k - 2)y_k - 4.$$

The equality (1) holds if and only if $|A| = y_k, |B| = n - 1 - d_T(s) - y_k$ and $d_T(x) = 2$ for $x \in B$. The equality (2) holds if and only if $T - u_i \cong T_{n-1,k,y_k}$ and $d_T(s) = \Delta = n - ky_k$.

Hence, $M_2(T) \leq (n - ky_k)[n - (k - 1)y_k] + (4k - 2)y_k - 4$ with equality if and only if $T \cong T_{n,k,y_k}$.

**Theorem 3.4** Let $T$ be a tree of order $n$ with distance $k$-domination number $\gamma_k \geq 3$. Then

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

and

$$M_2(T) \leq (n - ky_k)[n - (k - 1)y_k] + (4k - 2)y_k - 4,$$

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

**Proof** Let $T \in T_{n,k,y_k}$ 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 $S_T \neq \emptyset$, then we suppose that $T \in \{T^* \in T_{n,k,y_k} \mid |N_T(S_T)| = 1\}$ by Lemma 2.8 for establishing the maximum Zagreb indices of trees among $T_{n,k,y_k}$. If $v_d \in S_T \neq \emptyset$, 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 $\{v_0, v_1, v_d, v_d + 1\} \subseteq D$ 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 $T_i \cong S_{v_i(T')}$. Then $T' \in T_{n,k,y_k}$. By Lemma 2.2, we have $M_i(T) \leq M_i(T')$, $i = 1, 2$, with equality if and only if $T \cong T'$.

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

$$T'' = T' - \bigcup_{i \in \{1, \ldots, k\} \setminus \{i_0\}} \left\{v_i x \mid x \in N_T(v_i) \setminus \{v_{i-1}, v_{i+1}\}\right\}$$

$$+ \bigcup_{i \in \{1, \ldots, k\} \setminus \{i_0\}} \left\{v_i x \mid x \in N_T(v_i) \setminus \{v_{i-1}, v_{i+1}\}\right\}.$$
and

$$\tilde{T}'' = T' - \bigcup_{i \in \{1, \ldots, k\} \setminus \{i_1\}} \{v_i x \mid x \in N_{T'}(v_i) \setminus \{v_{i-1}, v_{i+1}\}\}$$

$$+ \bigcup_{i \in \{1, \ldots, k\} \setminus \{i_1\}} \{v_{i+1} x \mid x \in N_{T'}(v_i) \setminus \{v_{i-1}, v_{i+1}\}\}.$$ 

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

Suppose that $|N_{T''}(v_i) \setminus \{v_{i-1}, v_{i+1}\}| = |N_{\tilde{T}''}(v_i) \setminus \{v_{i-1}, v_{i+1}\}| = m$, $m \geq 0$. Let

$$T''' = T'' - \{v_{i-1} x \mid x \in N_{T''}(v_{i-1}) \setminus \{v_{i-2}, v_{i+1}\}\}$$

$$+ \{v_{i+1} x \mid x \in N_{T''}(v_{i+1}) \setminus \{v_{i-1}, v_{i+1}\}\}$$

$$\tilde{T}''' = \{v_i x \mid x \in N_{T''}(v_i) \setminus \{v_{i-1}, v_{i+1}\}\}$$

$$+ \{v_{i+1} x \mid x \in N_{\tilde{T}''}(v_{i+1}) \setminus \{v_{i-1}, v_{i+1}\}\}.$$ 

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 $\bigcup_{i=0}^{k} N_{T''}(v_i) \setminus \{v_0, \ldots, v_k\}$ 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

$$M_1(T''') = M_1(T') = 4 + (d_{T'}(v_{k+1}) + m)^2 - (2 + m)^2 - d_{T'''}^2(v_{k+1})$$

$$= 2m (d_{T'}(v_{k+1}) - 2) \geq 0,$$

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

\[
M_2(T''') - M_2(\overline{T}''') = 6 + (d_{\overline{T}'''}(v_{k+1}) + m)\left( m + \sum_{x \in N_{\overline{T}'''}(v_{k+1})} d_{\overline{T}'''}(x) \right) \\
- (m + 2)(m + 3) - d_{\overline{T}'''}(v_{k+1}) \sum_{x \in N_{\overline{T}'''}(v_{k+1})} d_{\overline{T}'''}(x) \\
= m\left[ d_{\overline{T}'''}(v_{k+1}) + \sum_{x \in N_{\overline{T}'''}(v_{k+1})} d_{\overline{T}'''}(x) - 5 \right] \\
\geq 0,
\]

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

\[
M_2(T''') - M_2(\overline{T}''') = 8 + (d_{\overline{T}'''}(v_{k+1}) + m)\left( m + \sum_{x \in N_{\overline{T}'''}(v_{k+1})} d_{\overline{T}'''}(x) \right) \\
- (m + 2)(m + 4) - d_{\overline{T}'''}(v_{k+1}) \sum_{x \in N_{\overline{T}'''}(v_{k+1})} d_{\overline{T}'''}(x) \\
= m\left[ d_{\overline{T}'''}(v_{k+1}) + \sum_{x \in N_{\overline{T}'''}(v_{k+1})} d_{\overline{T}'''}(x) - 6 \right] \\
\geq 0.
\]

Also, \( M_2(T''') - M_2(\overline{T}''') = 0 \) if and only if at least one of the following conditions holds:

1. \( m = 0 \), namely, \( \overline{T}''' \cong T''' \);
2. \( d_{\overline{T}'''}(v_k) = d_{\overline{T}'''}(v_{k+1}) = d_{\overline{T}'''}(v_{k+2}) = 2 \).

If \( i_1 \neq 1 \) and \( i_1 = k \), then

\[
M_2(T''') - M_2(\overline{T}''') = 4 + (d_{\overline{T}'''}(v_{k+1}) + m)\left( m + 2 + \sum_{x \in N_{\overline{T}'''}(v_{k+1}) \setminus \{v_k\}} d_{\overline{T}'''}(x) \right) \\
- (m + 2)(m + 2) - d_{\overline{T}'''}(v_{k+1}) \left( \sum_{x \in N_{\overline{T}'''}(v_{k+1}) \setminus \{v_k\}} d_{\overline{T}'''}(x) + m + 2 \right) \\
= m\left( \sum_{x \in N_{\overline{T}'''}(v_{k+1}) \setminus \{v_k\}} d_{\overline{T}'''}(x) - 2 \right) \\
\geq 0.
\]

As a result, \( M_2(T''') - M_2(\overline{T}''') = 0 \) if and only if at least one of the following conditions holds:

1. \( m = 0 \), which implies that \( \overline{T}''' \cong T''' \);
2. \( d_{\overline{T}'''}(v_{k+1}) = d_{\overline{T}'''}(v_{k+2}) = 2 \).

In what follows, we prove \( M_2(T''') \leq (n - k\gamma_k)(n - k\gamma_k + 1) + 4(k\gamma_k - 1) \) 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 \( T''' \cong T_{\mu,k,\gamma_k} \) by induction on \( \gamma_k \). 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

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

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 $d_{T''}(v_{k+1}) = \Delta = n-k\gamma_k$. 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, $M_1(T) \leq M_1(T') \leq M_1(T'') \leq M_1(T''-\{v_0\}) = (n-k\gamma_k)(n-k\gamma_k + 1) + 4(k\gamma_k - 1)$ 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. $T \cong T' \cong T'' \cong T_{n,k,\gamma_k}$;
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

\[
n - (k+1)\gamma_k \geq |N_{T''}(v_0) \setminus \{v_{i_0-1}, v_{i_0+1}\}|.
\]

Hence,

\[
d_{T''}(v_{k+1}) = d_{T''}(v_{k+1}) - |N_{T''}(v_0) \setminus \{v_{i_0-1}, v_{i_0+1}\}| \\
\geq d_{T''}(v_{k+1}) - \left[n - (k+1)\gamma_k\right] \\
= \gamma_k \geq 3,
\]

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

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

The equality holds if and only if $T''-\{v_0, \ldots, v_{k-1}\} \cong T_{n-k,k,\gamma_k-1}$ and $d_{T''}(v_{k+1}) = \Delta = n-k\gamma_k$.

In consideration of $d_{T''}(v) = 2$ for $i = 1, \ldots, k$, the equality holds if and only if $T'' \cong T_{n,k,\gamma_k}$.

Hence, if $i_3 \neq 1$, then $M_2(T) \leq M_2(T') \leq M_2(T'') \leq M_2(T''') \leq M_2(T''') \leq (n-k\gamma_k)[n-(k-1)\gamma_k] + (4k-2)\gamma_k - 4$, with equality if and only if at least one of the following conditions holds:
(1) \( T \cong T' \cong T'' \cong T_{n,k}\gamma_k \);
(2) \( T \cong T' \cong T'' \), where \( d_{T'}(v_k) = d_{T'}(v_{k+1}) = d_{T'}(v_{k+2}) = 2 \) and \( T'' \cong T_{n,k}\gamma_k \).

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

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

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. \( \square \)

**Remark 3.5** Borovičanin 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 \( T_{n,k}\gamma_k \cong T_{n,\gamma} \), \( T_{n,k,2} \cong T_{n,\gamma} \), \( i \in \{1, \ldots, k\} \), when \( k = 1 \). Let \( T \) be an \( n \)-vertex tree with distance \( k \)-domination number \( \gamma_k \). 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 \( \gamma_k = 1 \), \( T \cong T_{n,k,2}^{i} \), \( i \in \{1, \ldots, k\} \), 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 \( \gamma_k = 1 \), \( T \cong T_{n,k,2}^{i} \), \( i \in \{2, \ldots, k\} \), when \( k \geq 2 \) and \( \gamma_k = 2 \), or \( T \cong T_{n,k}\gamma_k \) otherwise.

**Appendix**

*Proof* Either \( M_1(G_1) > M_1(G) \) or \( M_1(G_2) > M_1(G) \), \( i = 1, 2 \), 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.
Let $G^* = G - \{x_1, \ldots, x_r, y_1, \ldots, y_t\}$, $d_{G^*}(u) = a$ and $d_{G^*}(v) = b$. Then

$$M_1(G_1) - M_1(G) = (a + r + 1)^2 + (b + t - 1)^2 - (a + r)^2 - (b + t)^2$$

$$= 2(a + r - b - t + 1)$$

and

$$M_1(G_2) - M_1(G) = (a + r - 1)^2 + (b + t + 1)^2 - (a + r)^2 - (b + t)^2$$

$$= 2(b + t - a - r + 1)$$

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

$$M_2(G_1) - M_2(G) = (a + r + 1) \left( \sum_{x \in N_{G^*}(u)} d_G(x) + r + 1 \right)$$

$$+ (b + t - 1) \left( \sum_{x \in N_{G^*}(v)} d_G(x) + t - 1 \right)$$

$$- (a + r) \left( \sum_{x \in N_{G^*}(u)} d_G(x) + r \right) - (b + t) \left( \sum_{x \in N_{G^*}(v)} d_G(x) + t \right)$$

$$= \sum_{x \in N_{G^*}(u)} d_G(x) - \sum_{x \in N_{G^*}(v)} d_G(x) + 2r - 2t + a - b + 2$$

and

$$M_2(G_2) - M_2(G) = (a + r - 1) \left( \sum_{x \in N_{G^*}(u)} d_G(x) + r - 1 \right)$$

$$+ (b + t + 1) \left( \sum_{x \in N_{G^*}(v)} d_G(x) + t + 1 \right)$$

$$- (a + r) \left( \sum_{x \in N_{G^*}(u)} d_G(x) + r \right) - (b + t) \left( \sum_{x \in N_{G^*}(v)} d_G(x) + t \right)$$

$$= \sum_{x \in N_{G^*}(v)} d_G(x) - \sum_{x \in N_{G^*}(u)} d_G(x) + 2t - 2r + b - a + 2.$$
If \( u \in N_G(v) \), then

\[
M_2(G_1) - M_2(G) = (a + r + 1) \left( \sum_{x \in N_G(u) \setminus \{v\}} d_G(x) + r + 1 \right) + (b + t - 1) \left( \sum_{x \in N_G(v) \setminus \{u\}} d_G(x) + t - 1 \right) \\
+ (a + r + 1)(b + t - 1) - (a + r) \left( \sum_{x \in N_G(u) \setminus \{v\}} d_G(x) + r \right) \\
- (b + t) \left( \sum_{x \in N_G(v) \setminus \{u\}} d_G(x) + t \right) - (a + r)(b + t) \\
= \sum_{x \in N_{G^*}(u) \setminus \{v\}} d_G(x) - \sum_{x \in N_{G^*}(v) \setminus \{u\}} d_G(x) + r - t + 1
\]

and

\[
M_2(G_2) - M_2(G) = (a + r - 1) \left( \sum_{x \in N_{G^*}(u) \setminus \{v\}} d_G(x) + r - 1 \right) + (b + t + 1) \left( \sum_{x \in N_{G^*}(v) \setminus \{u\}} d_G(x) + t + 1 \right) \\
+ (a + r - 1)(b + t + 1) - (a + r) \left( \sum_{x \in N_{G^*}(u) \setminus \{v\}} d_G(x) + r \right) \\
- (b + t) \left( \sum_{x \in N_{G^*}(v) \setminus \{u\}} d_G(x) + t \right) - (a + r)(b + t) \\
= \sum_{x \in N_{G^*}(v) \setminus \{u\}} d_G(x) - \sum_{x \in N_{G^*}(u) \setminus \{v\}} d_G(x) + t - r + 1.
\]

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

\[ \square \]

Acknowledgements

This work is financially supported by the National Natural Science Foundation of China (No. 11401004) and the Natural Science Foundation of Anhui Province of China (No. 1408085QA03).

Competing interests

The authors declare that they have no competing interests.

Authors’ contributions

All authors read and approved the final manuscript.

Publisher’s Note

Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Received: 25 September 2017 Accepted: 15 December 2017 Published online: 10 January 2018

References

1. Borovičanin, B, Furtula, B: On extremal Zagreb indices of trees with given domination number. Appl. Math. Comput. 279, 208-218 (2016)
2. Dobrynin, A, Kochetova, AA: Degree distance of a graph: a degree analogue of the Wiener index. J. Chem. Inf. Comput. Sci. 34, 1082-1086 (1994)
3. Dobrynin, A, Entringer, R, Gutman, I: Wiener index of trees: theory and applications. Acta Appl. Math. 66, 211-249 (2001)
54. Vasilyeva, A., Dardab, R., Stevanović, D.: Trees of given order and independence number with minimal first Zagreb index.

53. Lang, R.L., Deng, X.L., Lu, H.: Bipartite graphs with the maximal value of the second Zagreb index. J. Inequal. Appl. 2013, Article ID 180 (2013)

52. Gutman, I., Trinajstić, N.: Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons. Chem. Phys. Lett. 17, 535-538 (1972)

51. Gutman, I., Trinajstić, N.: Multiplicative Zagreb indices of trees. Bull. Soc. Math. Banja Luka 18, 17-23 (2011)

50. Hosamani, S.M., Basavanagoud, B.: New upper bounds for the first Zagreb index. MATCH Commun. Math. Comput. Chem. 74, 97-101 (2015)

49. Zhan, F.Q., Qiao, Y.F., Cai, J.L.: Unicyclic and bicyclic graphs with minimal augmented Zagreb index. J. Inequal. Appl. 2015, Article ID 126 (2015)

48. Balaban, A.T., Motoc, I., Bonchev, D., Mekenyan, O.: Topological indices for structure-activity correlations. Top. Curr. Chem. 114, 21-35 (1983)

47. Toledeschi, R., Componi, V.: Handbook of Molecular Descriptors. Wiley-VCH, Weinheim (2000)

46. Gutman, I., Trinajstić, N., Wilcox, C.F.: Graph theory and molecular orbitals. XII. Aromatic polyenes. J. Chem. Phys. 53, 3399-3405 (1975)

45. Nikolić, S., Kovačević, G., Miličević, A., Trinajstić, N.: The Zagreb indices 30 years after. Croat. Chem. Acta 76, 113-124 (2003)

44. Gutman, I., Das, K.C.: The first Zagreb index 30 years after. MATCH Commun. Math. Comput. Chem. 50, 427-438 (2000)

43. Milovanović, E.I., Milovanović, I.Z., Doličanin, E.C., Glogić, E.: A note on the first reformulated Zagreb index. Appl. Math. Comput. 273, 16-20 (2016)

42. Vasilyeva, A., Dardab, R., Stevanović, D.: Trees of given order and independence number with minimal first Zagreb index. MATCH Commun. Math. Comput. Chem. 55, 439-446 (2006)

41. Liu, B., Gutman, I.: Upper bounds for Zagreb indices of connected graphs. MATCH Commun. Math. Comput. Chem. 77, 775-782 (2014)

40. Furtula, B., Gutman, I.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 59, 233-239 (2005)

39. Liu, B., Deng, X.L., Lu, H.: Bipartite graphs with the maximal value of the second Zagreb index. Bull. Malays. Math. Sci. Soc. 36, 1-6 (2013)

38. Vasilyeva, A., Dardab, R., Stevanović, D.: Trees of given order and independence number with minimal first Zagreb index. MATCH Commun. Math. Comput. Chem. 62, 291-306 (2010)

37. Zhang, S.G., Zhang, H.L.: Unicyclic graphs with the smallest and largest first general Zagreb index. MATCH Commun. Math. Comput. Chem. 55, 9-18 (2005)

36. Liu, B., Deng, X.L., Lu, H.: Bipartite graphs with the maximal value of the second Zagreb index. Bull. Malays. Math. Sci. Soc. 38, 1-11 (2015)

35. Vasilyeva, A., Dardab, R., Stevanović, D.: Trees of given order and independence number with minimal first Zagreb index. MATCH Commun. Math. Comput. Chem. 62, 291-306 (2010)

34. Liu, B., Deng, X.L., Lu, H.: Bipartite graphs with the maximal value of the second Zagreb index. Bull. Malays. Math. Sci. Soc. 38, 1-11 (2015)

33. Gutman, I., Trinajstić, N.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 54, 233-239 (2005)

32. Gutman, I., Trinajstić, N.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 54, 233-239 (2005)

31. Vasilyeva, A., Dardab, R., Stevanović, D.: Trees of given order and independence number with minimal first Zagreb index. MATCH Commun. Math. Comput. Chem. 62, 291-306 (2010)

30. Zhang, S.G., Zhang, H.L.: Unicyclic graphs with the smallest and largest first general Zagreb index. MATCH Commun. Math. Comput. Chem. 55, 9-18 (2005)

29. Milovanović, E.I., Milovanović, I.Z., Doličanin, E.C., Glogić, E.: A note on the first reformulated Zagreb index. Appl. Math. Comput. 273, 16-20 (2016)

28. Furtula, B., Gutman, I.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 54, 233-239 (2005)

27. Vasilyeva, A., Dardab, R., Stevanović, D.: Trees of given order and independence number with minimal first Zagreb index. MATCH Commun. Math. Comput. Chem. 62, 291-306 (2010)

26. Furtula, B., Gutman, I.: A forgotten topological index. J. Math. Chem. 53, 1184-1190 (2015)

25. Hosamani, S.M., Basavanagoud, B.: New upper bounds for the first Zagreb index. MATCH Commun. Math. Comput. Chem. 74, 97-101 (2015)

24. Gutman, I., Trinajstić, N.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 54, 233-239 (2005)

23. Furtula, B., Gutman, I.: A forgotten topological index. J. Math. Chem. 53, 1184-1190 (2015)

22. Gutman, I., Trinajstić, N., Wilcox, C.F.: Graph theory and molecular orbitals. XII. Aromatic polyenes. J. Chem. Phys. 53, 3399-3405 (1975)

21. Nikolić, S., Kovačević, G., Miličević, A., Trinajstić, N.: The Zagreb indices 30 years after. Croat. Chem. Acta 76, 113-124 (2003)

20. Balaban, A.T., Motoc, I., Bonchev, D., Mekenyan, O.: Topological indices for structure-activity correlations. Top. Curr. Chem. 114, 21-35 (1983)

19. Toledeschi, R., Componi, V.: Handbook of Molecular Descriptors. Wiley-VCH, Weinheim (2000)

18. Gutman, I., Trinajstić, N., Wilcox, C.F.: Graph theory and molecular orbitals. XII. Aromatic polyenes. J. Chem. Phys. 53, 3399-3405 (1975)

17. Gutman, I.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 54, 233-239 (2005)

16. Gutman, I., Trinajstić, N.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 54, 233-239 (2005)

15. Gutman, I., Trinajstić, N.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 54, 233-239 (2005)

14. Milovanović, E.I., Milovanović, I.Z., Doličanin, E.C., Glogić, E.: A note on the first reformulated Zagreb index. Appl. Math. Comput. 273, 16-20 (2016)

13. Furtula, B., Gutman, I.: A forgotten topological index. J. Math. Chem. 53, 1184-1190 (2015)

12. Hosamani, S.M., Basavanagoud, B.: New upper bounds for the first Zagreb index. MATCH Commun. Math. Comput. Chem. 74, 97-101 (2015)

11. Milovanović, E.I., Milovanović, I.Z., Doličanin, E.C., Glogić, E.: A note on the first reformulated Zagreb index. Appl. Math. Comput. 273, 16-20 (2016)

10. Furtula, B., Gutman, I.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 54, 233-239 (2005)

9. Milovanović, E.I., Milovanović, I.Z., Doličanin, E.C., Glogić, E.: A note on the first reformulated Zagreb index. Appl. Math. Comput. 273, 16-20 (2016)

8. Furtula, B., Gutman, I.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 54, 233-239 (2005)

7. Milovanović, E.I., Milovanović, I.Z., Doličanin, E.C., Glogić, E.: A note on the first reformulated Zagreb index. Appl. Math. Comput. 273, 16-20 (2016)

6. Gutman, I., Trinajstić, N.: Multiplicative Zagreb indices of trees. MATCH Commun. Math. Comput. Chem. 54, 233-239 (2005)

5. Milovanović, E.I., Milovanović, I.Z., Doličanin, E.C., Glogić, E.: A note on the first reformulated Zagreb index. Appl. Math. Comput. 273, 16-20 (2016)

4. Balaban, A.T., Chiriac, A, Motoc, I., Simon, Z.: Steric Fit in Quantitative Structure-Activity Relations. Lecture Notes in Chemistry, vol. 15, pp. 22-27. Springer, Berlin (1980)
48. Das, K.C., Gutman, I.: Some properties of the second Zagreb index. MATCH Commun. Math. Comput. Chem. 52, 103-112 (2004)
49. Hua, H.B., Zhang, S.G., Xu, K.X.: Further results on the eccentric distance sum. Discrete Appl. Math. 160, 170-180 (2012)
50. Deng, H.Y.: A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs. MATCH Commun. Math. Comput. Chem. 57, 597-616 (2007)
51. Meir, A., Moon, J.W.: Relations between packing and covering numbers of a tree. Pac. J. Math. 61, 225-233 (1975)
52. Topp, J., Volkmann, L.: On packing and covering numbers of graphs. Discrete Math. 96, 229-238 (1991)