

Research Article

On the Zagreb indices of graphs with given Roman domination number

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Abstract: Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The two Zagreb indices $M_1 = \sum_{v \in V(G)} d_G^2(v)$ and $M_2 = \sum_{uv \in E(G)} d_G(u)d_G(v)$ are vertex degree based graph invariants that have been introduced in the 1970s and extensively studied ever since. In this paper, we first give a lower bound on the first Zagreb index of trees with given Roman domination number and we characterize all extremal trees. Then we present upper bound for Zagreb indices of unicyclic and bicyclic graphs with given Roman domination number.

Keywords: Zagreb index, Roman domination number, tree, unicyclic graph, bicyclic graph

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1. Introduction

All graphs considered in this paper are simple and connected. Let $G = (V, E)$ be a graph with vertex set $V = V(G)$ and edge set $E = E(G)$. An edge connecting

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two vertices u and v in the graph G is denoted by uv . The *degree* of a vertex u is denoted by $d_G(u)$ (or $d(u)$ for short) and it is the number of edges that are incident with u in the graph G . A vertex u in G is called *pendant* if $d(u) = 1$. The maximum vertex degree in a graph G is denoted by $\Delta(G)$ (or shortly Δ). For any vertex $v \in V$, the *open neighbourhood* of v is the set $N(v) = \{u \in V \mid uv \in E\}$ and the *closed neighbourhood* is the set $N[v] = N(v) \cup \{v\}$. As usual, by P_n , C_n and T_n we denote the path, cycle and tree on n vertices, respectively. The n -vertex graph G is said to be unicyclic or bicyclic graph if it has n or $n + 1$ edges, respectively. Let U_n and B_n denote the set of unicyclic and bicyclic graphs with n vertices, respectively. For other notation and terminologies which are not defined here, please refer the book by West [17].

A subset $D \subseteq V(G)$ is a *dominating set* of G if every vertex $V(G) \setminus D$ has a neighbor in D . The *domination number* of G , denoted by $\gamma(G)$, is the minimum cardinality of a dominating set of G . A subset $D \subseteq V(G)$ is a *total dominating set*, abbreviated as TDS, of G if every vertex G has a neighbor in D and G must be isolated-free. The *total domination number* of G , denoted by $\gamma_t(G)$, is the minimum cardinality of a total dominating set of G and was introduced by Cockayne *et al.* [9]. Domination in graphs has been an active research area in graph theory [12, 13].

For a graph $G = (V, E)$, let $f : V \rightarrow \{0, 1, 2\}$ be a function, and let (V_0, V_1, V_2) be the ordered partition of V induced by f , where $V_i = \{v \in V \mid f(v) = i\}$ and $|V_i| = n_i$, for $i = 0, 1, 2$. Note that there exists a 1 – 1 correspondence between the functions $f : V \rightarrow \{0, 1, 2\}$ and the ordered partitions (V_0, V_1, V_2) of V . Thus, we will write $f = (V_0, V_1, V_2)$.

A function $f = (V_0, V_1, V_2)$ is a *Roman dominating function* (RDF) if $V_2 \succ V_0$, where \succ means that the set V_2 dominates the set V_0 , i.e. $V_0 \subseteq N[V_2] \setminus V_2$. The weight of f is $f(V) = \sum_{v \in V} f(v) = 2n_2 + n_1$. The *Roman domination number*, denoted $\gamma_R(G)$ (or γ_R for short), equals the minimum weight of an RDF of G , and we say that a function $f = (V_0, V_1, V_2)$ is a γ_R -function if it is an RDF with $f(V) = \gamma_R(G)$. For more detail on Roman domination and its variant see [6–8].

The *first Zagreb index* M_1 and the *second Zagreb index* M_2 of graph G are defined as

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

and

$$M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v)$$

where $d_G(v)$ is the degree of vertex v in G .

The Zagreb indices has been studied extensively, see [3, 14, 16] and references therein. Relationships between various topological indices and domination number of graphs have been the focus of interest of the researchers for quite many years, and this direction is continuously vital, see [2, 4, 10, 15]. Specifically, Borovićanin and Furtula [4] investigated extremal Zagreb indices of trees with given domination number. Mojdeh *et al.* [15] obtained some upper bounds on the Zagreb indices of trees, unicyclic and

bicyclic graphs with given total domination number. Du *et al.* [11] and Ahmad Jamri *et al.* [1] determined the trees with maximum first and second Zagreb indices when Roman domination number is fixed, respectively.

In this paper, we first give a lower bound on the first Zagreb index of trees with given Roman domination number and we characterize all extremal trees. Then we present upper bound for Zagreb indices of unicyclic and bicyclic graphs with given Roman domination number.

2. Preliminary Results

In this section, we recall some known results that are useful for our main theorems. Let $\mathbb{T}(n, \gamma_R)$ be the set of n -vertex trees whose Roman domination number is γ_R , where $n \geq \max \left\{ \lceil \frac{3\gamma_R - 5}{2} \rceil, \gamma_R + 3 \right\}$.

Assume $T = (n_1, n_2, n_3, n_4, n_5)$ to represent a tree $T \in \mathbb{T}(n, \gamma_R)$ having n_i branches H_i of T at v , for $1 \leq i \leq 5$. It is trivial to obtain the following equations, see [1, 11].

$$M_1(T) = (n - \gamma_R + 1)^2 + n_1 + 5n_2 + 11n_3 + 15n_4 + 19n_5. \tag{1}$$

and

$$\begin{aligned} M_2(T) = & (n - \gamma_R + 1)n_1 + (2n - 2\gamma_R + 4)n_2 \\ & + (3n - 3\gamma_R + 9)n_3 + (3n - 3\gamma_R + 14)n_4 \\ & + (3n - 3\gamma_R + 19)n_5. \end{aligned} \tag{2}$$

Du *et al.* [11] obtained the upper bound of the first Zagreb index of trees with given Roman domination number as follows:

Theorem 1. [11] *Let $T \in \mathbb{T}(n, \gamma_R)$, where $n \geq \max \left\{ \lceil \frac{3\gamma_R - 5}{2} \rceil, \gamma_R + 3 \right\}$. Then*

$$M_1(T) \leq \begin{cases} n^2 - (2\gamma_R - 3)n + \gamma_R^2 + 2\gamma_R - 8 & \text{if } \gamma_R \text{ is even} \\ n^2 - (2\gamma_R - 3)n + \gamma_R^2 + 2\gamma_R - 9 & \text{if } \gamma_R \text{ is odd.} \end{cases}$$

In particular,

- *When γ_R is even, the equality holds if and only if*

$$T = \left(\frac{2n - 3\gamma_R + 4}{2}, 0, \frac{\gamma_R - 2}{2}, 0, 0 \right).$$

- *When γ_R is odd, the equality holds if and only if*

$$T = \left(\frac{2n - 3\gamma_R + 3}{2}, 1, \frac{\gamma_R - 3}{2}, 0, 0 \right) \text{ or } T = \left(\frac{2n - 3\gamma_R + 5}{2}, 0, \frac{\gamma_R - 5}{2}, 1, 0 \right).$$

By using similar method, Ahmad Jamri *et al.* [1] determined the upper bound of the second Zagreb index of trees with given Roman domination number as follows:

Theorem 2. [1] Let $T \in \mathbb{T}(n, \gamma_R)$, where $n \geq \max \left\{ \lceil \frac{3\gamma_R - 5}{2} \rceil, \gamma_R + 3 \right\}$. Then

$$M_2(T) \leq \begin{cases} (n-1)(n-\gamma_R+1) + 3\gamma_R - 6 & \text{if } \gamma_R \text{ is even} \\ (n-1)(n-\gamma_R+1) + 3\gamma_R - 7 & \text{if } \gamma_R \text{ is odd} \end{cases}.$$

For the even γ_R , the equality holds if and only if $T = \left(\frac{2n-3\gamma_R+4}{2}, 0, \frac{\gamma_R-2}{2}, 0, 0 \right)$. For the odd γ_R , the equality holds if and only if $T = \left(\frac{2n-3\gamma_R+3}{2}, 1, \frac{\gamma_R-3}{2}, 0, 0 \right)$ or $T = \left(\frac{2n-3\gamma_R+5}{2}, 0, \frac{\gamma_R-5}{2}, 1, 0 \right)$.

3. Lower bound for the first Zagreb index of trees with given Roman domination number

In this section, we obtain the lower bound for the first Zagreb index of trees with given Roman domination number.

We consider the following family \mathcal{F} of graphs, which we define recursively. For any $k \geq 1$ we consider the path with $3k$ vertices in \mathcal{F} and we construct new graphs in the family in two ways.

- (i) If $T' \in \mathcal{F}$ satisfies that there exists $v \in V(T')$ such that $d(v) = 2$ and $f(v) = 2$ belongs to a Roman dominating function in T' , and we take any path P , whose consecutive vertices are $w_1, w_2, \dots, w_{3k+1}$, then the graph T with $V(T) = V(T') \cup V(P)$ and $E(T) = E(T') \cup E(P) \cup \{vw_1\}$, belongs to \mathcal{F} .
- (ii) If $T' \in \mathcal{F}$, v is a leaf in T' and we take any path P , whose consecutive vertices are w_1, w_2, \dots, w_{3k} , then the graph T with $V(T) = V(T') \cup V(P)$ and $E(T) = E(T') \cup E(P) \cup \{vw_1\}$, belongs to \mathcal{F} .

By using a simple induction, we can see that for any tree $T \in \mathcal{F}$, $M_1(T) = 6n(T) - 3\gamma_R(T) - 6$.

Theorem 3. Let T be a tree with order n and Roman domination number γ_R . Then

$$M_1(T) \geq 6n - 3\gamma_R - 6, \tag{3}$$

with equality if and only if $T \in \mathcal{F}$.

Proof. We prove the theorem by induction on n . It can easily be checked that the result holds for $n \leq 4$. Assume the result holds for all trees of order $n' < n$ and let T be a tree of order $n \geq 5$. Suppose first that $\Delta = 2$. Then $T \cong P_n$ and we have $M_1(T) = 4n - 6$ and $\gamma_R(T) = \lceil \frac{2n}{3} \rceil$. Now it can easily be seen that $4n - 6 \geq 6n - 3\lceil \frac{2n}{3} \rceil - 6$, and also equality holds if $n = 3k$ for any $k \geq 1$.

Next, suppose that $\Delta \geq 3$ and let v_1, v_2, \dots, v_{d+1} be a diametral path of T such that $d_T(v_2)$ is maximized. Clearly, v_1 and v_{d+1} are pendant vertices. Let $T' = T - v_1$. We consider two cases.

Case 1. Assume that $\gamma_R(T') = \gamma_R(T) - 1$.

Then clearly $d_T(v_2) \in \{2, 3\}$. By the induction hypothesis we have

$$\begin{aligned} M_1(T) &= M_1(T') + 2d_T(v_2) \\ &\geq 6(n-1) - 3(\gamma_R(T) - 1) - 6 + 2d_T(v_2) \\ &= 6n - 3\gamma_R(T) - 6 + 2d_T(v_2) - 3 \\ &> 6n - 3\gamma_R(T) - 6. \end{aligned}$$

Case 2. Assume that $\gamma_R(T') = \gamma_R(T)$.

We distinguish two subcases.

Subcase 2.1. $d_T(v_2) \geq 3$.

Then we have

$$\begin{aligned} M_1(T) &= M_1(T') + 2d_T(v_2) \\ &\geq 6(n-1) - 3\gamma_R(T') - 6 + 2d_T(v_2) \\ &= 6n - 3\gamma_R(T) - 6 + 2(d_T(v_2) - 3) \\ &\geq 6n - 3\gamma_R(T) - 6. \end{aligned} \tag{4}$$

Assume that the equality holds in (4). Then the two inequalities occurring in (4) become equalities, that is $M_1(T') = 6(n-1) - 3\gamma_R(T') - 6$ and $d_T(v_2) = 3$. By the induction hypothesis we have $T' \in \mathcal{F}$. On the other hand, we deduce from $\gamma_R(T') = \gamma_R(T)$ that there is a $\gamma_R(T')$ -function f such that $f(v_2) = 2$. Thus T can be obtained from T' as construction (i) and so $T \in \mathcal{F}$.

Subcase 2.2. $d_T(v_2) = 2$.

In such a case, if f is a $\gamma_R(T)$ -function, then $f(v_2) = 2$, $f(v_3) = 0$ and $f(u) \leq 1$ for every $u \in N(v_3) \setminus \{v_2\}$. It follows from the choice of f and $\gamma_R(T') = \gamma_R(T)$ that $d_T(v_3) = 2$. If we take $T'' = T - \{v_1, v_2, v_3\}$, then we have $\gamma_R(T) = \gamma_R(T'') + 2$ and by the induction hypothesis we have

$$\begin{aligned} M_1(T) &= M_1(T'') + 2d_T(v_4) + 8 \\ &\geq 6(n-3) - 3(\gamma_R(T) - 2) - 6 + 2d_T(v_4) + 8 \\ &= 6n + 3\gamma_R(T) - 6 + 2(d_T(v_4) - 2) \\ &\geq 6n - 3\gamma_R - 6. \end{aligned} \tag{5}$$

Assume that the equality holds in (5). Then the inequalities occurring in (5) become equalities, that is $M_1(T'') = 6(n - 1) - 3\gamma_R(T'') - 6$ and $d_T(v_4) = 2$. By the induction hypothesis we have $T'' \in \mathcal{F}$. Thus T can be obtained from T as construction (ii) and so $T \in \mathcal{F}$. \square

We conclude this section with the following open problem.

Problem 1. Study the lower bound for the second Zagreb index of trees in terms of the order and the Roman domination number.

4. Upper bound for Zagreb indices of unicyclic and bicyclic graphs with given Roman domination number

In this section, we first present an upper bound for Zagreb indices of unicyclic and bicyclic graphs with a given Roman domination number.

We first obtain the following result.

Lemma 1. *Let G be a graph and $f = (V_0, V_1, V_2)$ be a $\gamma_R(G)$ -function. Then for an edge e of G , if $G - e$ does not have isolated vertex, then $\gamma_R(G - e) \in \{\gamma_R(G), \gamma_R(G) + 1\}$.*

Proof. Let $f = (V_0, V_1, V_2)$ be a $\gamma_R(G)$ -function and $e = uv$ be an edge of G . If G has an edge uv and $f(u) = f(v) = 0$, then $f = (V_0, V_1, V_2)$, where $V_0 = (V - V_1 - V_2) \cup \{u, v\}$, defines a Roman dominating function of $G - e$. Hence, $\gamma_R(G - e) = |V_1| + 2|V_2| = \gamma_R(G)$. If $f(u) = 2$ and $f(v) = 0$, then $f = (V_0, V_1, V_2)$, where $V_0 = N(u) \cup \{v\}$, $V_1 = V - N[u]$, and $V_2 = \{u\}$, defines a Roman dominating function of $G - e$. Hence, $\gamma_R(G - e) = \gamma_R(G) + 1$. \square

Now, we obtain an upper bound for the first Zagreb index of unicyclic graph G with given Roman domination number and maximum degree.

Theorem 4. *Let U_n be an unicyclic graph on $n \geq \max \left\{ \lceil \frac{3\gamma_R - 2}{2} \rceil, \gamma_R + 4 \right\}$ vertices with maximum degree Δ and Roman domination number γ_R . Then*

$$M_1(U_n) \leq \begin{cases} n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 4\Delta - 10 & \text{if } \gamma_R \text{ is even} \\ n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 4\Delta - 9 & \text{if } \gamma_R \text{ is odd.} \end{cases}$$

Proof. Let $e = uv$ be an edge of the cycle of U_n so that $T = U_n - e$ is a tree and that $\Delta(T) = \Delta(U_n) = \Delta$. By Lemma 1 we have $\gamma_R(T) \in \{\gamma_R(U_n), \gamma_R(U_n) + 1\}$ and it follows from our assumption that $n \geq \max \left\{ \lceil \frac{3\gamma_R(T) - 5}{2} \rceil, \gamma_R(T) + 3 \right\}$. If $\gamma_R(T)$ is

even, then by Theorem 1, we have

$$\begin{aligned}
 M_1(U_n) &= M_1(T) + (d(u))^2 - (d(u) - 1)^2 + (d(v))^2 - (d(v) - 1)^2 \\
 &= M_1(T) + 2(d(u) + d(v) - 1) \\
 &\leq n^2 - (2\gamma_R(T) - 3)n + (\gamma_R(T))^2 + 2\gamma_R(T) - 8 + 2(2\Delta - 1) \\
 &= n^2 - (2\gamma_R(T) - 3)n + (\gamma_R(T))^2 + 2\gamma_R(T) + 4\Delta - 10.
 \end{aligned} \tag{6}$$

Assume that $\gamma_R(T)$ is odd. By Theorem 1, we have

$$\begin{aligned}
 M_1(U_n) &= M_1(T) + (d(u))^2 - (d(u) - 1)^2 + (d(v))^2 - (d(v) - 1)^2 \\
 &= M_1(T) + 2(d(u) + d(v) - 1) \\
 &\leq n^2 - (2\gamma_R(T) - 3)n + (\gamma_R(T))^2 + 2\gamma_R(T) - 9 + 2(2\Delta - 1) \\
 &= n^2 - (2\gamma_R(T) - 3)n + (\gamma_R(T))^2 + 2\gamma_R(T) + 4\Delta - 11.
 \end{aligned} \tag{7}$$

Now, there exists two cases using Lemma 1. If $\gamma_R(T) = \gamma_R(U_n) = \gamma_R$, then the result is clear by (6) and (7).

Assume that $\gamma_R(T) = \gamma_R(U_n) + 1 = \gamma_R + 1$. Then we replace $\gamma_R(T)$ with $\gamma_R(U_n) + 1 = \gamma_R + 1$ in above equation. If γ_R is even, then $\gamma_R(T)$ is odd and by applying (7) and the fact that $\gamma_R(G) \leq 4n(G)/5$ for any graph G (see [5]), we have

$$\begin{aligned}
 M_1(U_n) &\leq n^2 - (2(\gamma_R + 1) - 3)n + (\gamma_R + 1)^2 + 2(\gamma_R + 1) + 4\Delta - 11 \\
 &= n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 - 2(n - \gamma_R) + 2\gamma_R + 4\Delta - 8 \\
 &\leq n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 4\Delta - 8 - 2 \left\lceil \frac{n}{5} \right\rceil \\
 &\leq n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 4\Delta - 10.
 \end{aligned}$$

If γ_R is odd, then $\gamma_R(T)$ is even and by applying (6) and the fact that $\gamma_R(G) \leq 4n(G)/5$ for any graph G , we have

$$\begin{aligned}
 M_1(U_n) &\leq n^2 - (2(\gamma_R + 1) - 3)n + (\gamma_R + 1)^2 + 2(\gamma_R + 1) + 4\Delta - 10 \\
 &= n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 - 2(n - \gamma_R) + 2\gamma_R + 4\Delta - 7 \\
 &\leq n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 4\Delta - 7 - 2 \left\lceil \frac{n}{5} \right\rceil \\
 &\leq n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 4\Delta - 9.
 \end{aligned}$$

□

Next we determine an upper bound for the second Zagreb index for unicyclic graphs with given Roman domination number and maximum degree of G .

Theorem 5. Let U_n be an unicyclic graph with $n \geq \max \left\{ \lceil \frac{3\gamma_R - 2}{2} \rceil, \gamma_R + 4 \right\}$ vertices, maximum degree Δ and Roman domination number γ_R . Then

$$M_2(U_n) \leq \begin{cases} (n-1)(n-\gamma_R+1) + 3\gamma_R + 3\Delta^2 - 2\Delta - 6 & \text{if } \gamma_R \text{ is even} \\ (n-1)(n-\gamma_R+1) + 3\gamma_R + 3\Delta^2 - 2\Delta - 7 & \text{if } \gamma_R \text{ is odd.} \end{cases}$$

Proof. Let $e = uv$ be an edge of the cycle of U_n so that $T = U_n - e$ be a tree and $\Delta(T) = \Delta(U_n) = \Delta$. Using Lemma 1 and the assumption we have $n \geq \max \left\{ \lceil \frac{3\gamma_R(T)-5}{2} \rceil, \gamma_R(T) + 3 \right\}$.

If $\gamma_R(T)$ is even, then by Theorem 2 we have

$$\begin{aligned} M_2(U_n) &= M_2(T) + d(u)d(v) + \sum_{z \in N(u), z \neq v} d(z) + \sum_{z \in N(v), z \neq u} d(z) \\ &\leq (n-1)(n-\gamma_R(T)+1) + 3\gamma_R(T) - 6 + \Delta^2 + 2\Delta(\Delta-1). \end{aligned} \quad (8)$$

Likewise, if $\gamma_R(T)$ is odd, then we have

$$\begin{aligned} M_2(U_n) &= M_2(T) + d(u)d(v) + \sum_{z \in N(u), z \neq v} d(z) + \sum_{z \in N(v), z \neq u} d(z) \\ &\leq (n-1)(n-\gamma_R(T)+1) + 3\gamma_R(T) - 7 + \Delta^2 + 2\Delta(\Delta-1). \end{aligned} \quad (9)$$

If $\gamma_R(T) = \gamma_R(U_n) = \gamma_R$, then the result is clear. Assume that $\gamma_R(T) = \gamma_R(U_n) + 1 = \gamma_R + 1$. Then we replace $\gamma_R(T)$ with $\gamma_R(U_n) + 1 = \gamma_R + 1$ in above equation. If γ_R is even, then $\gamma_R(T)$ is odd and by applying (9), we have

$$\begin{aligned} M_2(U_n) &\leq (n-1)(n-(\gamma_R+1)+1) + 3(\gamma_R+1) - 7 + \Delta^2 + 2\Delta(\Delta-1) \\ &\leq (n-1)(n-\gamma_R+1) + 3\gamma_R - 7 + 3\Delta^2 - 2\Delta + 4 - n \\ &= (n-1)(n-\gamma_R+1) + 3\gamma_R + 3\Delta^2 - 2\Delta - 9. \end{aligned}$$

If γ_R is odd, then $\gamma_R(T)$ is even and by applying (8), we have

$$\begin{aligned} M_2(U_n) &\leq (n-1)(n-(\gamma_R+1)+1) + 3(\gamma_R+1) - 6 + \Delta^2 + 2\Delta(\Delta-1) \\ &\leq (n-1)(n-\gamma_R+1) + 3\gamma_R - 6 + 3\Delta^2 - 2\Delta + 4 - n \\ &= (n-1)(n-\gamma_R+1) + 3\gamma_R + 3\Delta^2 - 2\Delta - 8. \end{aligned}$$

□

Now we present an upper bound for Zagreb indices of bicyclic graph G with given Roman domination number.

Theorem 6. Let B_n be an bicyclic graph with $n \geq \max \left\{ \lceil \frac{3\gamma_R - 2}{2} \rceil, \gamma_R + 4 \right\}$ vertices, maximum degree Δ and Roman domination number γ_R . Then

$$M_1(B_n) \leq \begin{cases} n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 6\Delta - 12 & \text{if } \gamma_R \text{ is even} \\ n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 6\Delta - 11 & \text{if } \gamma_R \text{ is odd.} \end{cases}$$

Proof. Let $U_n = B_n - e$, where $e = uv$ be an edge of one of the cycles of B_n such that $\Delta(U_n) = \Delta(B_n) = \Delta$. By Lemma 1, $\gamma_R(U_n) \in \{\gamma_R(B_n), \gamma_R(B_n) + 1\}$. Then $M_1(B_n) = M_1(U_n) + 2d(u) + 2d(v) - 2$. We consider four cases.

Case 1. Assume that $\gamma_R(U_n) = \gamma_R(B_n) = \gamma_R$ and γ_R is even.

By Theorem 4, we have

$$\begin{aligned} M_1(B_n) &= M_1(U_n) + 2(2\Delta - 1) \\ &\leq n^2 - (2\gamma_R(U_n) - 3)n + (\gamma_R(U_n))^2 + 2\gamma_R(U_n) + 2\Delta - 10 + 2(2\Delta - 1) \\ &= n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 6\Delta - 12 \end{aligned}$$

Case 2. Assume that $\gamma_R(U_n) = \gamma_R(B_n) = \gamma_R$ and γ_R is odd.

$$\begin{aligned} M_1(B_n) &= M_1(U_n) + 2(2\Delta - 1) \\ &\leq n^2 - (2\gamma_R(U_n) - 3)n + (\gamma_R(U_n))^2 + 2\gamma_R(U_n) + 2\Delta - 9 + 2(2\Delta - 1) \\ &= n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 6\Delta - 11 \end{aligned}$$

Case 3. Assume that $\gamma_R(B_n - e) = \gamma_R(B_n) + 1 = \gamma_R + 1$ and γ_R is even.

By Theorem 4, we have

$$\begin{aligned} M_1(B_n) &= M_1(U_n) + 2(2\Delta - 1) \\ &\leq n^2 - (2\gamma_R(U_n) - 3)n + (\gamma_R(U_n))^2 + 2\gamma_R(U_n) + 2\Delta - 10 + 2(2\Delta - 1) \\ &\leq n^2 - (2(\gamma_R + 1) - 3)n + (\gamma_R + 1)^2 + 2(\gamma_R + 1) + 2\Delta - 10 + 2(2\Delta - 1) \\ &= n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 - 2(n - \gamma_R) + 3 + 2\gamma_R + 6\Delta - 12 \\ &\leq n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 6\Delta - 12 \end{aligned}$$

Case 4. Assume that $\gamma_R(B_n - e) = \gamma_R(B_n) + 1 = \gamma_R + 1$ and γ_R is odd.

As above we have

$$\begin{aligned} M_1(B_n) &= M_1(U_n) + 2(2\Delta - 1) \\ &\leq n^2 - (2\gamma_R(U_n) - 3)n + (\gamma_R(U_n))^2 + 2\gamma_R(U_n) + 2\Delta - 9 + 2(2\Delta - 1) \\ &\leq n^2 - (2(\gamma_R + 1) - 3)n + (\gamma_R + 1)^2 + 2(\gamma_R + 1) + 2\Delta - 9 + 2(2\Delta - 1) \\ &= n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 - 2(n - \gamma_R) + 3 + 2\gamma_R + 6\Delta - 11 \\ &\leq n^2 - (2\gamma_R - 3)n + (\gamma_R)^2 + 2\gamma_R + 6\Delta - 11, \end{aligned}$$

and the proof is complete. □

We now determine an upper bound of the second Zagreb index of bicyclic graph G .

Theorem 7. *Let B_n be an bicyclic graph with $n \geq \max \left\{ \lceil \frac{3\gamma_R - 2}{2} \rceil, \gamma_R + 4 \right\}$ vertices, maximum degree Δ vertices and Roman domination number γ_R . Then*

$$M_2(B_n) \leq \begin{cases} (n-1)(n-\gamma_R+1) + 3\gamma_R + 6\Delta^2 - 4\Delta - 6 & \text{if } \gamma_R \text{ is even} \\ (n-1)(n-\gamma_R+1) + 3\gamma_R + 6\Delta^2 - 4\Delta - 7 & \text{if } \gamma_R \text{ is odd.} \end{cases}$$

Proof. Let $U_n = B_n - e$, where $e = uv$ be an edge of one of the cycles of B_n such that $\Delta(U_n) = \Delta(B_n) = \Delta$. By Lemma 1, $\gamma_R(U_n) \in \{\gamma_R(B_n), \gamma_R(B_n) + 1\}$. Clearly, we have $M_2(B_n) = M_2(U_n) + 2d(u) + 2d(v) - 2$. We consider four cases.

Case 1. Assume that $\gamma_R(B_n - e) = \gamma_R(B_n) = \gamma_R$ and γ_R is even. Using Theorem 5, we obtain

$$\begin{aligned} M_2(B_n) &= M_2(U_n) + d(u)d(v) + \sum_{z \in N(u), z \neq v} d(z) + \sum_{z \in N(v), z \neq u} d(z) \\ &\leq (n-1)(n-\gamma_R(U_n)+1) + 3\gamma_R(U_n) + 3\Delta^2 - 2\Delta - 6 + \Delta^2 + 2\Delta(\Delta-1) \\ &= (n-1)(n-\gamma_R+1) + 3\gamma_R + 6\Delta^2 - 4\Delta - 6. \end{aligned}$$

Case 2. Assume that $\gamma_R(B_n - e) = \gamma_R(B_n) = \gamma_R$ and γ_R is odd. As above we have

$$\begin{aligned} M_2(B_n) &= M_2(U_n) + d(u)d(v) + \sum_{z \in N(u), z \neq v} d(z) + \sum_{z \in N(v), z \neq u} d(z) \\ &\leq (n-1)(n-\gamma_R(U_n)+1) + 3\gamma_R(U_n) + 3\Delta^2 - 2\Delta - 7 + \Delta^2 + 2\Delta(\Delta-1) \\ &= (n-1)(n-\gamma_R+1) + 3\gamma_R + 6\Delta^2 - 4\Delta - 7. \end{aligned}$$

Case 3. Assume that $\gamma_R(B_n - e) = \gamma_R(B_n) = \gamma_R$ and γ_R is even. As in the Case 1, we have

$$\begin{aligned} M_2(B_n) &= M_2(U_n) + d(u)d(v) + \sum_{z \in N(u), z \neq v} d(z) + \sum_{z \in N(v), z \neq u} d(z) \\ &\leq (n-1)(n-\gamma_R(U_n)+1) + 3\gamma_R(U_n) + 3\Delta^2 - 2\Delta - 6 + \Delta^2 + 2\Delta(\Delta-1) \\ &\leq (n-1)(n-(\gamma_R+1)+1) + 3(\gamma_R+1) + 3\Delta^2 - 2\Delta - 6 + \Delta^2 + 2\Delta(\Delta-1) \\ &\leq (n-1)(n-\gamma_R+1) + 3\gamma_R + 6\Delta^2 - 4\Delta - 5. \end{aligned}$$

Case 4. Assume that $\gamma_R(B_n - e) = \gamma_R(B_n) = \gamma_R$ and γ_R is odd. As above we have

$$\begin{aligned} M_2(B_n) &= M_2(U_n) + d(u)d(v) + \sum_{z \in N(u), z \neq v} d(z) + \sum_{z \in N(v), z \neq u} d(z) \\ &\leq (n-1)(n-\gamma_R(U_n)+1) + 3\gamma_R(U_n) + 3\Delta^2 - 2\Delta - 7 + \Delta^2 + 2\Delta(\Delta-1) \\ &\leq (n-1)(n-(\gamma_R+1)+1) + 3(\gamma_R+1) + 3\Delta^2 - 2\Delta - 7 + \Delta^2 + 2\Delta(\Delta-1) \\ &\leq (n-1)(n-\gamma_R+1) + 3\gamma_R + 6\Delta^2 - 4\Delta - 8, \end{aligned}$$

and the proof is complete. \square

The following problem arise from Theorems 4-7 immediately.

Problem 2. Study the lower bound for Zagreb indices of unicyclic and bicyclic graphs with given Roman domination number.

5. Concluding remarks

This paper is devoted to the investigation of relationship between the Zagreb indices and Roman domination number of trees. More precisely, we establish a lower bound of the first Zagreb index of trees in terms of Roman domination number, and all the tree(s) attaining the equality are characterized. We also obtain upper bound for Zagreb indices of unicyclic and bicyclic graphs in terms of Roman domination number. As a possible sequel in the future, it is interesting to investigate the relationship between the Zagreb indices (or other well-known topological indices, e.g., Randić index, Wiener index) and other types of domination number of graphs.

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