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The minimum Zagreb indices for unicyclic graphs with fixed Roman domination number

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Abstract: Let $G = (V, E)$ be a graph with the vertex set V and the edge set E. The first Zagreb index of a graph G is defined to be the sum of squares of degrees of all the vertices of the graph. The second Zagreb index of the graph G is the sum of the $d(u)d(v)$ for every edge $uv \in E$, where $d(u)$ and $d(v)$ denote the degree of the vertices $u, v \in V$. In this paper, we propose new lower bounds of the Zagreb indices of unicyclic graphs in terms of the order and the Roman domination number. We prove that $4n - 2\left(\gamma_R - \lceil \frac{2n}{3} \rceil\right)$ and $4n - 3\left(\gamma_R - \lceil \frac{2n}{3} \rceil\right)$ are the sharp lower bounds for the first Zagreb index and the second Zagreb index, respectively. Also, we characterize the extremal trees for these lower bounds.

Keywords: Roman domination number, unicyclic graphs, Zagreb indices.

AMS Subject classification: 05C69, 05C35

1. Introduction

We consider finite, undirected and simple graphs. Let $G = (V, E)$ be a simple undirected graph with $|V(G)| = n$ vertices and $|E(G)| = m$ edges. For a vertex $v \in V(G)$,

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the degree of v, written by $d_G(v)$ or $d(v)$, is the number of edges incident with v. A pendant vertex is a vertex of degree 1. Assume that $PV(G) = \{v : d(v) = 1\}$. For two vertices u and v $(u \neq v)$, the distance between u and v, denoted by $d(u, v)$, is the number of edges in the shortest path joining u and v. The open neighborhood of a vertex $v \in V$ is denoted by $N(u) = \{u \in V | uv \in E\}$, while its closed neighborhood is given by $N[u] = N(u) \cup \{u\}$. We use $G - x$, $G - xy$ and $G + uv$ to denote the graph obtained from G by deleting the vertex $x \in V(G)$, the edge $xy \in E(G)$ and adding an edge $uv \notin E(G)$, where $x, y \in V(G)$.
Let C_k be a cycle of length k. Unicyclic graphs U_n are connected graphs of order n and size n that contain exactly one cycle. For other notation and terminologies which are not defined here, please refer to the book by West [20].

For a graph $G = (V, E)$, let $f : V \to \{0, 1, 2\}$, and let (V_0, V_1, V_2) be the ordered partition of V induced by f, where $V_i = \{v \in V | f(v) = i\}$ and $|V_i| = n_i$, for $i = 0, 1, 2$. Note that there exists a $1 - 1$ correspondence between the functions $f : V \to \{0, 1, 2\}$ and the ordered partitions (V_0, V_1, V_2) of $V(G)$. 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 $f(V) = \sum_{v \in V(G)} f(v) = 2n_2 + n_1$ [8].

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 and $f(V) = \gamma_R(G)$. For some most recent research on the Roman domination number of graphs, see [16, 17, 19].

The *first Zagreb index* M_1 and the *second Zagreb index* M_2 of graph G are defined as [12]

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

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.

Many results were obtained on the bounds of the Zagreb indices in graphs [6, 7, 15]. In [13], an extremal tree with the maximum second Zagreb index in the class of trees with a given degree sequence was characterized. Liu and Liu characterized an extremal unicyclic graph that achieves the maximum second Zagreb index in the class of unicyclic graphs with a given degree sequence [14]. Zhou in [23] obtained sharp upper bounds for the Zagreb indices of a graph. Das et al. proposed some upper and lower bounds on the second Zagreb index in terms of the order, the minimum degree and the maximum degree in a graph [9, 10]. In [5], Behtoei et al. determined the extremal graph with the maximal first Zagreb index among all graphs with an edge or vertex connectivity k.

Xu in [21] investigated the Zagreb indices of graphs with a given clique number. Ali et al. [4] obtained extremal graphs of the second Zagreb index among all the connected molecular n-vertex graphs with cyclomatic number $v \geq 3$. Stankov et al. [18] established new inequalities involving the first Zagreb index, the inverse degree index and the modified first Zagreb index. Some new and old bounds on the first Zagreb index are given as corollaries of the obtained inequalities.

Yan et al. [22] established the bounds for the second Zagreb index of unicyclic graphs and characterized the extremal graphs. Ahmad Jamri et al. [2] proposed a lower bound on the first Zagreb index of trees with a given Roman domination number and characterized all extremal trees. Furthermore, the upper bound for Zagreb indices of unicyclic and bicyclic graphs with a given Roman domination number are investigated. In [3], Ahmad Jamri et al. presented a lower bound on the second Zagreb index of trees with n vertices and Roman domination number. The upper bounds on the first and second Zagreb indices of trees with a given Roman domination number were studied in [1, 11].

In this paper, we obtain new lower bounds for the Zagreb indices of unicyclic graphs using the order and the Roman domination number.

2. Extremal unicyclic graphs for the Zagreb indices with a given Roman domination number

First, we obtain a lower bound for the first Zagreb index of unicyclic graphs with n vertices and Roman domination number γ_R. To do this, we consider

$$\mathcal{U}^+_{n,k} = \{G \in \mathcal{U}_{n,k} : M_1(G) \text{ is minimum}\}.$$

We first give the following lemma that will be used in the proof of Theorem 1.

Lemma 1. *Let $G \in \mathcal{U}^+_{n,k}$ be a unicyclic graph with order n and k leaves with the minimum Roman domination number in $\mathcal{U}_{n,k}$. For any $uv \in E(G)$ with $d(v) = 1$, then $d(u) \geq 3$.*

Proof. We consider the path $P = v_0v_1 \ldots v_s (s \geq 2)$ of G such that $d(v_0) = 1$, $d(v_s) \geq 3$ and $d(v_i) \geq 2$ for $1 \leq i \leq s-1$. Let $w_1w_2 \in E(G)$ with $d_G(w_i) \geq 2$, $i = 1, 2$. We take $G' = G - \{w_1w_2, v_{s-1}v_s\} + \{w_1v_{s-1}, w_2v_0\}$. Thus, $G^{'} \in U_{n,k}$. But we obtain

$$M_1(G') - M_1(G) = 4 + \big(d(v_s) - 1\big)^2 - 1 - d(v_s)^2 = 4 - 2d(v_2) < 0.$$

a contradiction with the choice of G. □

We consider the family $\mathcal{F}$ of graphs which includes cycles of order at least 3 and graphs obtained as follows.

Suppose that $G' \in \mathcal{F}$ is a cycle of order $3q$ or $3q+1$. The conservative vertices on cycle G' are $x_1, x_2, \ldots, x_{3q}$ or $x_1, x_2, \ldots, x_{3q+1}$ where $q \geq 0$. We construct the graph G by adding a vertex v_1 with $deg(v_1) = 1$ to one of the vertices G' (assume that x_1). Therefore, the graph G where $V(G) = V(G') \cup \{v_1\}$ and $E(G) = E(G') \cup \{v_1 x_1\}$, belongs to $\mathcal{F}$ (see Figure 1).

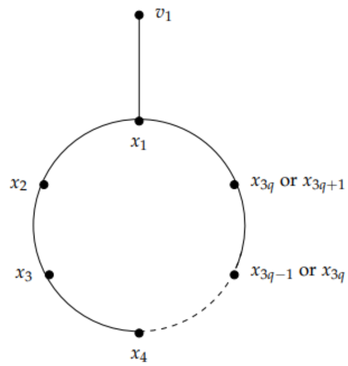

Figure 1. **The graphs of Family $\mathcal{F}$.**

Lemma 2. *Let G be an unicyclic graph of order n and Roman domination number γ_R. If $G \in \mathcal{F}$, then*

$$M_1(G) = 4n - 2\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right),$$

Proof. To simplify the calculations, we consider

$$g(n, \gamma_R) = 4n - 2\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right).$$

If G is a cycle with n vertices we can easily check that the result is true. Let $G \in \mathcal{F}$ with n vertices where $n \equiv 1, 2 \ (mod\ 3)$ be unicyclic with a cycle of order $n-1$ shown in Figure 1. Using the proof of Theorem 5 for the graph G of order $n \equiv 1, 2 \ (mod\ 3)$, we have $\gamma_R = \lceil \frac{2(n-1)}{3} \rceil$ and consequently $g(n, \gamma_R) = 4n + 2$. Since the sequence degree of graph G shown in Figure 1 is $(1, 3, 2, 2, \ldots, 2)$, thus the first Zagreb index equals to $M_1(G) = 1 + 9 + 4(n-2) = 4n + 2$. Therefore, the result is completed.

□

Theorem 1. *Let U_n be a unicyclic graph with order n and Roman domination number γ_R. Then*

$$M_1(U_n) \geq 4n - 2\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right),$$

where the equality holds if and only if $G \in \mathcal{F}$.

Proof. Using again the function

$$g(n,\gamma_R) = 4n - 2\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right).$$

Let G be an unicyclic graph of order n with k leaves where $0 \leq k \leq n-3$. Suppose that G contains a unique cycle C of order q with labeled vertices w_i for $i = 1,\dots,q$. Let $f = (V_0, V_1, V_2)$ be a γ_R-function of graph G.

If $k = 0$, then $G \simeq C_n$. Since $M_1(C_n) = 4n$ and $\gamma_R(C_n) = \lceil \frac{2n}{3} \rceil$, we have $g(n,\gamma_R) = 4n$. Therefore, $M_1(C_n) = g(n,\gamma_R)$. If $k = 1$, then G has only a vertex of degree 1. Let $uv \in E$ such that $d(v) = 1$. Thus, for $x \in V(G) \setminus \{u,v\}$ we have $d(x) = 2$ and $d(u) = 3$. In this case, $u \in V_2$ and $v \in V_0$. Therefore, $\gamma_R(C_{n-1}) = \lceil \frac{2(n-1)}{3} \rceil$ and $M_1(G) = 4n+2$. If $n \equiv 0 \ (mod\ 3)$, then $g(n,\gamma_R) = 4n$ and we have $M_1(G) > g(n,\gamma_R)$ and if $n \equiv 1,2 \ (mod\ 3)$, then $g(n,\gamma_R) = 4n+2$ and consequently, $M_1(G) = g(n,\gamma_R)$. Therefore, we suppose that $k \geq 2$ and the result is true for any unicyclic U_n with $k-1$ leaves. We prove that the result holds when U_n has n vertices and k leaves.

Suppose that $G \in \mathcal{U}^+_{n,k}$. Let $v_1 \in PV(G)$ with $uv_1 \in E(G)$. Then using Lemma 1, $d(u) = t \geq 3$. Let $N(u) \cap PV(G) = \{v_1,\dots,v_r\}$ and $N(u) \setminus PV(G) = \{x_1,\dots,x_{t-r}\}$. Then, $t - r \geq 1$ and all $d(x_i) = d_i \geq 2$. We study the following cases.

Case 1. Let $f(v_1) = 0$. So, $f(u) = 2$ and in this case, we consider the following cases.

Case 1.1. Assume that $u \in V(C)$ and $N(u) \cap V(C) = \{x_1, x_2\}$ such that $d(u) \geq 3$ and $d(x_i) \geq 2$ for $i = 1, 2$. In such that, the vertices of cycle C are $x_2ux_1w_1w_2\dots w_{q-3}$ such that $d(w_i) \geq 2$ for $i = 1,\dots,q-3$ and according to the labeling of vertices on cycle C, we consider $x_2 = w_{q-2}$, $u = w_{q-1}$, $x_1 = w_q$.

Case 1.1.1. We suppose that the set V_2 has at least one of the vertices x_1 and x_2. Without loss of generality, we suppose that $f(x_1) = 2$. Then we take $G_1 = G - ux_1 + v_1x_1$. In such a case, we have $\gamma_R(G_1) = \gamma_R(G)$ and $G_1 \in \mathcal{U}_{n,k-1}$. Therefore, we get

$$\begin{aligned} M_1(G) &= M_1(G_1) + 2t - 4 \\ &\geq g(n,\gamma_R) + 2 \\ &> g(n,\gamma_R). \end{aligned}$$

Case 1.1.2. We suppose that $f(x_1) = f(x_2) = 0$. Then we consider the path $x_1w_1w_2$ on cycle C. We consider two new cases.

i) If $f(w_1) = 2$ then, we take $G_1 = G - ux_1 + v_1x_1$ and we follow Case 1.1.1. Therefore, we have $\gamma_R(G_1) = \gamma_R(G)$ and $G_1 \in \mathcal{U}_{n,k-1}$. Consequently, $M_1(G) > g(n,\gamma_R)$.

ii) Assume that $f(w_1)=0$. In this case, we take $G_1 = G - v_1$. Thus, we have $G_1 \in \mathcal{U}_{n-1,k-1}$. Since $f(v_1) = f(x_1) = f(x_2) = 0$ and $f(u) = 2$, thus $\gamma_R(G_1) = \gamma_R(G)$. Therefore, we obtain

$$\begin{aligned} M_1(G) &= M_1(G_1) + 2t \\ &\geq 4(n-1) - 2\left(\gamma_R - \left\lceil \frac{2(n-1)}{3} \right\rceil\right) + 6 \\ &\geq 4n - 2\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right) + 2 \\ &\geq g(n, \gamma_R) + 2 \\ &> g(n, \gamma_R). \end{aligned}$$

Case 1.2. Assume that $u \notin V(C)$. We consider the path $v_1 u x_1 y_1 \cdots y_l w_1$ such that $w_1 \in V(C)$, $d(v_1) = 1$, $d(u) = t \geq 3$, $d(x_1) = d_1 \geq 2$, $d(w_1) \geq 3$ and $d_{y_i} \geq 2$ for $1 \leq i \leq l$.

Case 1.2.1. Let $f(x_1) = 2$. Then, we take $G_2 = G - ux_1 + v_1x_1$. In this case, we have $\gamma_R(G_2) = \gamma_R(G)$ and $G_2 \in \mathcal{U}_{n,k-1}$. So, $M_1(G_2) \geq g(n, \gamma_R)$. We obtain

$$\begin{aligned} M_1(G) &= M_1(G_2) + 2t - 4 \\ &\geq g(n, \gamma_R) + 2 \\ &> g(n, \gamma_R). \end{aligned}$$

Case 1.2.2. Let $f(x_1) = 0$. We consider $G_2 = G - v_1$ and in such a case, $G_2 \in \mathcal{U}_{n,k-1}$ and $\gamma_R(G_2) = \gamma_R(G)$. Therefore, we have

$$\begin{aligned} M_1(G) &= M_1(G_2) + 2t \\ &\geq g(n-1, \gamma_R) + 6 \\ &\geq 4(n-1) - 2\left(\gamma_R - \left\lceil \frac{2(n-1)}{3} \right\rceil\right) + 6 \\ &\geq 4n - 2\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right) + 2 \\ &= g(n, \gamma_R) + 2 \\ &> g(n, \gamma_R). \end{aligned}$$

Case 2. Let $f(v_1) = 1$ and $f(u) = 0$. We consider the following cases.

Case 2.1. Assume that $u \in V(C)$ and the vertices of cycle C are $x_2 u x_1 w_1 w_2 \ldots w_{q-3}$ such that $d(w_i) \geq 2$, $1 \leq i \leq q-3$, $d(x_1), d(x_2) \geq 2$, $d(u) = t \geq 3$ and according to the labeling of vertices on cycle C, $x_2 = w_{q-2}$, $u = w_{q-1}$, $x_1 = w_q$.

Case 2.1.1. We suppose that at least one of $f(x_1)$ and $f(x_2)$ equals 0 for $i = 1, 2$. Without loss of generality, we suppose that $f(x_1) = 0$. Thus, we take $G_1' = G - x_1u+$

v_1x_1. Therefore, we have $G_1' \in \mathcal{U}_{n,k-1}$ and $\gamma_R(G_1') = \gamma_R(G)$. Similar to Case 1.1.1, we obtain

$$\begin{aligned} M_1(G) &= M_1(G_1') + 2t - 4 \\ &\geq g(n, \gamma_R) + 2 \\ &> g(n, \gamma_R). \end{aligned}$$

Case 2.1.2. Assume that $x_1, x_2 \notin V_0$. Since each vertex of V_0 is adjacent to at most a vertex of V_1, thus $\{f(x_1), f(x_2)\} \in \{1, 2\}$. Thus, we have two new cases.

i) We suppose one of the vertices x_1 or x_2 is at the set V_1. Without loss of generality, we consider $f(x_1) = 1$ and $f(x_2) = 2$. In this case, we take $G_1' = G - ux_1 + v_1x_1$. Therefore, $G_1' \in \mathcal{U}_{n,k-1}$ and $\gamma_R(G_1') = \gamma_R(G)$. So, we have $M_1(G_1') \geq g(n, \gamma_R)$. Similar to Case 2.1.1, we obtain $M_1(G) > g(n, \gamma_R)$.

ii) We suppose that $f(x_1) = f(x_2) = 2$. In such a case, we take $G' = G - v_1$. Therefore, $G' \in \mathcal{U}_{n-1,k-1}$ and $\gamma_R(G') = \gamma_R(G) - 1$. Thus, we obtain

$$\begin{aligned} M_1(G) &= M_1(G') + 2t \\ &\geq f(n-1, \gamma_R - 1) + 6 \\ &\geq 4(n-1) - 2\left(\gamma_R - 1 - \left\lceil \frac{2(n-1)}{3} \right\rceil\right) + 6 \\ &\geq 4n - 2\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right) + 4 \\ &= g(n, \gamma_R) + 4 \\ &> g(n, \gamma_R). \end{aligned}$$

Case 2.2. Assume that $u \notin V(C)$. We consider the path $v_1ux_1y_1 \cdots y_lw_1$ in G such that $d(v_1) = 1$, $d(u) = t \geq 3$, $d(x_1) = d_1 \geq 2$, $d(w_1) \geq 3$ and $d_{y_i} \geq 2$ for $1 \leq i \leq l$.

Case 2.2.1. Let $x_1 \in V_0$. Since $f(u) = 0$ and $f(v_1) = 1$ thus, $deg(u) = 3$. We consider $G_2' = G - ux_1 + v_1x_1$ that in such a case, we have $G_2' \in \mathcal{U}_{n,k-1}$ and $\gamma_R(G_2') = \gamma_R(G)$. Thus, $M_1(G_2') > g(n, \gamma_R)$. Similar to the above discussions, we obtain

$$\begin{aligned} M_1(G) &= M_1(G_2') + 2 \\ &\geq f(n, \gamma_R) + 2 \\ &> f(n, \gamma_R). \end{aligned}$$

Case 2.2.2. Let $f(x_1) = 2$. In this case, we take $G_2' = G - v_1$ and we have,

$G'_2 \in \mathcal{U}_{n-1,k-1}$ and $\gamma_R(G'_2) = \gamma_R(G) - 1$. Therefore, we have

$$\begin{aligned} M_1(G) &= M_1(G'_2) + 2t \\ &\geq g(n-1, \gamma_R - 1) + 6 \\ &\geq 4(n-1) - 2\left(\gamma_R - \left\lceil \frac{2(n-1)}{3} \right\rceil\right) + 6 \\ &\geq 4n - 2\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right) + 4 \\ &= g(n, \gamma_R) + 4 \\ &> g(n, \gamma_R). \end{aligned}$$

This then completes the proof. □

Here, we obtain the lower bound for the second Zagreb index of unicyclic graphs with a given Roman domination number. To do this, we recall some known results that are useful for our main results.

Suppose that $\mathcal{U}_{n,k} = \{G : G \textit{ is unicyclic graph with } n \textit{ vertices and } k \textit{ leaves},\ 0 \leq k \leq n-3\}$. We consider

$$\mathcal{U}^*_{n,k} = \{G \in \mathcal{U}_{n,k} : M_2(G) \textit{ is minimum}\}.$$

Lemma 3. [22] *Let $G \in \mathcal{U}^*_{n,k}$ be an unicyclic graph of order n and k leaves with the Roman domination number in $\mathcal{U}_{n,k}$. For any $uv \in E(G)$ with $d(v) = 1$, then $d(u) \geq 3$.*

Lemma 4. [8] *For cycle C_n, $\gamma_R(C_n) = \lceil \frac{2n}{3} \rceil$.*

Lemma 5. *Let G be an unicyclic graph of order n and Roman domination number γ_R. if $G \in \mathcal{F}$, then*

$$M_2(G) = 4n - 3\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right).$$

Proof. To simplify the calculations, we denote

$$f(n, \gamma_R) = 4n - 3\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right).$$

If $G \in \mathcal{F}$ is a cycle with n vertices then we can easily check that the result is true. We suppose that the graph $G \in \mathcal{F}$ is the graph shown in Figure 1. Therefore, G is an unicyclic graph of order n where $n \equiv 1, 2$ $(mod\ 3)$ and G contains a cycle of order $n-1$. Thus, one can consider $\gamma_R(C_{n-1})$-function for graph G. So, $\gamma_R(G) = \lceil \frac{2(n-1)}{3} \rceil$ and consequently,

$$f(n, \gamma_R) = 4n - 3\left(\left\lceil \frac{2(n-1)}{3} \right\rceil - \left\lceil \frac{2n}{3} \right\rceil\right) = 4n + 3.$$

On the other hand, it can be easily obtained that $M_2(G) = 4n + 3$. Therefore, the result is completed. □

Theorem 2. *Let U_n be an unicyclic graph of order n and Roman domination number γ_R. Then*

$$M_2(U_n) \geq 4n - 3\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right),$$

which the equality holds if and only if $G \in \mathcal{F}$.

Proof. Using again the function

$$f(n, \gamma_R) = 4n - 3\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right).$$

Let G be an unicyclic graph of order n with k leaves where $0 \leq k \leq n-3$. Suppose that G contains a unique cycle C of order q with labeled vertices w_i for $i = 1, \ldots, q$. Let $f = (V_0, V_1, V_2)$ be a γ_R-function of graph G.

If $k = 0$, then $G \cong C_n$. Since $M_2(C_n) = 4n$ and $\gamma_R(C_n) = \left\lceil \frac{2n}{3} \right\rceil$, we have $f(n, \gamma_R) = 4n$. Therefore, $M_2(C_n) = f(n, \gamma_R)$. If $k = 1$, then G has only a vertex of degree 1. Let $uv \in E$ such that $d(v) = 1$. Thus, for $x \in V(G) \setminus \{u, v\}$ we have $d(x) = 2$ and $d(u) = 3$. In this case, $u \in V_2$ and $v \in V_0$. Therefore, $\gamma_R(C_{n-1}) = \left\lceil \frac{2(n-1)}{3} \right\rceil$ and $M_2(G) = 4n + 3$. Since $f(n, \gamma_R) = 4n$, for $n \equiv 0$ $(mod\ 3)$ and $f(n, \gamma_R) = 4n + 3$, for $n \equiv 1, 2$ $(mod\ 3)$ then, $M_2(G) \geq f(n, \gamma_R)$. Therefore, we assume that $k \geq 2$ and the result is true for any unicyclic U_n with $k - 1$ leaves. We investigate that it is true when U_n has n vertices and k leaves.

Suppose that $G \in \mathcal{U}^*_{n,k}$. Let $v_1 \in PV(G)$ with $uv_1 \in E(G)$. Then using Lemma 3, $d(u) = t \geq 3$. Let $N(u) \cap PV(G) = \{v_1, \ldots, v_r\}$ and $N(u) \setminus PV(G) = \{x_1, \ldots, x_{t-r}\}$. Then, $t - r \geq 1$ and all $d(x_i) = d_i \geq 2$. We study the following cases.

Case 1. We suppose that $f(v_1) = 0$. Thus, $f(u) = 2$ and in this case, we consider the following cases.

Case 1.1 Assume that $u \in V(C)$ and $N(u) \cap V(C) = \{x_1, x_2\}$ such that $d(u) \geq 3$ and $d(x_i) \geq 2$ for $i = 1, 2$. In such that, the vertices of cycle C are $x_2 u x_1 w_1 w_2 \ldots w_{q-3}$ such that $d(w_i) \geq 2$ for $i = 1, \ldots, q-3$ and according to the labeling of vertices on cycle C, we consider $x_2 = w_{q-2}$, $u = w_{q-1}$, $x_1 = w_q$.

Case 1.1.1. We suppose that the set V_2 has at least one of the vertices x_1 and x_2. Without loss of generality, we suppose that $f(x_1) = 2$. Then we take $G' = G - ux_1 + v_1 x_1$. In such a case, we have $\gamma_R(G') = \gamma_R(G)$ and $G' \in \mathcal{U}_{n,k-1}$. Therefore, we obtain

$$\begin{aligned}
M_2(G) &= M_2(G') + (t-2)d_1 + (r+t) - 1 - 2(t-1) + \sum_{i=2}^{t-r} d_i \\
&= M_2(G') + (t-2)d_1 + (r-t) + \sum_{i=2}^{t-r} d_i + 1 \\
&\geq M_2(G') + 2(t-2) + (r-t) + 2(t-r-1) + 1 \\
&\geq M_2(G') + 2t + (t-r) - 5 \\
&\geq f(n, \gamma_R) + 2 \\
&> f(n, \gamma_R).
\end{aligned}$$

Case 1.1.2. We suppose that $f(x_1) = f(x_2) = 0$. Then we consider the path $x_1w_1w_2$ on cycle C. We consider two new cases.

i) If $f(w_1) = 2$, then we take $G' = G - ux_1 + v_1x_1$ and we follow the case 1.1.1. Therefore, we have $\gamma_R(G') = \gamma_R(G)$ and $G' \in \mathcal{U}_{n,k-1}$. Consequently, $M_2(G) > f(n, \gamma_R)$.

ii) Assume that $f(w_1) = 0$. In this case, we take $G_1 = G - v_1$. Thus we have $G_1 \in \mathcal{U}_{n,k-1}$. Since $f(v_1) = f(x_1) = f(x_2) = 0$ and $f(u) = 2$, thus $\gamma_R(G_1) = \gamma_R(G)$. Therefore, we get

$$\begin{aligned}
M_2(G) &= M_2(G_1) + (t+r) + \sum_{i=1}^{t-r} d_i - 1 \\
&\geq M_2(G_1) + (t+r) + 2(t-r) - 1 \\
&= M_2(G_1) + 2t + (t-r) - 1 \\
&\geq f(n-1, \gamma_R) + 6 \\
&= 4(n-1) - 3\left(\gamma_R - \left\lceil \frac{2(n-1)}{3} \right\rceil\right) + 6 \\
&= 4n - 3\left(\gamma_R - \left\lceil \frac{2(n-1)}{3} \right\rceil\right) + 2 \\
&\geq 4n - 3\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right) + 2 \\
&= f(n, \gamma_R) + 2 \\
&> f(n, \gamma_R).
\end{aligned}$$

Case 1.2. We suppose that $u \notin V(C)$. We consider the path $v_1ux_1y_1 \ldots y_lw_1$ such that $w_1 \in V(C)$, $d(v_1) = 1$, $d(u) = t \geq 3$, $d(x_1) = d_1 \geq 2$, $d(w_1) \geq 3$ and $d_{y_i} \geq 2$ for $1 \leq i \leq l$.

Case 1.2.1. Assume that $f(x_1) = 2$. Then we take $G_2 = G - ux_1 + v_1x_1$. In this case, we have $\gamma_R(G') = \gamma_R(G)$ and $G' \in \mathcal{U}_{n,k-1}$. So, $M_2(G') \geq f(n, \gamma_R)$. We obtain

$$\begin{aligned}
M_2(G) &= M_2(G') + (t-2)d_1 + (r-t+1) + \sum_{i=2}^{t-r} d_i \\
&\geq M_2(G') + 2(t-2) + (r-t+1) + 2(t-r-1) \\
&= M_2(G') + 2t + (t-r) - 3 \\
&\geq M_2(G') + 6 + 1 - 3 \\
&\geq f(n, \gamma_R) + 4 \\
&> f(n, \gamma_R).
\end{aligned}$$

Case 1.2.2. Let $f(x_1) = 0$. We consider $G_1 = G - v_1$ and in such a case, $G_1 \in \mathcal{U}_{n,k-1}$ and $\gamma_R(G_1) = \gamma_R(G)$. Therefore, we have

$$\begin{aligned}
M_2(G) &= M_2(G_1) + (t+r) + \sum_{i=1}^{t-r} d_i - 1 \\
&\geq M_2(G_1) + 2t + (t-r) - 1 \\
&\geq M_2(G_1) + 6 \\
&\geq f(n-1, \gamma_R) + 6 \\
&= 4n - 3\left(\gamma_R - \left\lceil \frac{2(n-1)}{3} \right\rceil\right) + 2 \\
&\geq f(n, \gamma_R) + 2 \\
&> f(n, \gamma_R).
\end{aligned}$$

Case 2. We suppose that $f(v_1) = 1$ and $f(u) = 0$. We consider the following cases.

Case 2.1. Assume that $u \in V(C)$ and the vertices of cycle C are $x_2ux_1w_1w_2 \ldots w_{q-3}$ such that $d(w_i) \geq 2$, $1 \leq i \leq q-3$, $d(x_1), d(x_2) \geq 2$, $d(u) = t \geq 3$ and according to the labeling of vertices on cycle C, $x_2 = w_{q-2}$, $u = w_{q-1}$, $x_1 = w_q$.

Case 2.1.1. We suppose that at least one of $f(x_1)$ and $f(x_2)$ equals 0 for $i = 1, 2$. Without loss of generality, we suppose that $f(x_1) = 0$. Thus we take $G' = G - x_1u + v_1x_1$. Therefore, we have $G' \in \mathcal{U}_{n,k-1}$ and $\gamma_R(G') = \gamma_R(G)$. Similar to Case 1.1.1, we obtain

$$\begin{aligned}
M_2(G) &= M_2(G') + (t-2)d_1 + (r+t) - 1 - 2(t-1) + \sum_{i=2}^{t-r} d_i \\
&= M_2(G') + (t-2)d_1 + (r-t) + \sum_{i=2}^{t-r} d_i + 1 \\
&\geq M_2(G') + 2t + (t-r) - 5 \\
&\geq f(n, \gamma_R) + 2 \\
&> f(n, \gamma_R).
\end{aligned}$$

Case 2.1.2. Assume that $x_1, x_2 \notin V_0$. Since each vertex of V_0 is adjacent to at most two vertices of V_1, thus $\{f(x_1), f(x_2)\} \in \{1, 2\}$. So we have two new cases.

i) We suppose one of the vertices x_1 or x_2 is in the set V_1. Without loss of generality, we consider $f(x_1) = 1$ and $f(x_2) = 2$. In this case, we take $G'_1 = G - ux_1 + v_1x_1$. Therefore, $G' \in \mathcal{U}_{n,k-1}$ and $\gamma_R(G') = \gamma_R(G)$. Thus, we have $M_2(G') \geq f(n, \gamma_R)$. Similar to Case 2.1.1, we obtain $M_2(G) > f(n, \gamma_R)$.

ii) Let $f(x_1) = f(x_2) = 2$. Therefore, $d(x_1) \geq 3$ or $d(x_2) \geq 3$. Assume that $d(x_1) \geq 3$. If $N(x_1) \cap PV(G) \neq \emptyset$, then there is a vertex $s \in PV(G)$ such that $sx_1 \in E$, $d(s) = 1$, $d(x_1) \geq 3$, $f(s) = 0$ and $f(x_1) = 2$. Therefore, by considering $x_1 = u$ and $s = v_1$, we have Case 1 and the result follows.

Otherwise, we take $G_1 = G - v_1$ and we have $\gamma_R(G_1) = \gamma_R(G) - 1$. Therefore, we obtain

$$\begin{aligned}
M_2(G) &= M_2(G_1) + (t + r) + \sum_{i=1}^{t-r} d_i - 1 \\
&\geq M_2(G_1) + 2t + (t - r) - 1 \\
&\geq M_2(G_1) + 6 \\
&\geq f(n - 1, \gamma_R - 1) + 6 \\
&= 4(n - 1) - 3\left(\gamma_R - 1 - \left\lceil \frac{2(n-1)}{3} \right\rceil\right) + 6 \\
&= 4n - 3\left(\gamma_R - \left\lceil \frac{2(n-1)}{3} \right\rceil\right) + 5 \\
&= 4n - 3\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right) + 5 \\
&\geq f(n, \gamma_R) + 5 \\
&> f(n, \gamma_R).
\end{aligned}$$

Case 2.2. Assume that $u \notin V(C)$. We consider the path $v_1ux_1y_1 \ldots y_lw_1$ in G such that $d(v_1) = 1$, $d(u) = t \geq 3$, $d(x_1) = d_1 \geq 2$, $d(w_1) \geq 3$ and $d_{y_i} \geq 2$ for $1 \leq i \leq l$.

Case 2.2.1. Let $x_1 \in V_0$. Then we consider $G' = G - ux_1 + v_1x_1$ that in such a case, we have $G'_2 \in \mathcal{U}_{n,k-1}$ and $\gamma_R(G') = \gamma_R(G)$. So, $M_2(G') > f(n, \gamma_R)$. Similar to the above discussions, we obtain

$$\begin{aligned}
M_2(G) &= M_2(G') + (t - 2)d_1 + (r - t) + \sum_{i=2}^{t-r} d_i + 1 \\
&\geq M_2(G') + 2(t - 2) + (r - t) + 2(t - r - 1) + 1 \\
&= f(n, \gamma_R) + 2t + (t - r) - 5 \\
&\geq f(n, \gamma_R) + 2 \\
&> f(n, \gamma_R).
\end{aligned}$$

Case 2.2.2. We suppose that $f(x_1) = 2$. So, we take $G_1 = G - v_1$ and we have $\gamma_R(G_1) = \gamma_R(G) - 1$. Therefore, we obtain

$$\begin{aligned} M_2(G) &= M_2(G_1) + (t+r) + \sum_{i=1}^{t-r} d_i - 1 \\ &\geq M_2(G_1) + 2t + (t-r) - 1 \\ &\geq M_2(G_1) + 6 \\ &\geq f(n-1, \gamma_R - 1) + 6 \\ &= 4n - 3\left(\gamma_R - \left\lceil \frac{2n}{3} \right\rceil\right) + 5 \\ &> f(n, \gamma_R). \end{aligned}$$

Consequently, the result completes. □

3. Concluding remaks

The purpose of this research is to look at the link between the Zagreb indices and the Roman domination number of unicyclic graphs. We provided the lower bound for the Zagreb indices of unicyclic graphs in terms of the order and Roman domination number, and characterize such graphs that attain the equality case.

To conclude this paper, we suggest the following open problem.

Problem Determine the upper and lower bounds for other degree-based topological indices of unicyclic graphs using the order and Roman domination number.

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References

[1] A.A.S. Ahmad Jamri, R. Hasni, M. Kamran Jamil, and D.A. Mojdeh, *Maximum second Zagreb index of trees with given Roman domination number*, Trans. Comb. **12** (2023), no. 1, 1–10.
https://doi.org/10.22108/toc.2022.128323.1848.

[2] A.A.S. Ahmad Jamri, R. Hasni, and S.K. Said Husain, *On the Zagreb indices of graphs with given Roman domination number*, Commun. Comb. Optim. **8** (2023), no. 1, 141–152.
https://doi.org/10.22049/cco.2021.27439.1263.

[3] A.A.S. Ahmad Jamri, F. Movahedi, R. Hasni, and M.H. Akhbari, *A lower bound for the second Zagreb index of trees with given Roman domination number*, Commun. Comb. Optim. **8** (2023), no. 2, 391–396.
https://doi.org/10.22049/CCO.2022.27553.1288.

[4] A. Ali, K.C. Das, and S. Akhter, *On the extremal graphs for second Zagreb index with fixed number of vertices and cyclomatic number*, Miskolc Math. Notes **23** (2022), no. 1, 41–50.
http://dx.doi.org/10.18514/MMN.2022.2382.

[5] A. Behtoei, M. Jannesari, and B. Taeri, *Maximum Zagreb index, minimum hyper-Wiener index and graph connectivity*, Appl. Math. Lett. **22** (2009), no. 10, 1571–1576.
https://doi.org/10.1016/j.aml.2009.05.001.

[6] B. Borovićanin and B. Furtula, *On extremal Zagreb indices of trees with given domination number*, Appl. Math. Comput. **279** (2016), 208–218.
https://doi.org/10.1016/j.amc.2016.01.017.

[7] B. Borovićanin, B. Furtula, and I. Gutman, *Bounds for Zagreb indices*, MATCH Commun. Math. Comput. Chem. **78** (2017), 17–100.

[8] E.J. Cockayne, P.A. Dreyer Jr, S.M. Hedetniemi, and S.T. Hedetniemi, *Roman domination in graphs*, Discrete Math. **278** (2004), no. 1-3, 11–22.
https://doi.org/10.1016/j.disc.2003.06.004.

[9] K.C. Das, I. Gutman, and B. Zhou, *New upper bounds on Zagreb indices*, J. Math. Chem. **46** (2009), no. 2, 514–521.
https://doi.org/10.1007/s10910-008-9475-3.

[10] K.C. Das, K. Xu, and J. Nam, *Zagreb indices of graphs*, Front. Math. China **10** (2015), no. 3, 567–582.
https://doi.org/10.1007/s11464-015-0431-9.

[11] Z. Du, A.A.S. Ahmad Jamri, R. Hasni, and D.A. Mojdeh, *Maximal first Zagreb index of trees with given Roman domination number*, AIMS Math. **7** (2022), no. 7, 11801–11812.

[12] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), no. 4, 535–538.
https://doi.org/10.1016/0009-2614(72)85099-1.

[13] M. Liu and B. Liu, *The second Zagreb indices and Wiener polarity indices of trees with given degree sequences*, MATCH Commun. Math. Comput. Chem. **67** (2012), no. 2, 439.

[14] ———, *The second Zagreb indices of unicyclic graphs with given degree sequences*, Discrete Appl. Math. **167** (2014), 217–221.
https://doi.org/10.1016/j.dam.2013.10.033.

[15] D.A. Mojdeh, M. Habibi, L. Badakhshian, and Y. Rao, *Zagreb indices of trees,*

unicyclic and bicyclic graphs with given (total) domination, IEEE Access **7** (2019), 94143–94149.
https://doi.org/10.1109/ACCESS.2019.2927288.

[16] A. Poureidi, N.A.A. Aziz, N. Jafari Rad, and H. Kamarulhaili, *Computing strong Roman domination of trees and unicyclic graphs in linear time*, Bull. Malays. Math. Sci. Soc. **45** (2022), no. 5, 2509–2523.
https://doi.org/10.1007/s40840-022-01301-4.

[17] S.S. Shirkol, P.P. Kumbargoudra, and M.M. Kaliwal, *On Roman domination in middle graphs*, J. Shanghai Jiaotong Univ. **17** (2021), no. 7, 10–18.

[18] S.D. Stankov, M.M. Matejić, I.Z. Milovanović, E.I. Milovanović, and S.B. Bozkurt Altindağ, *Some new bounds on the first Zagreb index*, Electron. J. Math. **1** (2021), 101–107.

[19] D. Thakkar and S. Badiyani, *Total Roman domination number of graphs*, TWMS J. Apl. Eng. Math. **12** (2022), no. 2, 445–455.

[20] D.B. West, *Introduction to Graph Theory*, Prentice hall Upper Saddle River, 2001.

[21] K. Xu, *The Zagreb indices of graphs with a given clique number*, Appl. Math. Lett. **24** (2011), no. 6, 1026–1030.
https://doi.org/10.1016/j.aml.2011.01.034.

[22] Z. Yan, H. Liu, and H. Liu, *Sharp bounds for the second Zagreb index of unicyclic graphs*, J. Math. Chem. **42** (2007), no. 3, 565–574.
https://doi.org/10.1007/s10910-006-9132-7.

[23] B. Zhou, *Zagreb indices*, MATCH Commun. Math. Comput. Chem **52** (2004), no. 1, 113–118.