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Short Note

A lower bound for the second Zagreb index of trees with given Roman domination number

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Abstract: For a (molecular) graph, the second Zagreb index $M_2(G)$ is equal to the sum of the products of the degrees of pairs of adjacent vertices. Roman dominating function RDF of G is a function $f : V(G) \to \{0, 1, 2\}$ satisfying the condition that every vertex with label 0 is adjacent to a vertex with label 2. The weight of an RDF f is $w(f) = \sum_{v \in V(G)} f(v)$. The Roman domination number of G, denoted by $\gamma_R(G)$, is the minimum weight among all RDF in G. In this paper, we present a lower bound on the second Zagreb index of trees with n vertices and Roman domination number and thus settle one problem given in [On the Zagreb indices of graphs with given Roman domination number, Commun. Comb. Optim. DOI: 10.22049/CCO.2021.27439.1263 (article in press)].

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1. Introduction

Throughout this paper, all graphs are simple, undirected and connected. Let $G = (V, E)$ be such a graph, where $V = V(G)$ is the vertex set and $E = E(G)$ is the edge set of G. For any vertex $v \in V$, the open neighbourhood of v is the set $N(v) = \{u \in V \mid uv \in E\}$. The *degree* of a vertex u is denoted by $\deg(u)$ (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 which $\deg(u) = 1$ is called a pendant vertex. The diameter of a tree is the longest path between two leaves. We use $T - \{u_1, \ldots, u_k\}$ to denote the tree obtained from T by deleting the vertices $u_1, \ldots, u_k$ of T. As usual, by P_n we denote the path on n vertices. For other undefined notations and terminologies from graph theory, please refer to the book [11].
A chemical molecule can be viewed as a graph. In the molecular graph, the vertices represent the atoms of the molecule and the edges are chemical bonds. A topological index is a mathematical parameter used for studying various properties of this molecule. The degree-based topological indices, such as the Zagreb indices, have been extensively researched for many decades. The first Zagreb index $M_1(G)$ (the second Zagreb index $M_2(G)$ as well) was first introduced by Gutman and Trinajstić [10], and has been closely related to many chemical properties [10, 14]. The Zagreb indices $M_1(G)$ and $M_2(G)$ are defined as

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

and

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

Further study about the Zagreb indices can be found in [3, 9, 13, 14].

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. Domination in graphs has been an active research area in graph theory [11].

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 $V_i = \{v \in V \mid f(v) = i\}$ and $|V_i| = n_i$, for $i = 0, 1, 2$. Note that there exists a $1-1$ correspondence between the functions $f : V \to \{0, 1, 2\}$ 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. any vertex in V_0 has a neighbor in 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 and $f(V) = \gamma_R(G)$. For more details on Roman domination number and its variants, see [5] 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, 7, 12], the surveys [3, 13] and references therein. Specifically, Borovićanin and Furtula [4] investigated extremal Zagreb indices of trees with given domination number. Mojdeh *et al.* [12] obtained some upper bounds on the Zagreb indices of trees, unicyclic and bicyclic graphs with given total domination number. Ahmad Jamri *et al.* [1] obtained a lower bound of the first Zagreb index of trees with a given Roman domination number. They also determined the upper bound for Zagreb indices of unicyclic and bicyclic graphs with given Roman domination number, and characterized the extremal graphs. In the same paper, the authors posed the following problem.
Problem 1. Study the lower bound for the second Zagreb index of trees in terms of the order and the Roman domination number.
In this paper, we present a lower bound on the second Zagreb index of trees with n vertices and Roman domination number and thus settle Problem 1.

2. A lower bound for the second Zagreb index of trees in terms of the order and Roman domination number

We first give the following lemma.

Lemma 1. [6] *For $n \geq 3$, $\gamma_R(P_n) = \lceil \frac{2n}{3} \rceil$.*

We obtain the lower bound for the second Zagreb index of trees with given Roman domination number as follows.

Theorem 1. *Let T be a tree with order n and Roman domination number γ_R. Then*

$$M_2(T) \geq \frac{14n}{3} - \gamma_R - 8. \tag{1}$$

The equality holds if and only if $T \cong P_n$ where $n \equiv 0 \pmod 3$.

Proof. We proceed by induction on the order n. The results is immediate for any tree of order $n \geq 4$ with equality if and only if $T = P_3$. Assume that $n \geq 5$ and the result is true for any tree T' of order $n' < n$. Let T be a tree of order n. First let $\Delta(T) = 2$. Then $T \cong P_n$. If $n \equiv r \pmod 3$, then using Lemma 1, $\gamma_R = \gamma_R(P_n) = \frac{2n+r}{3}$ and we obtain

$$\begin{aligned} M_2(P_n) &= 4 + 4(n-3) \\ &= 4n - 8 + \frac{2n+r}{3} - \gamma_R \\ &= \frac{14n}{3} - \gamma_R - 8 + \frac{r}{3} \\ &\geq \frac{14n}{3} - \gamma_R - 8, \end{aligned}$$

and equality holds if and only if $n \equiv 0 \pmod 3$.
Now, suppose that $\Delta(T) \geq 3$ and let $v_1v_2 \dots v_d$ be a diametral path of T. Clearly, v_1 and v_d are pendant vertices. Let $T' = T - v_1$. One can easily seen that $\gamma_R(T) - 1 \leq \gamma_R(T') \leq \gamma_R(T)$ and $M_2(T) = M_2(T') + \deg_T(v_3) + 2(\deg_T(v_2) - 1)$. If $\max\{\deg_T(v_2), \deg_T(v_3)\} \geq 3$ or $\deg_T(v_2) = \deg_T(v_3) = 2$ and $\gamma_R(T) - 1 = \gamma_R(T')$, then using the induction hypothesis on T' we get

$$\begin{aligned} M_2(T) &\geq M_2(T') + \deg_T(v_3) + 2(\deg_T(v_2) - 1) \\ &\geq \frac{14(n-1)}{3} - \gamma_R(T') - 8 + \deg_T(v_3) + 2(\deg_T(v_2) - 1) \\ &\geq \frac{14n}{3} - \gamma_R(T) - 8 + 5 - \frac{14}{3} \\ &> \frac{14n}{3} - \gamma_R(T) - 8. \end{aligned}$$

Hence we assume that $\deg_T(v_2) = \deg_T(v_3) = 2$ and $\gamma_R(T) = \gamma_R(T')$. Then for any $\gamma_R(T)$-function f, we must have $f(v_1) = f(v_3) = 0$ and $f(v_2) = 2$. Therefore we can see that $\gamma_R(T) = \gamma_R(T - \{v_1, v_2, v_3\}) + 2$. Let $T'' = T - \{v_1, v_2, v_3\}$. Thus, $\gamma_R(T'') = \gamma_R(T) - 2$. Since $\Delta(T) \geq 3$, we have $|V(T'')| \geq 3$. One can easily check that $M_2(T) - M_2(T'') \geq 6 + 2\deg_T(v_4) + \sum_{v \in N(v_4) - \{v_3\}} \deg_T(v)$. If $\max\{\deg_T(v_4), \deg_T(v_5)\} \geq 3$, then using the induction hypothesis on T'' and the fact $\gamma_R(T'') = \gamma_R(T) - 2$ we obtain

$$\begin{aligned} M_2(T) &\geq M_2(T'') + 6 + 2\deg_T(v_4) + \sum_{v \in N(v_4) - \{v_3\}} \deg_T(v) \\ &\geq \frac{14(n-3)}{3} - (\gamma_R(T) - 2) - 8 + 6 + 2\deg_T(v_4) + \deg_T(v_5) \\ &= \frac{14n}{3} - \gamma_R(T) - 8 + +2\deg_T(v_4) + \deg_T(v_5) - 6 \\ &> \frac{14n}{3} - \gamma_R(T) - 8. \end{aligned}$$

Hence we assume that $\deg_T(v_4) = \deg_T(v_5) = 2$. We deduce from $\Delta(T) \geq 3$ that $\Delta(T'') \geq 3$. Now using the induction hypothesis on T'' and the fact $\gamma_R(T'') =$

$\gamma_R(T) - 2$ we obtain

$$\begin{aligned} M_2(T) &\geq M_2(T'') + 6 + 2\deg_T(v_4) + \sum_{v \in N(v_4)-\{v_3\}} \deg_T(v) \\ &> \frac{14(n-3)}{3} - (\gamma_R(T) - 2) - 8 + 6 + 2\deg_T(v_4) + \deg_T(v_5) \\ &= \frac{14n}{3} - \gamma_R(T) - 8 + +2\deg_T(v_4) + \deg_T(v_5) - 6 \\ &= \frac{14n}{3} - \gamma_R(T) - 8. \end{aligned}$$

This completes the proof. □

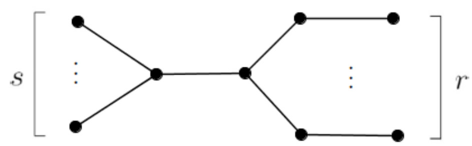

Figure 1. **The graph $T_{s,r}$.**

Remark 1. In [8], a lower bound of the second Zagreb index for any tree T of order n is obtained as $M_2(T) \geq 4n - 8$. We show that the proposed bound in Theorem 1 is better than the obtained bound in [8] for some trees.
If the relation (1) is better that $4n - 8$, then we obtain

$$\frac{14n}{3} - \gamma_R - 8 \geq 4n - 8.$$

Therefore, we obtain $\frac{14n}{3} - 4n \geq \gamma_R$ and consequently, $\gamma_R \leq \frac{2n}{3}$. Hence, the lower bound of the second Zagreb index in Theorem 1 is better that the lower bound $4n - 8$ for any tree of order n with condition $\gamma_R(T) \leq \frac{2n}{3}$. The tree $T_{s,r}$ $(s, r \geq 2)$ illustrated in Figure 1, has $n = s + 2r + 2$ vertices and $\gamma_R(T_{r,s}) = 4 + r$. It can easily seen that $\gamma_R(T) \leq \frac{2n}{3}$. Therefore, for tree $T \simeq T_{s,r}$, the bound (1) is better than the bound $4n - 8$.

3. Concluding remarks

The purpose of this research is to look at the link between the second Zagreb index and the Roman domination number of trees. We provide a lower bound for the second Zagreb index of trees in terms of Roman domination number, and characterizing all tree(s) that attain the equality case. We settled Problem 1 in [1].

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