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On the minimum second Zagreb index of trees with small parameters

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Abstract: The second Zagreb index M_2 is one of the oldest vertex-degree-based molecular structure descriptors, introduced in the 1970s. Recently, there has been a great interest in studying extremal graphs that minimize (or maximize) second Zagreb index in different classes of graphs. In this paper, lower bounds on the second Zagreb index of trees with given small parameters such as diameter, matching number and domination number are determined and the extremal trees are characterized, as well.

Keywords: second Zagreb index, diameter, matching number, domination number

1 Introduction

All graphs considered in this paper are simple, connected graphs. Let $G = (V,E)$ be such a graph, where $V = V(G)$ is its vertex set and $E = E(G)$ is its edge set. An edge connecting two vertices u and v in the graph G is denoted by uv. The degree $d_G(v)$ (or $d(v)$ for short) of a vertex $v \in V(G)$ is the number of edges that are incident with v in the graph G. By $N_G(v)$ we denote the neighborhood of a vertex v in G (the set of vertices adjacent to a vertex v in G). A vertex v for which $d_G(v) = 1$ is called a pendent vertex.

By $G - v$ and $G - uv$ we denote the graph obtained from G by deleting vertex $v \in V(G)$ and edge $uv \in E(G)$, respectively. Similarly, $G + uv$ is obtained from G by adding an edge $uv \notin E(G)$.

For any two distinct vertices u and v in G, the distance between u and v is the number of edges in a shortest path joining u and v. The diameter D of G is the maximum distance between any two vertices of G.

A matching of a graph is a set of mutually independent edges in a graph (set of edges with no common vertices). The *matching number* $\beta(G)$ of the graph G is the number of edges in a maximum matching. It is known that $\beta(G) = 0$ if and only if G is an empty graph.

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The *domination number* $\gamma(G)$ of a graph G is the minimum cardinality of a subset D of $V(G)$ such that each vertex of G that is not contained in D is adjacent to at least one vertex of D. A subset D is called minimum dominating set of G.

A graph T that has n vertices and $n-1$ edges is called a *tree*. As usual, by P_n and $K_{1,n-1}$ we denote the path and the star on n vertices, respectively. For other undefined notations and terminology from graph theory, the readers are referred to [4] .

Molecular structure descriptors (topological indices) are used in mathematical chemistry to describe the properties of chemical compounds. Some of the well studied molecular structure descriptors are the *first* and *second Zagreb indices,* $M_1(G)$ and $M_2(G)$, respectively. They were introduced in 1972 by Gutman and Trinajstić [10, 11], as follows

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

and

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

These indices reflect the extent of branching within the molecular carbon-atom skeleton, which allows them to be viewed as molecular structure descriptors [1, 16]. The main properties of M_1 and M_2 were summarized in [12, 15, 3] and the references therein.

There has been great interest in studing extremal graphs that minimize (or maximize) Zagreb indices in different classes of graphs, recently [5, 6, 7, 13, 17]. Despite the large number of papers concerning these indices, few papers have been published in which the minimum value of these indices in different classes has been determined [9, 18].

In this paper we determine the sharp lower bounds for the second Zagreb index of trees with some fixed small parameters, such as diameter, matching number and domination number, and characterize extremal trees that attain these bounds, as well. Similar results, concerning Harary index, another molecular structure descriptor, have been obtained in [8].

The following result follows immediately from the definition of the second Zagreb index and will be used in the sequel.

Lemma 1.1. *Let G be a connected graph with u, v as its nonadjacent vertices and $e \in E(G)$. Then*

(i) $M_2(G+uv) > M_2(G)$,

(i) $M_2(G-e) < M_2(G)$.

2 On the minimum second Zagreb index of trees with small diameter

Denote by $\mathscr{T}_{n,D}$ the set of trees of order n and diameter D. The star $K_{1,n-1}$ is the only element in $\mathscr{T}_{n,2}$. The trees in $\mathscr{T}_{n,3}$ are of the form $T_1(a,b)$, where $\min(a,b) \geqslant 1$ (Figure 1). In paper [19] Zogić and Glogić characterized the trees from $\mathscr{T}_{n,3}$ attaining the minimum second Zagreb index.

Theorem 2.1. *[19] For $T \in \mathscr{T}_{n,3}$ we have*

$$M_2(T) \geqslant \begin{cases} \frac{3}{4}n^2 - n, \text{ if } n \text{ is even}, \\ \frac{3}{4}n^2 - n + \frac{1}{4}, \text{ if } n \text{ is odd}. \end{cases}$$

The equality holds if and only if $T \cong T_1(a,b)$ with $a = \dfrac{n-2}{2}$ when n is even and $a = \dfrac{n-1}{2}$ or $a = \dfrac{n-3}{2}$ when n is odd.

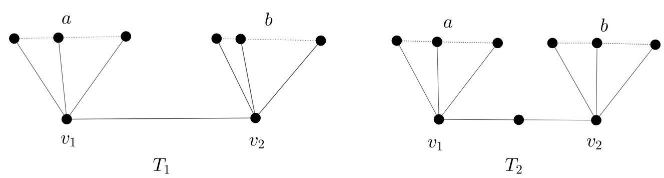

Fig. 1. Tree with $D = 3$

Next, we consider the trees with diameter 4. Let $\mathscr{T}_{n,4}$ be a set of trees with n vertices and diameter $D = 4$. The trees in $\mathscr{T}_{n,4}$ are of the form $T_4(m; a_1, a_2, \ldots, a_k)$ with $m \geqslant 0$, as shown in Figure 2, where $\sum_{i=1}^{k} a_i + m + k + 1 = n$. For $2 \leqslant k \leqslant n-3$, if $m = 0$ and $d(v) = k$, we denote these trees by $T(a_1, a_2, \ldots, a_k)$. In addition, if the numbers a_i, $i = 1, 2, \ldots, k$, are almost all the same, i.e., $|a_i - a_j| \leqslant 1$ for $1 \leqslant i < j \leqslant k$, we denote the tree $T(a_1, a_2, \ldots, a_k)$ by $T^*(n,k)$.

In paper [19] the authors obtained some results concerning trees from $\mathscr{T}_{n,4}$ with minimal second Zagreb index, but unfortunately they made some mistakes, so here we give the correct proofs.

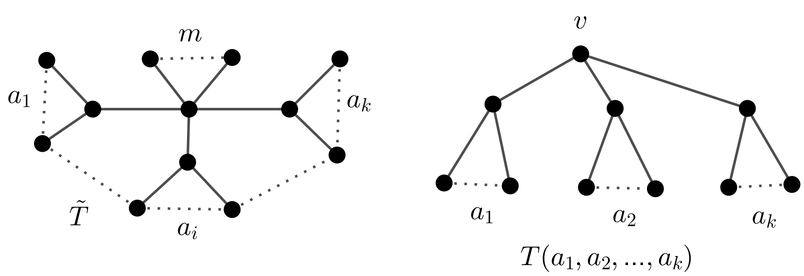

Fig. 2. Trees with $D = 4$

Lemma 2.1. *For any tree of order $n \geqslant 5$ of the form $\widetilde{T} = T_4(m; a_1, a_2, \ldots, a_k) \in \mathscr{T}_{n,4}$, where $k \geqslant 2$ and $m \geqslant 1$, there exists a tree of the same order of the form $T = T(b_1, b_2, \ldots, b_k)$ such that $M_2(T) < M_2(\widetilde{T})$.*

Proof. Suppose, without lost of generality, that $a_1 \leqslant a_2 \leqslant \cdots \leqslant a_k$ and set $T' = T(m-1; a_1+1, a_2, \ldots, a_k)$. Then it holds

$$M_2(\widetilde{T}) = (m+3)\sum_{i=1}^{k}(a_i+1) + \sum_{i=1}^{k} a_i(a_i+1) + m(m+3)$$

and

$$M_2(T') = (m+2)\sum_{i=2}^{k}(a_i+1) + (m+2)(a_1+2) + \sum_{i=2}^{k} a_i(a_i+1) + \\ + (a_1+1)(a_1+2) + (m-1)(m+2),$$

implying

$$M_2(\widetilde{T}) - M_2(T') = \sum_{i=1}^{k} a_i + k + m - 2a_1 - 2 > 0.$$

The last inequality holds as $\sum_{i=1}^{k} a_i \geqslant ka_1 \geqslant 2a_1$ and $k+m-2 > 0$, so the result follows. $\square$

Theorem 2.2. *Let $T \in \mathscr{T}_{n,4}$. Then*

$$M_2(T) \geqslant \frac{(n-1)(k_0^2 - k_0 + n - 1)}{k_0}$$

with equality if and only if $T \cong T^*(n,k_0)$, where $k_0 = \lfloor \sqrt{n-1} \rfloor$ or $k_0 = \lceil \sqrt{n-1} \rceil$.

Proof. Having in mind Lemma 2.1 we conclude that the extremal tree which attains the minimum second Zagreb index must be of the form $T(a_1, a_2, \ldots, a_k)$. As

$$M_2(T(a_1,a_2,\ldots,a_k)) = k\sum_{i=1}^{k}(a_i+1) + \sum_{i=1}^{k} a_i(a_i+1) = \sum_{i=1}^{k} a_i^2 + (k+1)\sum_{i=1}^{k} a_i + k^2$$

and $\sum_{i=1}^{k} a_i = n-k-1$, we obtain

$$M_2(T(a_1,a_2,\ldots,a_k)) = \sum_{i=1}^{k} a_i^2 + k(n-2) + n - 1.$$

In addition, the sum $\sum_{i=1}^{k} a_i^2$ is minimized when the numbers a_i, $i = 1,2,\ldots,k$, are almost all the same, i.e., $a_i = \frac{n-k-1}{k}$. So, in order to obtain the minimum second Zagreb index of trees from $\mathscr{T}_{n,4}$ we need to determine the minimum of the function

$$f(k) = \frac{(n-k-1)^2}{k} + k(n-2) + n - 1,$$

i.e.,

$$f(k) = \frac{(n-1)(k^2-k+n-1)}{k}.$$

If we take the derivative with respect to k we obtain

$$\frac{df(k)}{dk} = \frac{(n-1)(k^2-n+1)}{k^2}$$

and $\dfrac{d^2 f(k)}{dk^2} = \frac{2(n-1)^2}{k^3} > 0$, so $f(k)$ has only one minimum value which is attained at the point k_0 such that $\dfrac{(n-1)(k^2-n+1)}{k^2} = 0$, i.e., $k_0 = \sqrt{n-1}$. Having in mind that k_0 must be an integer, we conclude that $k_0 = \lfloor \sqrt{n-1} \rfloor$ or $k_0 = \lceil \sqrt{n-1} \rceil$. □

3 Trees with small matching number

Let $\mathscr{M}_{n,\beta}$ be the set of trees on n vertices with matching number β. The unique tree with matching number $\beta = 1$ is the star $K_{1,n-1}$.

The set $\mathscr{M}_{n,2}$ contains trees of the form T_1 with $a+b = n-2$ and $\min(a,b) \geqslant 1$, as well as the trees of the form T_2 with $a+b = n-3$ and $\max(a,b) \geqslant 1$ (see Figure 3).

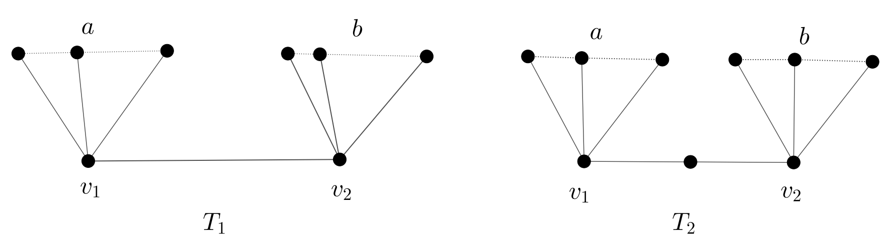

Fig. 3. Trees with matching number 2

Theorem 3.1. *If $T \in \mathscr{M}_{n,2}$, then*

$$M_2(T) \geqslant \begin{cases} \dfrac{n^2}{2}, \text{ if } n \text{ is even}, \\ \dfrac{n^2-1}{2}, \text{ if } n \text{ is odd}. \end{cases}$$

The equality holds if and only if $T \cong T_2$ with $a = \dfrac{n-2}{2}$ or $a = \dfrac{n-4}{2}$ when n is even and $a = \dfrac{n-3}{2}$ when n is odd.

Proof. If $T \in \mathscr{M}_{n,2}$, then T must be of the form T_1 or T_2. If T is of the form T_1, i.e., $T = T_1(a,b)$, where $1 \leqslant a \leqslant b$, let $T^* = T_2(a-1,b)$. If $a = 1$, then $T_1(a,b) \cong T_2(a-1,b)$, so in the sequel we assume that $2 \leqslant a \leqslant b$. As $M_2(T) = a^2 - a(n-2) + (n-1)^2$ and $M_2(T^*) = 2a^2 + 2a - 2an + n^2 - n$, we obtain

$$M_2(T) - M_2(T^*) = (a-1)(n-1-a) > 0,$$

since $a < n-2$. Thus, the tree from $\mathscr{M}_{n,2}$ with minimal second Zagreb index is of the form T_2. It is easily obtained that

$$M_2(T_2) = 2a^2 + 6a - 2an + n^2 - 3n + 4 = 2\left(a - \frac{n-3}{2}\right)^2 + \frac{n^2-1}{2}.$$

If n is even, then the above expression is minimized for $a = \dfrac{n-2}{2}$ or $a = \dfrac{n-4}{2}$ and $M_2(T) \geqslant \dfrac{n^2}{2}$.

If n is odd, then the above expression is minimized for $a = \dfrac{n-3}{2}$ and $M_2(T) \geqslant \dfrac{n^2-1}{2}$, as desired. $\square$

Recall that the independence number of a graph G, denoted by $\alpha(G)$, is the cardinality of maximal independent sets of G, where an independent set of G is the subset $S \subseteq V(G)$ of mutually non-adjacent vertices in a graph G. It is known that $\alpha(T) + \beta(T) = n$, where T is a tree on n vertices, so the results stated in this section can be viewed as the minimal second Zagreb index of trees with a given independence number equal to $n-1$ and $n-2$. In fact, we will prove that these trees attain minimum second Zagreb index among all connected graphs with a given independence number equal to $n-1$ and $n-2$. Denote by $\mathscr{G}_{n,\alpha}$ the set of all connected graphs on n vertices with a given independence number α. The case $\alpha = n-1$ is trivial, since the star $K_{1,n-1}$ is the unique element in $\mathscr{G}_{n,n-1}$.

Let us now consider the case $\alpha = n-2$. The graphs $T_1(a,b), T_2(a,b)$ displayed in Figure 3 belong to $\mathscr{G}(n, n-2)$.

Suppose G is the graph attaining the minimum second Zagreb index in $\mathscr{G}(n, n-2)$ and let $S = \{v_3, v_4, \ldots, v_n\}$ be the maximal independent set in G. Any vertex from S is adjacent to at least one of the vertices v_1 and v_2. As $\alpha = n-2$, we conclude that $N_G(v_1) \setminus \{v_2\} \neq \emptyset$ and $N_G(v_2) \setminus \{v_1\} \neq \emptyset$.

If $N_G(v_1) \setminus \{v_2\} \cap N_G(v_2) \setminus \{v_1\} = \emptyset$, then $G \cong T_1(a,b)$. Otherwise, by Lemma 1.1 $|N_G(v_1) \setminus \{v_2\} \cap N_G(v_2) \setminus \{v_1\}| = 1$, implying $G \cong T_2(a,b)$. Then, by Theorem 3.1, we conclude that the tree $T_2(a, n-3-a)$ attain the minimum second Zagreb index among all graphs from $\mathscr{G}_{n,n-2}$, with $a = \dfrac{n-2}{2}$ or $a = \dfrac{n-4}{2}$ for even n and $a = \dfrac{n-3}{2}$ for odd n.

4 On the minimum second Zagreb index of trees with small domination number

Denote by $\mathscr{D}_{n,\gamma}$ the set of trees on n vertices with domination number γ. The star $K_{1,n-1}$ is the only element in $\mathscr{D}_{n,1}$.

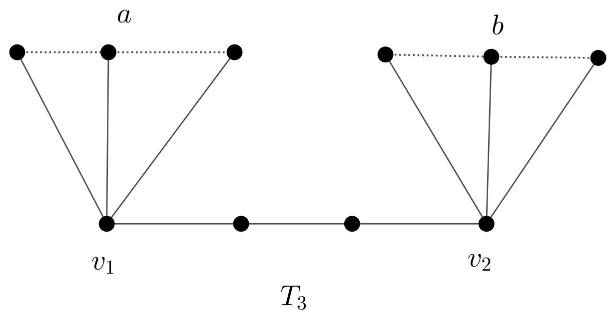

Fig. 4. Tree of the form $T_3(a,b)$ with domination number 2

The trees from $\mathscr{D}_{n,2}$ must be of the form $T_1(a,b)$, $T_2(a,b)$ (see Figure 3) or $T_3(a,b)$ (Figure 4), where $a+b=n-4$, $a,b \geqslant 0$. We proved that for any tree of type T_1 there exists a tree of type T_2 with smaller second Zagreb index. In an analogous manner it can be proved that for any tree of type T_2 there exists a tree of type T_3 with smaller second Zagreb index. Thus, in order to characterize the trees from $\mathscr{D}_{n,2}$ attaining the minimum second Zagreb index we need to consider only the trees of type T_3.

Theorem 4.1. *If $T \in \mathscr{D}_{n,2}$, then*

$$M_2(T) \geqslant \begin{cases} \dfrac{n^2-2n+8}{2}, & \textit{if } n \textit{ is even,} \\ \dfrac{n^2-2n+9}{2}, & \textit{if } n \textit{ is odd.} \end{cases}$$

The equality holds if and only if $T \cong T_3$ with $a = \dfrac{n-4}{2}$ when n is even and $a = \dfrac{n-3}{2}$ or $a = \dfrac{n-5}{2}$ when n is odd.

Proof. It is easily seen that

$$M_2(T_3) = 2a^2+8a-2an+n^2-5n+12 = 2\left(a-\frac{n-4}{2}\right)^2+\frac{n^2-2n+8}{2}.$$

If n is even, then the above expression is minimized for $a = \dfrac{n-4}{2}$ and $M_2(T) \geqslant \dfrac{n^2-2n+8}{2}$.

If n is odd, then the above expression is minimized for $a = \dfrac{n-3}{2}$ or $a = \dfrac{n-5}{2}$ and $M_2(T) \geqslant \dfrac{n^2-2n+9}{2}$, as desired. $\square$

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