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TREES WITH THE MINIMAL SECOND ZAGREB INDEX

M. ELIASI[1] AND A. GHALAVAND[1]

Abstract. For simple graph G with edge set $E(G)$, the second Zagreb index of G is defined as $M_2(G) = \sum_{uv\in E(G)}[d_G(u)d_G(v)]$, where $d_G(v)$ is the degree of the vertex v in G. In this paper, we identify the nine classes of trees, which have the first to the sixth smallest second Zagreb indices, among all the trees of the order $n \geq 11$.

1. Introduction

Let G be a finite, connected, simple graph (an undirected graph containing no loops and no multiple edges) with the vertex set $V(G)$ and edge set $E(G)$. For vertex $v \in V(G)$, we denote the degree of v by $d_G(v)$ and the set of vertices adjacent to v by $N_G(v)$, respectively. The maximum vertex degree is denoted by $\Delta = \Delta(G)$. A pendent vertex of G is a vertex with degree one. If G is acyclic graph, then G is called a tree. Any tree with at least two vertices has at least two pendent vertices. The second Zagreb index, $M_2(G)$, is defined as follows:

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

The second Zagreb index is a topological index; real numbers related to a graph, which are invariant under graph isomorphisms. Topological indices have many applications in chemistry, biology, and other branches of science [5]. The second Zagreb index was found to occur in certain approximate expressions of the total π-electron energy of alternant hydrocarbons [7]. We encourage the reader to consult [2, 13, 19, 20] and [21] for the historical background, computational techniques, and mathematical properties of the second Zagreb index. Recently, a search for graphs in different classes with extreme values of the second Zagreb index has been conducted by many researchers,

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see [12, 17]. Goubko [6] described trees with the minimal second Zagreb index as among those with a fixed number of pendent vertices. Deng [4] presented a unified and simplified approach to the largest and smallest second Zagreb indices for trees, unicyclic graphs, and bicyclic graphs by introducing some transformations. In [1], the authors characterized trees with maximal and minimal M_2 as among those with a given number of segments or a given number of branching vertices. Vukicevic et al. [16] reported a simple approach to calculate the maximal value of M_2 for trees with a fixed number of vertices of a given degree. The extreme M_2 values of graphs with connectivity at most k, were obtained in [11, 18], and the M_2 bounds of unicyclic graphs were obtained by Yan et al. [17]. The sharp M_2 bounds of bipartite graphs with a given diameter were obtained in [9, 10]. Lang et al. [9] gave a necessary condition for a bipartite graph to attain the maximal value of the second Zagreb index. Further, Das and Gutman proved that the connected n-vertex graph with minimum second Zagreb index is an n-vertex tree and they demonstrated that the tree with minimum value of M_2 represents the path [3]. In [8], the first and second maximum values of the second Zagreb index in class of tetracyclic n-vertex graphs was presented.

In the above references, the authors obtained the first and second maximal M_2 or the first minimal M_2 in some classes of graphs. In this paper, we identify the nine classes of trees, which have the first to the sixth smallest second Zagreb indices among all the trees of the order $n \geq 11$.

2. Preliminaries

For subset E of $E(G)$, we denote the subgraph of G obtained by deleting the edges of E by $G - E$. If $E = \{uv\}$, the subgraphs $G - E$ will be written as $G - uv$ for short. In addition, for any two nonadjacent vertices x and y of graph G, let $G + xy$ be the graph obtained from G by adding an xy edge. The set of all n-vertex trees will be denoted by $\tau(n)$. We denote the path graph and the star graph (both with n vertices) by P_n and S_n, respectively. A non-increasing sequence $(d_1, d_2, \ldots, d_n)$ of nonnegative integers is said to be graphic if a finite simple graph G exists, with vertices $v_1, v_2, \ldots, v_n$, such that each v_i has degree d_i.

Further, suppose that $(d_1, d_2, \ldots, d_n) = (\underbrace{x_1, \ldots, x_1}_{\alpha_1 \text{ times}}, \underbrace{x_2, \ldots, x_2}_{\alpha_2 \text{ times}}, \ldots, \underbrace{x_t, \ldots, x_t}_{\alpha_t \text{ times}})$, where $d_1 = x_1 > x_2 > \ldots > x_t = d_n$ and $\alpha_1, \ldots, \alpha_t$ are positive integers, such that $\alpha_1 + \alpha_2 + \ldots + \alpha_t = n$. Then, we write, $(d_1, d_2, \ldots, d_n) = (x_1^{\alpha_1}, x_2^{\alpha_2}, \ldots, x_t^{\alpha_t})$. In addition, $T(x_1^{\alpha_1}, \ldots, x_m^{\alpha_m})$ represents the class of trees with α_i vertices of the degree x_i, $i = 1, \ldots, m$.

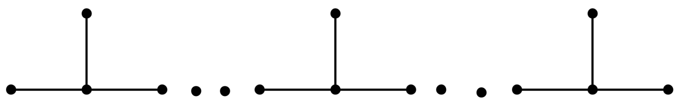
A rooted tree is a tree with a designated vertex called a root. If vertex v immediately precedes vertex w on the path from the root to w, then v is a parent of w and w is child of v. A leaf in a rooted tree is any vertex with no children and a vertex of degree 1. Vertices with the same parent are called siblings. Vertex w is called a descendant of vertex v if v is on the unique path from the root to w.

The subdivision of graph G is a new graph obtained by adding vertices inside the edges.

For a positive number $n \geq 11$, let:

$$\begin{aligned} T_9(n) =& \{T \in T(4^1, 2^{n-5}, 1^4) \mid m_{1,4}(T) = 3, m_{1,2}(T) = m_{2,4}(T) = 1 \text{ and } m_{2,2}(T) \\ & = n-6\} \\ T_{12}(n) =& \{T \in T(3^3, 2^{n-8}, 1^5) \mid m_{1,3}(T) = 5, m_{1,2}(T) = m_{3,3}(T) = 0, m_{2,3}(T) = 4 \\ & \text{and } m_{2,2}(T) = n-10\}, \end{aligned}$$

where $m_{i,j}(T)$ is the number of edges of T connecting the vertices of degrees i and j. In Figure 1, we illustrate the trees in $T_{12}(n)$, the BB tree.



BB

Figure 1. BB tree

For a graph G with $n \geq 3$ vertices and m edges, denote the number of vertices with degree i for $i = 1, 2, \ldots, n-1$, by n_i. For $1 \leq i \leq j \leq n-1$, when no confusion can arise, we shall simply write $m_{i,j}$ instead of $m_{i,j}(G)$. Now we have:

$$\begin{aligned} n =& n_1 + n_2 + \cdots + n_{n-1} \\ 2m =& n_1 + 2n_2 + \cdots + (n-1)n_{n-1} \\ n_1 =& m_{1,2} + m_{1,3} + \cdots + m_{1,n-1} \\ 2n_2 =& m_{1,2} + 2m_{2,2} + \cdots + m_{2,n-1} \\ & \vdots \\ (n-1)n_{n-1} =& m_{1,n-1} + m_{2,n-1} + \cdots + 2m_{n-1,n-1}. \\ M_2(G) =& \sum_{1 \leq i \leq j \leq n-1} m_{i,j}.i.j, \end{aligned} \tag{2.1}$$

where the last equality was given by Vukicevic et al. [16]. Note that if $G \in \tau(n)$, then $m = n-1$ and $n_1 \geq 2$. We start with the following lemma.

Lemma 2.1. *Let u be the root of rooted tree T and $d_T(u) \geq 3$. If v_0v_1 is a pendent edge in T $(d_T(v_0) \geq 2, d_T(v_1) = 1)$, then for each $u_1 \in V(T)$, in which u_1 and v_0 do not have same parent and $d_T(u) \geq d_T(v_0)$, $M_2(T - uu_1 + v_1u_1) < M_2(T)$ (Figure 2).*

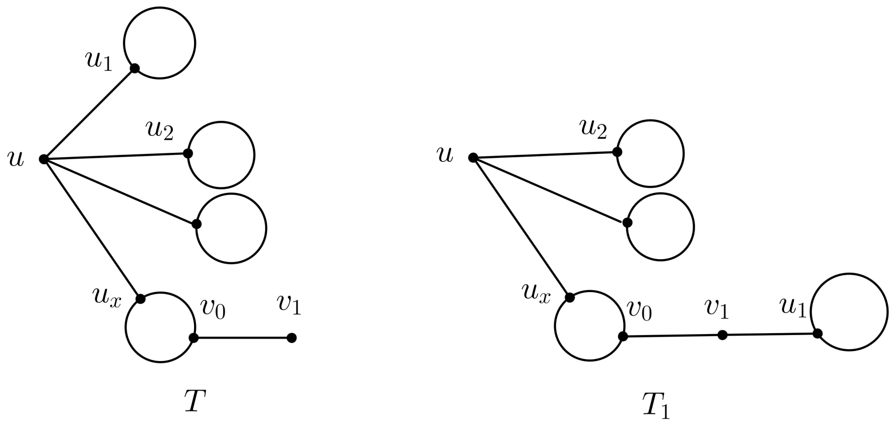


FIGURE 2. Trees T and T_1 in Lemma 2.1

Proof. Suppose that $T_1 = T - uu_1 + v_1u_1$, $d_T(u) = x, N_T(u) = \{u_1, \ldots, u_x\}$ and $d_T(u_i) = d_i$, for $i = 1, \ldots, x$ (Figure 2). If $u \neq v_0$, then

$$\begin{aligned}
M_2(T) - M_2(T_1) =& 1d_T(v_0) + d_T(u)d_T(u_1) + \sum_{i=2}^{x} d_T(u)d_i \\
& - 2d_T(v_0) - 2d_T(u_1) - \sum_{i=2}^{x}[d_T(u) - 1]d_i \\
=& - d_T(v_0) + (d_T(u) - 2)d_T(u_1) + \sum_{i=2}^{x} d_i \\
\geq& - d_T(v_0) + (d_T(u) - 2)d_T(u_1) + d_T(u) \\
\geq& (d_T(u) - 2)d_T(u_1) > 0,
\end{aligned}$$

because $d_x \geq 2$ and $d_i \geq 1$ for $2 \leq i \leq x - 1$.

Now, suppose that $u = v_0$. Without the loss of generality, we may assume that $u_x = v_1$. Since $d_T(u) \geq 3$, then:

$$\begin{aligned}
M_2(T) - M_2(T_1) =& d_T(u)d_T(u_1) + 1d_T(u) + \sum_{i=2}^{x-1} d_T(u)d_i \\
& - \sum_{i=2}^{x-1}[d_T(u) - 1]d_i - 2(d_T(u) - 1) - 2d_T(u_1) \\
=& - d_T(u) + 2 + d_T(u)d_T(u_1) - 2d_T(u_1) + \sum_{i=2}^{x-1} d_i \\
\geq& - d_T(u) + 2 + d_T(u)d_T(u_1) - 2d_T(u_1) + (d_T(u) - 2) \\
=& (d_T(u) - 2)d_T(u_1) > 0.
\end{aligned}$$

This completes the proof. $\square$

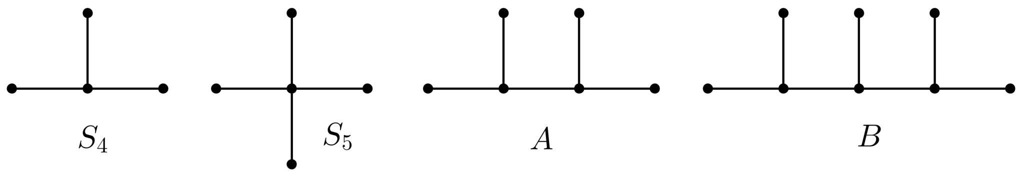


FIGURE 3. Trees S_4, S_5, A and B

Remark 2.1. Considering the proof of Lemma 2.1, one can see that if $d_T(u) = 3$ and $d_T(v_0) = 4$, then $M_2(T_1) \leq M_2(T)$.

In Figure 3 we illustrate the trees S_4, S_5, A and B that we need in the remainder of this paper.

Lemma 2.2. *Among all the subdivisions of S_5, with $n \geq 10$ vertices, the tree obtained by adding all the new vertices to one edge has the minimal second Zagreb index. If $T \in T(4^1, 2^{n-5}, 1^4)$, then $M_2(T) \geq 4n - 2$. Equality holds if and only if $T \in T_9(n)$.*

Proof. Let T be a subdivision graph of S_5, with $n \geq 11$ vertices. Then, $m = n-1$, $n_1 = 4$ and $n_4 = 1$. In addition, since $n \geq 11$, $m_{1,2}, m_{2,2}$ and $m_{2,4}$ are nonzero integers. By considering equation (2.1), we must obtain the minimum $2m_{1,2} + 4m_{2,2} + 4m_{1,4} + 8m_{2,4}$ with respect to

$$\begin{aligned}
n &= n_2 + 5, \\
4 &= m_{1,2} + m_{1,4}, \\
2n_2 &= m_{1,2} + 2m_{2,2} + m_{2,4}, \\
4 &= m_{1,4} + m_{2,4}.
\end{aligned}$$

Therefore, $m_{1,4} = 4 - m_{1,2}$, $m_{2,4} = m_{1,2}$, and $m_{2,2} = n - 5 - m_{1,2}$. So, $M_2(T) = 4n - 4 + 2m_{12}$. Hence, if $m_{1,2} = 1$, then the minimum value of M_2 is obtained. In this case, $m_{1,4} = 3$, $m_{2,4} = 1$, and thus $m_{2,2}(T) = n - 6$. $\square$

Lemma 2.3. *Among all the subdivisions of B, with $n \geq 11$ vertices, the trees in $T_{12}(n)$ have the minimal second Zagreb index. Moreover, if $T \in T(3^3, 2^{n-8}, 1^5)$ (a subdivision graph of B), then $M_2(T) \geq 4n - 1$. Equality holds if and only if T is a BB tree.*

Proof. Let T be a subdivision graph of B, with $n \geq 11$ vertices. Then, $m = n - 1$, $n_1 = 5$, and $n_3 = 3$. By considering equation (2.1), we must obtain the minimum $2m_{1,2} + 3m_{1,3} + 4m_{2,2} + 6m_{2,3} + 9m_{3,3}$ with respect to

$$\begin{aligned}
n &= n_2 + 8, \\
5 &= m_{1,2} + m_{1,3}, \\
2n_2 &= m_{1,2} + 2m_{2,2} + m_{2,3}, \\
9 &= m_{1,3} + m_{2,3} + 2m_{3,3}.
\end{aligned}$$

Therefore, $m_{1,3} = 5 - m_{1,2}$, $m_{2,2} = n - 10 - m_{1,2} + m_{3,3}$, and $m_{2,3} = 4 + m_{1,2} - 2m_{3,3}$. So, $M_2(T) = 4n - 1 + m_{1,2} + m_{3,3}$. Hence, if $m_{1,2} = 0 = m_{3,3}$, then the minimum value of M_2 is obtained. In this case, $m_{1,3} = 5$, $m_{2,3} = 4$, and thus $m_{2,2} = n - 10$. $\square$

3. Main Results

Theorem 3.1. *Let $\acute{T}$ be a tree in $\tau(n)$, where $n \geq 11$. If $\Delta(\acute{T}) \geq 4$ and $\acute{T} \notin T_9(n)$, then for each $T \in T_9(n)$, we have $M_2(T) < M_2(\acute{T})$.*

Proof. By induction on $\Delta(\acute{T})$. Suppose that $\Delta(\acute{T}) = 4$. Let $U_4 = \{u \in V(\acute{T}) \mid d_{\acute{T}}(u) = 4\}$ and fix $u_0 \in U_4$. If $U_4 \setminus \{u_0\} \neq \emptyset$, then by the repeated application of Lemma 2.1 on the vertices in $U_4 \setminus \{u_0\}$, $(|U_4| - 1)$-times, we arrive at tree T_m, in which u_0 is the only vertex of degree 4 in $V(T_m)$ and in which $M_2(T_m) < M_2(\acute{T})$. In addition, if $u \in V(T_m)$ and $u \neq u_0$, then $d_{T_m}(u) \leq 3$. Therefore, without the loss of generality, we suppose that u_0 is the only vertex of degree 4 in $\acute{T}$ and that the other vertices have degree almost 3. We consider the following cases.

Case 1: $n_3(\acute{T}) = 0$. Then, $\acute{T}$ is a subdivision graph of S_5, and by Lemma 2.2, $M_2(T) < M_2(\acute{T})$.

Case 2: $n_3(\acute{T}) > 0$. Let $U_3 = \{u \in V(\acute{T}) \mid d_{\acute{T}}(u) = 3\}$. Suppose that $u \in U_3$ and $N_{\acute{T}}(u) = \{u_1, u_2, u_3\}$, such that u is the root of $\acute{T}$ and u_2 is u_0 or u_2 is an ancestor of u_0. Then, according to Remark 2.1, if v_1 is a leaf in $\acute{T}$ such that u_3 is an ancestor of v_1, then $M_2(\acute{T} - uu_1 + v_1u_1) \leq M_2(\acute{T})$. By the repeated application of this process on the vertices in U_3, we arrive at a tree T_m, in which $M_2(T_m) \leq M_2(\acute{T})$, $n_3(T_m) = 0$ and u_0 is the only vertex of degree 4 in T_m. Therefore, by Case 1, $M_2(T) < M_2(T_m) \leq M_2(\acute{T})$.

Now, suppose that $\Delta(\acute{T}) > 4$ and $U_{\Delta(\acute{T})} = \{u \in V(\acute{T}) \mid d_{\acute{T}}(u) = \Delta(\acute{T})\}$. By the repeated application of Lemma 2.1 on the vertices in $U_{\Delta(\acute{T})}$, $|U_{\Delta(\acute{T})}|$-times, we arrive at a tree T_s, with $\Delta(T_s) = \Delta(\acute{T}) - 1$ and $M_2(T_s) < M_2(\acute{T})$. By the induction hypothesis, $M_2(T) < M_2(T_s)$, and hence $M_2(T) < M_2(\acute{T})$. $\square$

Theorem 3.2. *Let $\acute{T}$ be a tree with $\Delta(\acute{T}) = 3$, such that the number of its vertices of degree 3 is at least 3. Then, for each $T \in T_{12}(n)$, we have $M_2(T) \leq M_2(\acute{T})$.*

Proof. We consider the following cases.

Case 1: the number of vertices of degree 3 in $\acute{T}$ is equal to 3. Since $\Delta(\acute{T}) = 3$, $\acute{T}$ is a subdivision graph of B. Thus, by Lemma 2.3, $M_2(T) \leq M_2(\acute{T})$.

Case 2: $n_3(\acute{T}) \geq 4$. Let u_1, u_2 and u_3 be distinct vertices of degree 3 in $\acute{T}$ and let U_3 be the set of all vertices of degree 3 in $\acute{T}$. If $u \in U_3 \setminus \{u_1, u_2, u_3\}$, then by Lemma 2.1, we obtain tree T_1, in which $d_{T_1}(u) = 2$, and $M_2(T_1) \leq M_2(\acute{T})$. By repeating this argument $(|U_3| - 4)-$times, we obtain tree T_s, in which $\Delta(T_s) = 3$, $n_3(T_s) = 3$, and $M_2(T_s) \leq M_2(\acute{T})$. Case 1 shows that $M_2(T) \leq M_2(T_s)$. Therefore, $M_2(T) \leq M_2(\acute{T})$. $\square$

Let $T \in \tau(n)$, $T_9 \in T_9(n)$, and $n \geq 11$. We consider the following cases.

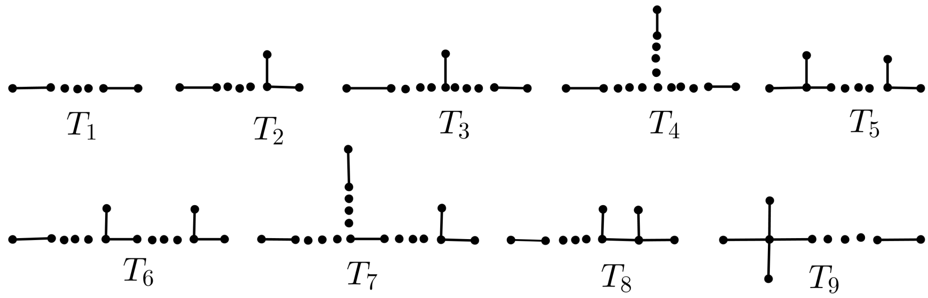


FIGURE 4. Trees in Theorem 3.3

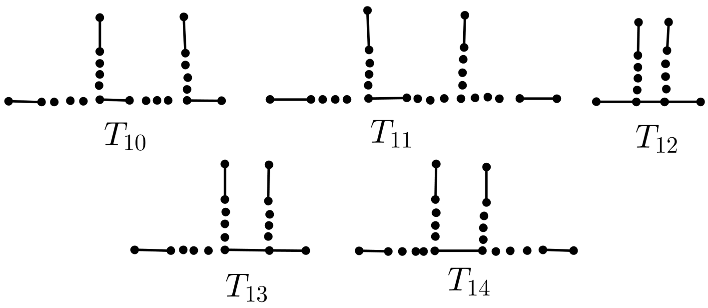


FIGURE 5. Some subdivision graphs of A

Case 1: $\Delta(T) \geq 4$. Then, by Theorem 3.1, $M_2(T_9) \leq M_2(T)$.

Case 2: $\Delta(T) = 3$. If $n_3(T) \geq 3$, then Theorem 3.2, shows that $M_2(BB) \leq M_2(T)$. Since $M_2(T_9) = 4n - 2 < 4n - 1 = M_2(BB)$, $M_2(T_9) < M_2(T)$. Now, suppose that $n_3(T) \leq 2$. If $n_3(T) = 1$, then T is a subdivision graph of S_4. As we illustrated in Figure 4, the subdivision graphs of S_4, are T_2, T_3, and T_4. It is easy to see that $M_2(T_2) = 4n - 6$, $M_2(T_3) = 4n - 5$, and $M_2(T_4) = 4n - 4$. If $n_3(T) = 2$, then T is a subdivision graph of A. As we illustrated in Figures 4 and 5, the subdivision graphs of A, are $T_5, T_6, \ldots, T_8, T_{10}, \ldots, T_{14}$. It is easy to see that $M_2(T_5) = 4n - 4$, $M_2(T_6) = 4n - 3$, $M_2(T_7) = M_2(T_8) = M_2(T_9) = 4n - 2$, $M_2(T_{10}) = M_2(T_{12}) = 4n - 1$, $M_2(T_{11}) = M_2(T_{13}) = 4n$, and $M_2(T_{14}) = 4n + 1$.

Case 3: $\Delta(T) = 2$. Then, $T \cong P_n$ and $M_2(T) = 4n - 8$. The above deductions, lead us the following theorem.

Theorem 3.3. *Suppose that T is a tree with $n(\geq 11)$ vertices, except $T_1, T_2, \ldots, T_9$, as illustrated in Figure 4. Then, we have*

$$\begin{aligned} M_2(T_1) <& M_2(T_2) < M_2(T_3) < M_2(T_4) = M_2(T_5) < M_2(T_6) < M_2(T_7) \\ =& M_2(T_8) = M_2(T_9) < M_2(T). \end{aligned}$$

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[1] Department of Mathematics,
Khansar Faculty of Mathematics and Computer Science,
P. O. Box 87915-85163, Khansar, Iran
E-mail address: eliasi@math.iut.ac.ir
E-mail address: Ali797ghalavand@gmail.com