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Maximal and Minimal Zagreb Indices of Trees with Fixed Number of Vertices of Maximum Degree

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Abstract

For a graph G, the first Zagreb index is defined as the sum of the squares of the vertex degrees, while the second Zagreb index is the sum of the products of the degrees of adjacent vertices. The aim of this paper is to completely characterize n-vertex trees with given $k \geq 1$ vertices that have a fixed maximum degree $\Delta \geq 3$ with respect to the maximal and minimal Zagreb indices. Furthermore, our results provide detailed insights into the structure of extremal trees and are equally applicable to the class of chemical trees.

1 Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_v(G)$ of a vertex v in a graph G is the number of vertices adjacent to v. The set of vertices of G that are adjacent to a vertex v is called neighborhood of v and is represented as $N_v(G)$. A vertex of degree 1 is called a pendant vertex. If a vertex has degree at least 3, it is called a branching vertex. The distance $d_G(u, v)$ between two vertices u and v in

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G is defined as the number of edges in the shortest path connecting u and v. The total number of vertices of degree i is denoted by $n_i(G)$. The total number of edges in G whose one end has degree i and other end has degree j is denoted by $m_{i,j}(G)$, where $i, j \in \{1, 2, \ldots, \Delta\}$. When there is no ambiguity, we write $d_v(G)$, $N_v(G)$, $d_G(u, v)$, $n_i(G)$ and $m_{i,j}(G)$ as d_v, N_v, $d(u, v)$, n_i and $m_{i,j}$, respectively.

A segment of a tree T is a path such that all the internal vertices of the path have a degree 2 and the terminal vertices are pendants or branching vertices. A segment with a pendant vertex at one end and a branching vertex at the other end is called a pendant path, while a segment with branching vertices at both ends is called an internal path. An n-vertex star S_n is a tree with one vertex of degree $n-1$ and all other $n-1$ vertices have degree 1. A double star graph $DS_{i,j}$ of order $i+j=n$ is a tree with exactly two non-pendant vertices of degree i and j, connected by an edge. A broom tree $B_{n,\Delta}$ on n vertices with maximum degree Δ is obtained from a star graph $S_{\Delta+1}$ by extending one of its pendant edges into a path of length $n-\Delta$. A (r, i, j)-dumbbell is a tree obtained by connecting S_{i+1} and S_{j+1} by a path of length $r \geq 1$, such that the number of pendant vertices adjacent to both S_{i+1} and S_{j+1} differ by at most 1. A sequence of non-increasing positive integers $\pi = (d_1, d_2, \ldots, d_n)$ is called a vertex degree sequence, if there exists a graph G with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ such that $d_{v_i} = d_i$ for all $i \in \{1, 2, \ldots, n\}$. For two disjoint sets E_1 and E_2 of $E(G)$, the graph $G - E_1 + E_2$ is obtained from G by removing the edges of E_1 from G and adding the edges of E_2 in G. When an edge is removed from the graph, its endpoints are not deleted, and when an edge is added, it makes two non-adjacent vertices adjacent.

In chemical graph theory, topological indices are widely used to predict and model various properties of chemical compounds. Among the pioneering are the first and second Zagreb indices, represented as M_1 and M_2, respectively. These indices resulted from studies on the total π-electron energy of molecular structures [12, 13], and are respectively defined as:

$$M_1(G) = \sum_{v \in V(G)} d_v^2(G) = \sum_{vu \in E(G)} (d_v(G) + d_u(G)),$$
$$M_2(G) = \sum_{vu \in E(G)} d_v(G) d_u(G).$$

The Zagreb indices have attracted significant interest in mathematical chemistry, with their properties and applications extensively studied in surveys [11, 22] and recent works [5, 8, 10, 15].

Finding trees that maximize or minimize graph indices within specific classes has been a major focus in chemical graph theory (see, for Zagreb indices [2, 4, 6, 7, 9, 16, 18, 26, 27]). The study of extremal trees with a given maximum degree has been extensively explored in the literature [1, 14, 21, 24]. Borovićanin et al. [4] characterized the maximal and minimal Zagreb indices of trees with a given number of vertices of maximum degree. A similar problem to [4] concerning the Wiener index has been solved in [17]. Thus, it is natural to consider the analogous problem of characterizing maximal and minimal n-vertex trees with $k \geq 1$ vertices of fixed maximum degree $\Delta \geq 3$.

Let T be an n-vertex tree with specified $k \geq 1$ vertices that have the fixed maximum degree $\Delta \geq 3$. Then

$$\left.\begin{aligned} &\sum_{i=1}^{\Delta-1} n_i + k = n, \\ &\sum_{i=1}^{\Delta-1} i n_i + \Delta k = 2(n-1), \end{aligned}\right\} \tag{1}$$

and
$$\sum_{\substack{j=1 \\ j \neq i}}^{\Delta} m_{j,i} + 2m_{i,i} = i n_i, \quad \forall\ i \in \{1, 2, \ldots, \Delta\}. \tag{2}$$

From (1), we obtain

$$n_1 = 2 + n_3 + 2n_4 + \cdots + (\Delta - 2)k.$$

This leads to

$$n_1 \geq 2 + k(\Delta - 2).$$

From (1), it follows that $n \geq n_1 + k$. Taking this into consideration with above inequality, we obtain

$$n \geq 2 + k(\Delta - 1).$$

Thus, the order n of T with the specified $k \geq 1$ vertices of fixed maximum degree $\Delta \geq 3$ must satisfy $n \geq 2 + k(\Delta - 1)$.

We define a class $\mathcal{T}_{n,\Delta,k}$ of n-vertex trees, where $n \geq 2 + k(\Delta - 1)$, containing exactly $k \geq 1$ vertices, each with a fixed maximum degree $\Delta \geq 3$. In this paper, we consider the following problem.

Problem 1. *Characterize all n-vertex trees in $\mathcal{T}_{n,\Delta,k}$ with maximal and minimal Zagreb indices.*

The characterization of trees with maximal and minimal Zagreb indices based on a given number of vertices having maximum degree [4] is distinct from **Problem 1**, as here we fix the values for k and Δ.

For fixed Δ and k, we illustrate examples of trees in $\mathcal{T}_{n,\Delta,k}$ for specific values of n in Figure 1. For instance, when $\Delta = 4$ and $k = 2$, we have $\mathcal{T}_{8,4,2} = \{T_1\}$, $\mathcal{T}_{9,4,2} = \{T_2, T_3\}$, $\mathcal{T}_{10,4,2} = \{T_4, \ldots, T_{10}\}$. Similarly, for $\Delta = 5$ and $k = 3$, the sets include $\mathcal{T}_{14,5,3} = \{T_{11}\}$, $\mathcal{T}_{15,5,3} = \{T_{12}, \ldots T_{14}\}$, $\mathcal{T}_{16,5,3} = \{T_{15}, \ldots, T_{29}\}$.

To find a solution to **Problem 1**, we first establish several key results. By using (1), the following result is true.

Lemma 1. *Let $T \in \mathcal{T}_{n,\Delta,k}$, where $\Delta = 3$. Then the vertex degree sequence of T is* $\pi_0 = (\underbrace{3, \ldots, 3}_{k}, \underbrace{2, \ldots, 2}_{n-2-2k}, \underbrace{1, \ldots, 1}_{2+k})$.

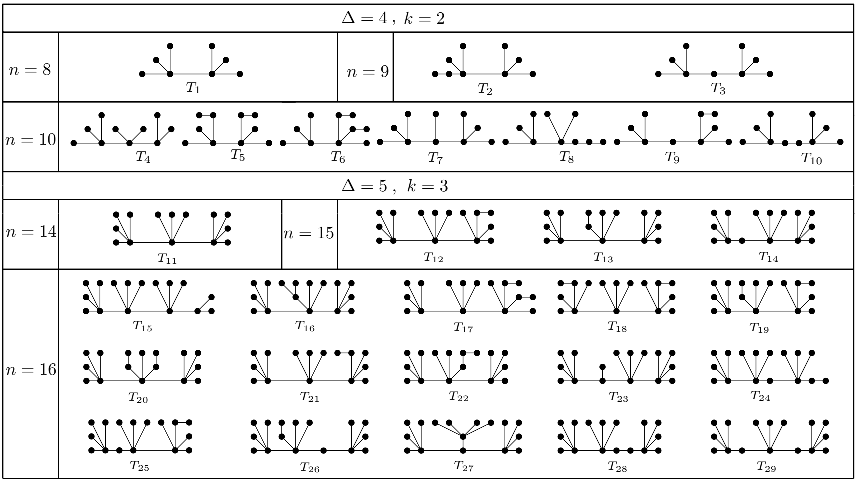

Figure 1. Examples of trees in $\mathcal{T}_{n,\Delta,k}$ for selected values of n with fixed Δ and k, where $\Delta \in \{4, 5\}$ and $k \in \{2, 3\}$.

Lemma 2. *For $T \in \mathcal{T}_{n,\Delta,k}$ with $\Delta \geq 4$, we have the following:*
(a) If $|\{v \in V(T) \mid 2 \leq d_v(T) \leq \Delta-2\}| = 0$, then $n-k \equiv 2 \pmod{(\Delta-2)}$. Moreover, T has the degree sequence

$$\pi_1 = (\underbrace{\Delta, \ldots, \Delta}_{k}, \underbrace{\Delta-1, \ldots, \Delta-1}_{\frac{n-2-k(\Delta-1)}{(\Delta-2)}}, \underbrace{1, \ldots, 1}_{\frac{n(\Delta-3)+2+k}{(\Delta-2)}}).$$

(b) If $|\{v \in V(T) \mid 2 \leq d_v(T) = i \leq \Delta-2\}| = 1$, then $n-k-i \equiv 1 \pmod{(\Delta-2)}$. Moreover, T has the degree sequence

$$\pi_2 = (\underbrace{\Delta, \ldots, \Delta}_{k}, \underbrace{\Delta-1, \ldots, \Delta-1}_{\frac{n-k(\Delta-1)-i-1}{(\Delta-2)}}, i, \underbrace{1, \ldots\ldots, 1}_{\frac{n(\Delta-3)+k-\Delta+i+3}{(\Delta-2)}}).$$

Proof. (a) In this case, (1) implies

$$\left.\begin{aligned} n &= n_1 + n_{\Delta-1} + k, \\ 2n-2 &= n_1 + (\Delta-1)n_{\Delta-1} + \Delta k. \end{aligned}\right\} \tag{3}$$

From (3), we obtain

$$n_1 = (\Delta - 3)n_{\Delta-1} + (\Delta - 2)k + 2. \tag{4}$$

Now substituting (4) in the first equation of (3), we obtain

$$n - k = (\Delta - 2)(n_{\Delta-1} + k) + 2.$$

This implies $n - k \equiv 2 \pmod{(\Delta - 2)}$. From the above equation, we have $n_{\Delta-1} = \frac{n-2-k(\Delta-1)}{\Delta-2}$. This with (4) implies that $n_1 = \frac{n(\Delta-3)+2+k}{\Delta-2}$. Thus we have π_1.

(b) In this case, (1) implies

$$\left.\begin{aligned} n &= n_1 + 1 + n_{\Delta-1} + k, \\ 2n - 2 &= n_1 + i + (\Delta - 1)n_{\Delta-1} + \Delta k. \end{aligned}\right\} \tag{5}$$

From (5), we obtain

$$n_1 = (\Delta - 3)n_{\Delta-1} + (\Delta - 2)k + i. \tag{6}$$

Now substituting (6) in the first equation of (5), we obtain

$$n - k = (\Delta - 2)(n_{\Delta-1} + k) + i + 1.$$

This implies $n - k - i \equiv 1 \pmod{(\Delta - 2)}$. From the above equation, we have $n_{\Delta-1} = \frac{n-k(\Delta-1)-i-1}{\Delta-2}$. This with (6) gives $n_1 = \frac{n(\Delta-3)+k-\Delta+i+3}{\Delta-2}$. Thus, we have our desired degree sequence π_2. ■

In the following lemma, we introduce a graph transformation that decreases the second Zagreb index of the modified graph compared to the original graph.

Lemma 3. *Let G be a graph containing an internal path $xy\,(d_x, d_y \geq 3)$ of length $l_1 = 1$ and another internal path of length $l_2 \geq 3$. Let G_1 be derived from G by replacing $l_1 = 1$ with $l_1 = 2$ and $l_2 \geq 3$ with $l_2 \geq 2$. Then $M_2(G_1) < M_2(G)$.*

Proof. Note that $d_w(G_1) = d_w(G)$ for all $w \in V(G)$. We obtain

$$M_2(G_1) - M_2(G) = 2d_x + 2d_y - 4 - d_x d_y.$$

Let us consider a function $f(z_1, z_2) = 2z_1 + 2z_2 - z_1 z_2$ with $z_1, z_2 \geq 3$. One can easily see that $f(z_1, z_2)$ is strictly decreasing in both z_1 and z_2. Then from the above, we obtain

$$M_2(G_1) - M_2(G) \leq f(3,3) - 4 = -1 < 0.$$

Hence $M_2(G_1) < M_2(G)$. ■

2 The first Zagreb index

In this section, we aim to find trees in $\mathcal{T}_{n,\Delta,k}$ with maximal and minimal first Zagreb index. For $\Delta = 3$, the extremal first Zagreb index for trees in $\mathcal{T}_{n,\Delta,k}$ directly follows from Lemma 1. Henceforth, in this section, we will consider the class $\mathcal{T}_{n,\Delta,k}$ for $\Delta \geq 4$.

Theorem 1. *Let $T \in \mathcal{T}_{n,\Delta,k}$ be a tree with $\Delta \geq 4$. Then*

$$M_1(T) \geq 4n + k(2 - 3\Delta + \Delta^2) - 6.$$

The equality holds if and only if T has the degree sequence
$(\underbrace{\Delta, \ldots, \Delta}_{k}, \underbrace{2, \ldots, 2}_{n-2+k(1-\Delta)}, \underbrace{1, \ldots, 1}_{2+k(\Delta-2)})$.

Proof. Let $T' \in \mathcal{T}_{n,\Delta,k}$ be a tree having a minimal first Zagreb index. We show that $n_i(T') = 0$ for each $i \in [3, \Delta - 1]$. On the contrary, assume that there exists a vertex $u \in V(T')$ such that $3 \leq d_u \leq \Delta - 1$. Without loss of generality, assume that u is chosen in such a way that there exists a pendant path from v to u, where v is a pendant vertex. Let $u_1, u_2 \in N_u$ and u_2 lies on the pendant u,v-path. We construct a tree $T_1 \in \mathcal{T}_{n,\Delta,k}$ from T' as follows:

$$T_1 = T' - uu_1 + vu_1.$$

Then $d_u(T_1) = d_u(T') - 1 = d_u - 1$, $d_v(T_1) = 2$ and $d_w(T_1) = d_w(T')$ for all $w \in V(T') \setminus \{u,v\}$. Thus

$$M_1(T_1) - M_1(T') = (d_u - 1)^2 + 2^2 - d_u^2 - 1 = 2(2 - d_u).$$

Since $d_u \geq 3$, we obtain $M_1(T_1) < M_1(T')$, which contradicts the choice of T'. Therefore, $n_i(T') = 0$ for each $i \in [3, \Delta - 1]$. From (1), we obtain that T' has the degree sequence $(\underbrace{\Delta, \ldots, \Delta}_{k}, \underbrace{2, \ldots, 2}_{n-2+k(1-\Delta)}, \underbrace{1, \ldots, 1}_{2+k(\Delta-2)})$. Hence

$$\begin{aligned} M_1(T') &= k\Delta^2 + 2^2\Big(n - 2 + k(1-\Delta)\Big) + 2 + k(\Delta - 2), \\ &= 4n + k(2 - 3\Delta + \Delta^2) - 6. \end{aligned}$$

This completes the proof. ■

In the next theorem, we determine upper bounds for the trees in $\mathcal{T}_{n,\Delta,k}$ with respect to the first Zagreb index when $\Delta \geq 4$ and characterize the maximal trees.

Theorem 2. *Let $T \in \mathcal{T}_{n,\Delta,k}$ be a tree with $\Delta \geq 4$. Then*

$$M_1(T) \leq \begin{cases} n(\Delta+1) + k(\Delta-1) - 2\Delta & \text{if } n - k \equiv 2(\text{mod } (\Delta - 2)), \\ (\Delta+1)(n-1) + k(\Delta-1) + i(i-\Delta) & \\ & \text{if } n - k - i \equiv 1(\text{mod } (\Delta - 2)), \end{cases}$$

where $i \in [2, \Delta - 2]$. Inequality becomes an equality if and only if T has the degree sequence π_1 for $n - k \equiv 2(\text{mod } (\Delta - 2))$, and inequality becomes an equality if and only if T has degree sequence π_2 for $n - k - i \equiv 1(\text{mod } (\Delta - 2))$, where π_1 and π_2 are defined in Lemma 2.

Proof. Let $T' \in \mathcal{T}_{n,\Delta,k}$ be a tree with the maximal first Zagreb index. We prove that $|\{v \in V(T') \mid 2 \leq d_v(T') \leq \Delta - 2\}| \leq 1$. Assume to the contrary, there exist two vertices $u, v \in V(T')$ such that $2 \leq d_u \leq d_v \leq (\Delta - 2)$. Let $u_1 \in N_u$ be such that u_1 does not lie on the u,v-path. We construct a tree $T_1 \in \mathcal{T}_{n,\Delta,k}$ from T' as follows:

$$T_1 = T' - uu_1 + vu_1.$$

Then $d_u(T_1) = d_u(T') - 1 = d_u - 1$, $d_v(T_1) = d_v(T') + 1 = d_v + 1$ and $d_w(T_1) = d_w(T')$ for all $w \in V(T') \setminus \{u, v\}$. We obtain

$$M_1(T_1) - M_1(T') = (d_u - 1)^2 - d_u^2 + (d_v + 1)^2 - d_v^2 = 2 + 2(d_v - d_u).$$

Since $d_v \geq d_u$, we obtain $M_1(T_1) > M_1(T')$, which is a contradiction to the choice of T'. Thus $|\{v \in V(T') \mid 2 \leq d_v(T') \leq \Delta - 2\}| \leq 1$. We now consider the following cases:

Case 1. When $|\{v \in V(T') \mid 2 \leq d_v(T') \leq \Delta - 2\}| = 0$, that is $n_i(T') = 0$ for all $i \in [2, \Delta - 2]$. From Lemma 2 (a), we have $n - k \equiv 2 \pmod{(\Delta - 2)}$, and T' has the degree sequence

$$\pi_1 = (\underbrace{\Delta, \ldots, \Delta}_{k}, \underbrace{\Delta - 1, \ldots, \Delta - 1}_{\frac{n-2-k(\Delta-1)}{\Delta-2}}, \underbrace{1, \ldots, 1}_{\frac{n(\Delta-3)+2+k}{\Delta-2}}).$$

Therefore

$$M_1(T') = n(\Delta + 1) + k(\Delta - 1) - 2\Delta.$$

Case 2. When $|\{v \in V(T') \mid 2 \leq d_v(T') = i \leq \Delta - 2\}| = 1$. From Lemma 2 (b), we obtain $n - k - i \equiv 1 \pmod{(\Delta - 2)}$, such that $n_i(T') = 1$. Therefore, T' has the degree sequence

$$\pi_2 = (\underbrace{\Delta, \ldots, \Delta}_{k}, \underbrace{\Delta - 1, \ldots, \Delta - 1}_{\frac{n-k(\Delta-1)-i-1}{\Delta-2}}, i, \underbrace{1, \ldots\ldots\ldots, 1}_{\frac{n(\Delta-3)+k-\Delta+i+3}{\Delta-2}}),$$

Hence

$$M_1(T') = (\Delta + 1)(n - 1) + k(\Delta - 1) + i(i - \Delta).$$

This completes the proof. ■

3 The second Zagreb index

In this section, we find trees in $\mathcal{T}_{n,\Delta,k}$ with the maximal and minimal second Zagreb index.

3.1 Maximal second Zagreb index

In this subsection, we first address **Problem 1** regarding the maximal second Zagreb index for $\Delta = 3$. By Lemma 1, a tree $T \in \mathcal{T}_{n,\Delta,k}$ with $\Delta = 3$ has the degree sequence $\pi_0 = (\underbrace{3,\ldots,3}_{k},\underbrace{2,\ldots,2}_{n-2-2k},\underbrace{1,\ldots,1}_{2+k})$.

We define a subclass $\mathcal{T}^1_{n,\Delta,k} \subseteq \mathcal{T}_{n,\Delta,k}$ of trees that satisfy the following conditions:

(i) Each tree in $\mathcal{T}^1_{n,\Delta,k}$ has a degree sequence π_0.

(ii) If $n < 3k+4$, then $m_{1,3} = 3k-n+4-n$, $m_{2,3} = n-2-2k$, $m_{1,2} = n-2-2k$ and $m_{3,3} = k-1$.

(iii) If $n \geq 3k+4$, then $m_{1,2} = k+2$, $m_{2,3} = k+2$, $m_{2,2} = n-3k-4$ and $m_{3,3} = k-1$.

We now prove the main result for the maximal second Zagreb index for trees in $\mathcal{T}_{n,\Delta,k}$ when $\Delta = 3$.

Theorem 3. *Let $T \in \mathcal{T}_{n,\Delta,k}$ be a tree with $\Delta = 3$. Then*

$$M_2(T) \leq \begin{cases} 5n+2k-13 & \text{if } n < 3k+4, \\ 4n+5k-9 & \text{if } n \geq 3k+4. \end{cases}$$

The equality holds if and only if T is in $\mathcal{T}^1_{n,\Delta,k}$.

Proof. Let T' be a tree with maximal second Zagreb index in $\mathcal{T}_{n,\Delta,k}$ such that $\Delta = 3$. From Lemma 1, the degree sequence of T' is

$$\pi_0 = (\underbrace{3,\ldots,3}_{k},\underbrace{2,\ldots,2}_{n-2-2k},\underbrace{1,\ldots,1}_{2+k}).$$

We now consider the following claims.

Claim 1. *T' holds $m_{3,3} = k-1$.*

Proof of Claim 1. Suppose to the contrary that T' contains $v_1v_2\ldots v_l$ ($l \geq 3$) such that $d_{v_1} = 3 = d_{v_l}$. Let $xy \in E(T')$ such that $d_x = 1$ and

$d_y \geq 2$. Now, construct a tree T_1 from T' as follows:

$$T_1 = T' - \{v_1v_2, v_{l-1}v_l, xy\} + \{v_1v_l, xv_2, v_{l-1}y\}.$$

Then note that $d_v(T_1) = d_v(T')$ for all $v \in V(T')$. We obtain

$$M_2(T_1) - M_2(T') = 9 - 6 + 2 - 6 + d_y = -1 + d_y > 0,$$

as $d_y \geq 2$. Consequently, $M_2(T_1) > M_2(T')$. This completes the proof of **Claim 1**.

Now by using degree sequence π_0 and **Claim 1** in (2), we obtain

$$\left.\begin{aligned} &m_{1,2} + m_{1,3} = 2 + k, \\ &m_{1,2} + 2m_{2,2} + m_{2,3} = 2(n - 2k - 2), \\ &m_{1,3} + m_{2,3} + 2(k-1) = 3k. \end{aligned}\right\} \tag{7}$$

Claim 2. *$m_{2,2}$ and $m_{1,3}$ cannot be simultaneously positive.*

Proof of Claim 2. Suppose to the contrary that T' contains $xy \in E(T')$ and $v_1v_2 \dots v_l$ ($l \geq 4$) simultaneously such that $d_y = 3 = d_{v_l}$ and $d_{v_1} = 1 = d_x$. We construct a tree $T_2 = T' - \{v_1v_2, v_2v_3, xy\} + \{xv_2, yv_2, v_1v_3\}$ from T' such that $d_v(T_2) = d_v(T')$ for all $v \in V(T')$. We obtain

$$M_2(T_2) - M_2(T') = 6 + 2 - 3 - 4 = 1 > 0.$$

Hence $M_2(T_2) > M_2(T')$. This proves the **Claim 2**.

We now consider the following two cases:

Case 1. When $n < 3k + 4$. In this case, we claim $m_{2,2} = 0$. Suppose on the contrary that $m_{2,2} > 0$. Since $n_2 = n - 2 - 2k < 3k + 4 - 2 - 2k = k + 2$, $m_{3,3} = k - 1$ and T' contains $n_1 = k + 2$ pendant paths. These along with $m_{2,2} > 0$ ensure that $m_{1,3} > 0$. By **Claim 2**, we conclude that $m_{2,2} = 0$. This with (7) implies that $m_{1,3} = 3k - n + 4$, $m_{1,2} = n - 2 - 2k$ and

$m_{2,3} = n - 2 - 2k$. Hence

$$\begin{aligned} M_2(T') &= 3^2(k-1) + 3(3k-n+4) + 2(n-2-2k) + 6(n-2-2k) \\ &= 5n + 2k - 13. \end{aligned}$$

Case 2. When $n \geq 3k+4$. In this case, we claim $m_{1,3} = 0$. On the contrary, assume that $m_{1,3} > 0$. Note that $n_2 = n-2-2k \geq k+2$. This with $m_{3,3} = k-1$, $m_{1,3} > 0$ and T' contains $n_1 = k+2$ pendant paths, verifies that $m_{2,2} > 0$. Then by **Claim 2**, we have $m_{1,3} = 0$. Using this in (7), we obtain $m_{1,2} = 2+k$, $m_{2,3} = k+2$ and $m_{2,2} = n-3k-4$. Thus

$$M_2(T') = 2(2+k) + 6(2+k) + 4(n-3k-4) + 3^2(k-1) = 4n + 5k - 9.$$

This completes the proof. ■

From now on, we consider the class $\mathcal{T}_{n,\Delta,k}$ for $\Delta \geq 4$ and introduce the definitions of BFS-ordering and majorization to characterize the structural properties of trees with maximal second Zagreb index. The BFS-ordering and majorization technique is a valuable method for localizing graph topological indices and has been extensively studied in the literature (for example see [19, 23]).

For a tree T with root vertex v_0, denote h_v by the distance between vertices v and v_0, and define $A_i(T)$ as: $A_i(T) = \{v \mid h_v = i \text{ and } v \in V(T)\}$. Thus $A_0(T) = \{v_0\}$. For details, we refer [19, 20, 29].

Definition 1. (**BFS-ordering, [19]**) Let T be a tree with root vertex v_0. A well-ordering $\prec$ of the vertices is called a breadth-first search ordering (BFS-ordering) if the following holds for all vertices $u, v \in V(T)$:

(i) $u \prec v$ implies $h_u \leq h_v$ and $d_u \geq d_v$.

(ii) If there are two edges $uu_1 \in E(T)$ and $vv_1 \in E(T)$ such that $u \prec v$, $h_u = h_{u_1} + 1$ and $h_v = h_{v_1} + 1$, then $u_1 \prec v_1$.

We call tree a BFS tree if the vertices have BFS-ordering. In some literature, a BFS-tree is also called a greedy tree (see, [20, 28]). We now define the majorization.

Definition 2. (**Majorization**) Given two non-increasing degree sequences $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$, we say that π' majors π, written by $\pi \lhd \pi'$, if the following conditions are met:

(*i*) $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$.

(*ii*) $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, \ldots, n-1$.

We define $\Gamma(\pi)$ as the class of connected graphs that have the degree sequence π. The following result will be important to build our argument.

Lemma 4. [19] *Let π and π' be two different non-increasing tree degree sequences with $\pi \lhd \pi'$. Let T^* and T^{**} be the trees with maximal second Zagreb indices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. Then $M_2(T^*) < M_2(T^{**})$.*

We now prove the following lemma.

Lemma 5. *Let $T \in \mathcal{T}_{n,\Delta,k}$ be a tree with the maximal second Zagreb index, where $\Delta \geq 4$. Then $|\{v \in V(T) \mid 2 \leq d_v(T) \leq \Delta - 2\}| \leq 1$.*

Proof. On the contrary, assume that there exist $u, v \in V(T)$ such that $2 \leq d_v \leq d_u \leq \Delta - 2$. It follows that the degree sequence of T is

$$\pi = (\underbrace{\Delta, \ldots, \Delta}_{k \geq 1}, \underbrace{\Delta - 1, \ldots, \Delta - 1}_{p \geq 0}, \underbrace{d_u, \ldots d_v, \ldots}_{q \geq 2}, 1, \ldots, 1).$$

We now construct a tree $T' \in \mathcal{T}_{n,\Delta,k}$ from T such that $d_u(T') = d_u(T) + 1$, $d_v(T') = d_v(T) - 1$ and $d_w(T') = d_w(T)$ for all $w \in V(T) \backslash \{u, v\}$. Then T' has the degree sequence

$$\pi' = (\underbrace{\Delta, \ldots, \Delta}_{k \geq 1}, \underbrace{\Delta - 1, \ldots, \Delta - 1}_{p \geq 0}, \underbrace{d_u + 1, \ldots, d_v - 1, \ldots}_{q \geq 2}, 1, \ldots, 1).$$

If d_i and $d_{i'}$ represent the entries of π and π', respectively, then

$$\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i, \tag{8}$$

and

$$\sum_{i=1}^{k+p+1} d'_i > \sum_{i=1}^{k+p+1} d_i.$$

This gives

$$\sum_{i=1}^{j} d'_i \geq \sum_{i=1}^{j} d_i, \quad \text{for all } j = 1, 2, \ldots, n-1. \tag{9}$$

From (8), (9) and Definition 2, we conclude that $\pi \lhd \pi'$ (π' majorizes π). Let $\Gamma(\pi)$ and $\Gamma(\pi')$ be the subclasses of trees in $\mathcal{T}_{n,\Delta,k}$ with degree sequences π and π', respectively. Let $T \in \Gamma(\pi)$ and $T' \in \Gamma(\pi')$ such that both T and T' have the maximal second Zagreb index in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. Then, by using Lemma 4, we obtain

$$M_2(T) < M_2(T'),$$

which contradicts the choice of T. Hence $|\{v \in V(T) \mid 2 \leq d_v(T) \leq \Delta - 2\}| \leq 1$. This completes the proof. ■

The following results are important in establishing our main theorem.

Proposition 4. **[29]** *For a given degree sequence π of some tree, there exists a unique tree T^* with degree sequence π having a BFS-ordering. Moreover, any two trees with the same degree sequences and having BFS-ordering are isomorphic.*

Lemma 6. **[19]** *Given a tree degree sequence π, the BFS-tree T^* has the maximum second Zagreb index in $\Gamma(\pi)$.*

Theorem 5. *Let $T \in \mathcal{T}_{n,\Delta,k}$ be a tree with the maximal second Zagreb index, where $\Delta \geq 4$. Then*

$$M_2(T) = \begin{cases} \Delta(k+2n-2) - \Delta^2 - k - n + 2 \\ \quad \textit{if } n < k\Delta^2 + (2-3k)(\Delta-1),\ n-k \equiv 2(\text{mod } (\Delta-2)), \\ \Delta^2(k-1) + 2(n\Delta - k\Delta + k - n) \\ \quad \textit{if } n \geq k\Delta^2 + (2-3k)(\Delta-1),\ n-k \equiv 2(\text{mod } (\Delta-2)), \\ \frac{1}{(\Delta-2)}\Big(n(2\Delta^2 - 5\Delta + 2) + \Delta^2(1-\Delta+k-i) + i^2(\Delta-2) \\ +k(2-3\Delta) + \Delta(3+2i) - 2\Big) \\ \textit{if } n < k\Delta^2 + (2-3k)(\Delta-1),\ n-k-i \equiv 1(\text{mod } (\Delta-2)), \\ \frac{1}{(\Delta-2)}\Big(n(\Delta^2 + 3 - 4\Delta) + k(\Delta^2(6 - 4\Delta + \Delta^2) - 1 - 3\Delta) \\ +i(\Delta - 1 + i\Delta - 2i) + \Delta(3-\Delta) - 1\Big) \\ \quad \textit{if } n = k\Delta^2 + (2-3k)(\Delta-1),\ n-k-i \equiv 1(\text{mod } (\Delta-2)), \\ \frac{1}{(\Delta-2)}\Big(2n(\Delta^2 - 3\Delta + 2) + k(6\Delta - 4 - 4\Delta^2 + \Delta^3) \\ +2(1-i^2) + \Delta(2i + 3\Delta - 3 - i\Delta - \Delta^2 + i^2)\Big) \\ \textit{if } n > k\Delta^2 + (2-3k)(\Delta-1), n-k-i \equiv 1(\text{mod } (\Delta-2)), \end{cases}$$

where $i \in [2, \Delta-2]$.

Proof. By Lemma 5, T has the degree sequence

$$\pi^* = (\underbrace{\Delta, \ldots, \Delta}_{k \geq 1}, \underbrace{\Delta-1, \ldots, \Delta-1}_{p \geq 0}, \underbrace{i}_{q \leq 1}, \underbrace{1, \ldots, 1}_{n-k-p-q}),$$

where $i \in [2, \Delta-2]$. Thus $T \in \Gamma(\pi^*) \subseteq \mathcal{T}_{n,\Delta,k}$. From Lemma 6, the BFS-tree maximizes the second Zagreb index within $\Gamma(\pi^*)$. Denote the BFS-tree by T_{BFS} in $\Gamma(\pi^*)$. By Proposition 4, it follows that T_{BFS} may or may not be isomorphic to T. Since both T and T_{BFS} are maximal in $\Gamma(\pi^*)$, it holds that $M_2(T) = M_2(T_{BFS})$. Therefore we focus on finding the $M_2(T_{BFS})$ by following BFS-ordering. From BFS-ordering, it is clear that

$$m_{\Delta,\Delta} = k - 1. \tag{10}$$

By using (10) in (2), we obtain

$$m_{1,\Delta} + \sum_{2\le i\le \Delta-2} m_{i,\Delta} + m_{\Delta-1,\Delta} + 2(k-1) = \Delta k,$$

that is,

$$m_{1,\Delta} + \sum_{2\le i\le \Delta-2} m_{i,\Delta} + m_{\Delta-1,\Delta} = k(\Delta-2)+2.$$

By Lemma 5, the tree T_{BFS} contains at most one vertex of degree $2 \le i \le \Delta - 2$, thus we can write the above equation as follows:

$$m_{1,\Delta} + m_{i,\Delta} + m_{\Delta-1,\Delta} = k(\Delta-2)+2. \tag{11}$$

By (11), one can see that that the total neighboring vertices of degree Δ, excluding the vertices having degree Δ, amount to $(\Delta-2)k+2$. From Lemma 5, we have $|\{v \in V(T_{BFS}) \mid 2 \le d_v(T_{BFS}) \le \Delta-2\}| \le 1$. We now discuss the proof in two cases:

Case 1. When $|\{v \in V(T_{BFS}) \mid 2 \le d_v(T_{BFS}) \le \Delta-2\}| = 0$.
By Lemma 2 (a), we obtain $n-k \equiv 2 \,(\mathrm{mod}\,(\Delta-2))$, and the degree sequence π^* of T_{BFS} becomes

$$\pi_1 = (\underbrace{\Delta,\ldots,\Delta}_{k}, \underbrace{\Delta-1,\ldots,\Delta-1}_{\frac{n-2-k(\Delta-1)}{\Delta-2}}, \underbrace{1,\ldots,1}_{\frac{n(\Delta-3)+2+k}{\Delta-2}}).$$

By using (10) and above degree sequence π_1 in (2), we derive

$$\left.\begin{aligned} m_{1,\Delta-1} + m_{1,\Delta} &= \frac{n(\Delta-3)+2+k}{\Delta-2}, \\ m_{1,\Delta-1} + 2m_{\Delta-1,\Delta-1} + m_{\Delta-1,\Delta} &= \frac{(\Delta-1)[n-2-k(\Delta-1)]}{\Delta-2}, \\ m_{1,\Delta} + m_{\Delta-1,\Delta} + 2(k-1) &= \Delta k. \end{aligned}\right\} \tag{12}$$

Since T_{BFS} follows BFS-ordering, so by (11), it is observed that if $n_{\Delta-1} < k(\Delta-2)+2$ then $m_{\Delta-1,\Delta-1} = 0$, $m_{1,\Delta} \ne 0$, and if $n_{\Delta-1} \ge k(\Delta-2)+2$, then $m_{1,\Delta} = 0$. We now consider the following cases:

Case 1.1. When $n < k\Delta^2 + (2-3k)(\Delta-1)$.
We obtain $n_{\Delta-1} < k(\Delta-2)+2$, and thus by (11), we conclude that $m_{1,\Delta} > n_{\Delta-1} - m_{\Delta-1,\Delta} \geq 0$. Since $m_{1,\Delta} > 0$, thus by BFS-ordering, one can see that $m_{\Delta-1,\Delta-1} = 0$. This with (12) implies that $m_{1,\Delta-1} = n+k(1-\Delta)-2$, $m_{\Delta-1,\Delta} = \frac{n+k(1-\Delta)-2}{(\Delta-2)}$ and $m_{1,\Delta} = \frac{k(\Delta^2-3\Delta+3)+2\Delta-n-2}{(\Delta-2)}$. Therefore

$$M_2(T_{BFS}) = \Delta\left(\frac{k(\Delta^2-3\Delta+3)+2\Delta-n-2}{\Delta-2}\right) + \Delta^2(k-1) + \Delta(\Delta-1)\left(\frac{n+k(1-\Delta)-2}{\Delta-2}\right) + (\Delta-1)(n+k(1-\Delta)-2).$$

Case 1.2. When $n \geq k\Delta^2 + (2-3k)(\Delta-1)$.
We obtain $n_{\Delta-1} \geq k(\Delta-2)+2$. By (11), it is evident that in a tree $T_{BFS} \in \mathcal{T}_{n,\Delta,k}$, the k vertices of degree Δ collectively have $(\Delta-2)k+2$ neighboring vertices that are not of degree Δ. Since $n_{\Delta-1} \geq k(\Delta-2)+2$, by BFS-ordering, one can infer that $m_{1,\Delta} = 0$. By using this in (12), we obtain $m_{1,\Delta-1} = \frac{n(\Delta-3)+2+k}{(\Delta-2)}$, $m_{\Delta-1,\Delta} = (\Delta-2)k+2$ and $m_{\Delta-1,\Delta-1} = \frac{n+2+k(3\Delta-\Delta^2-3)-2\Delta}{(\Delta-2)}$. Thus

$$M_2(T_{BFS}) = (\Delta-1)\left(\frac{n(\Delta-3)+2+k}{(\Delta-2)}\right) + \Delta(\Delta-1)\Big(k(\Delta-2)+2\Big) + \Delta^2(k-1) + (\Delta-1)^2\left(\frac{n+2+k(3\Delta-\Delta^2-3)-2\Delta}{(\Delta-2)}\right).$$

Case 2. When $|\{v \in V(T_{BFS}) \mid 2 \leq d_v(T_{BFS}) \leq \Delta-2\}| = 1$. Then there exists $i \in [2, \Delta-2]$ such that $n_i(T_{BFS}) = 1$ and $n_j(T_{BFS}) = 0$ for all $j \in [2, \Delta-2]$ with $j \neq i$. From Lemma 2 (b), we obtain $n-k-i \equiv 1 \,(\mathrm{mod}\,(\Delta-2))$ and degree sequence π^* of T_{BFS} becomes

$$\pi_2 = (\underbrace{\Delta,\ldots,\Delta}_{k}, \underbrace{\Delta-1,\ldots,\Delta-1}_{\frac{n-k(\Delta-1)-i-1}{(\Delta-2)}}, i, \underbrace{1,\ldots\ldots,1}_{\frac{n(\Delta-3)+k-\Delta+i+3}{(\Delta-2)}}).$$

From BFS-ordering, it is evident that $m_{1,i} = i-1$. This with above degree sequence π_2 and (10) in (2), we derive

$$\left.\begin{aligned}(i-1)+m_{1,\Delta-1}+m_{1,\Delta} &= \frac{n(\Delta-3)+k-\Delta+i+3}{(\Delta-2)},\\ (i-1)+m_{i,\Delta-1}+m_{i,\Delta} &= i,\\ m_{1,\Delta-1}+m_{i,\Delta-1}+2m_{\Delta-1,\Delta-1}+m_{\Delta-1,\Delta} &\\ &= \frac{(\Delta-1)[n-k(\Delta-1)-i-1]}{(\Delta-2)},\\ m_{1,\Delta}+m_{i,\Delta}+m_{\Delta-1,\Delta}+2(k-1) &= \Delta k.\end{aligned}\right\} \tag{13}$$

We now further consider the following cases:

Case 2.1. When $n < k\Delta^2+(1-3k)(\Delta-1)+i$.
We obtain $n_{\Delta-1}+n_i(=1) < k(\Delta-2)+2$, and thus by (11), we conclude that $m_{1,\Delta} > n_{\Delta-1}-m_{\Delta-1,\Delta}-m_{i,\Delta}+1$. From (13), we have $m_{i,\Delta}+m_{i,\Delta-1}=1$, which implies that $m_{i,\Delta}\leq 1$. It follows that $m_{1,\Delta} > n_{\Delta-1}-m_{\Delta-1,\Delta}-1+1 = n_{\Delta-1}-m_{\Delta-1,\Delta}\geq 0$, that is, $m_{1,\Delta}>0$. Since $m_{1,\Delta}>0$, by BFS-ordering, it follows that

$$m_{\Delta-1,\Delta-1}=0 \quad\text{and}\quad m_{i,\Delta-1}=0. \tag{14}$$

By using (14) in (13), we obtain $m_{i,\Delta}=1$, $m_{1,\Delta-1}=n-k(\Delta-1)-(i+1)$, $m_{\Delta-1,\Delta}=\frac{n-k(\Delta-1)-(i+1)}{\Delta-2}$ and $m_{1,\Delta}=\frac{k\Delta^2+3k(1-\Delta)-n+i+\Delta-1}{\Delta-2}$. Thus

$$\begin{aligned}M_2(T_{BFS}) &= (\Delta-1)\Big(n-k(\Delta-1)-(i+1)\Big)+\Delta^2(k-1)+i(i-1)\\ &\quad+\Delta(\Delta-1)\left(\frac{n-k(\Delta-1)-(i+1)}{\Delta-2}\right)+i\Delta\\ &\quad+\Delta\left(\frac{k\Delta^2+3k(1-\Delta)-n+i+\Delta-1}{\Delta-2}\right).\end{aligned}$$

Case 2.2. When $n = k\Delta^2+(1-3k)(\Delta-1)+i$.
From **Case 2.1**, clearly $m_{1,\Delta}>0$ for $n < k\Delta^2+(1-3k)(\Delta-1)+i$. In this case $n = k\Delta^2+(1-3k)(\Delta-1)+i$, thus by BFS-ordering, one can

infer that

$$m_{i,\Delta-1} = 0 \text{ and } m_{\Delta-1,\Delta-1} = 0. \tag{15}$$

We now claim that $m_{1,\Delta} = 0$ for $n = k\Delta^2 + (1-3k)(\Delta-1) + i$. On the contrary, we assume that $m_{1,\Delta} > 0$. One can observe that $m_{1,\Delta} > n_{\Delta-1} - m_{\Delta-1,\Delta} - m_{i,\Delta} + 1$. Together with (11), we obtain $n_{\Delta-1} + 1 < k(\Delta-2)+2$. This gives $n < k\Delta^2 + (1-3k)(\Delta-1)+i$, which is a contradiction. Therefore

$$m_{1,\Delta} = 0. \tag{16}$$

By using (15) and (16) in (13), we obtain $m_{1,\Delta-1} = \frac{(\Delta-3)(n-i)+k+1}{\Delta-2}$, $m_{i,\Delta} = 1$, $m_{\Delta-1,\Delta} = k(\Delta-2)+1$. Thus

$$M_2(T_{BFS}) = (\Delta-1)\left(\frac{(\Delta-3)(n-i)+k+1}{\Delta-2}\right) + i\Delta + i(i-1) + \Delta^2(k-1) + (\Delta)(\Delta-1)\Big(k(\Delta-2)+1\Big).$$

Case 2.3. When $n > k\Delta^2 + (1-3k)(\Delta-1) + i$.
This case implies that $n_{\Delta-1} + n_i(=1) > k(\Delta-2)+2$. By (11), it is evident that in a tree $T_{BFS} \in \mathcal{T}_{n,\Delta,k}$, the k vertices of degree Δ collectively have $(\Delta-2)k+2$ neighboring vertices other than those of degree Δ. Since $n > k\Delta^2 + (1-3k)(\Delta-1)+i$, by BFS-ordering, it is obvious that $m_{1,\Delta} = 0$ and $m_{i,\Delta} = 0$. These, together with (13) imply that $m_{i,\Delta-1} = 1$, $m_{1,\Delta-1} = \frac{n(\Delta-3)+k+i(3-\Delta)+1}{\Delta-2}$, $m_{\Delta-1,\Delta} = (\Delta-2)k+2$. and $m_{\Delta-1,\Delta-1} = \frac{n-\Delta k(\Delta-3)-3k-i-2\Delta+3}{\Delta-2}$. Thus

$$M_2(T_{BFS}) = (\Delta-1)\left(\frac{n(\Delta-3)+k+i(3-\Delta)+1}{\Delta-2}\right) + \Delta^2(k-1) + i(\Delta-1) + \Delta(\Delta-1)\Big((\Delta-2)k+2\Big) + i(i-1) + (\Delta-1)^2\left(\frac{n-\Delta k(\Delta-3)-3k-i-2\Delta+3}{\Delta-2}\right).$$

This completes the proof. ■

3.2 Minimal second Zagreb index

In this subsection, we find the minimal second Zagreb index of trees in $\mathcal{T}_{n,\Delta,k}$. First, we prove the following result when $k \geq 2$.

Lemma 7. *Let $T \in \mathcal{T}_{n,\Delta,k}$ be a tree with the minimal second Zagreb index, where $k \geq 2$. Then $n_1 = m_{1,\Delta}$.*

Proof. On the contrary, assume that there exists an edge $uu_1 \in E(T)$ such that $d_u = 1$ and $2 \leq d_{u_1} \leq \Delta - 1$. Let v be a vertex with $d_v = \Delta$ and $N_v = \{v_1, v_2, \ldots, v_\Delta\}$. Assume that v minimizes $d(u,v)$ among all vertices of degree Δ. Also, assume that v_Δ lies on the v,u-path. Thus, $d_{v_\Delta} \geq 2$. We consider the following two cases based on whether there exists a vertex of degree between 3 to $\Delta - 1$ on u, v_Δ-path.

Case 1. When there exists a vertex of degree between 3 to $\Delta - 1$ on u, v_Δ-path: Let z be the vertex on u, v_Δ-path such that $3 \leq d_z \leq \Delta - 1$. Without loss of generality, assume that z minimizes $d(u,z)$ among all vertices on the u, v_Δ-path whose degree lies between 3 and $\Delta - 1$. Let z_1 be the neighbor of z on the u,z-path. Then by the choice of z, we have $d_{z_1} = 2$. We construct a tree

$$T_1 = T - \{zz_1, vv_\Delta\} + \{vu, z_1v_\Delta\}.$$

Then $d_z(T_1) = d_z(T) - 1 = d_z - 1$, $d_u(T_1) = 2$ and $d_w(T_1) = d_w(T)$ for all $w \in V(T) \backslash \{z, u\}$.

If $z = u_1$, then $z_1 = u$ and $d_{u_1} \geq 3$. Let $u_1' \in N_{u_1}$ such that u_1' lies on u_1, v_Δ-path, where $d_{u_1'} \geq 2$. We obtain

$$\begin{aligned} M_2(T_1) - M_2(T) = 2\Delta - d_{u_1} + d_{v_\Delta}(2 - \Delta) + d_{u_1'}(d_{u_1} - 1) - d_{u_1'}d_{u_1} \\ + \sum_{y \in N_{u_1} \backslash \{u, u_1'\}} \Big(d_y(d_{u_1} - 1) - d_y d_{u_1}\Big). \end{aligned}$$

Since $d_{u_1} \geq 3$, it follows that $N_{u_1} \setminus \{u, u_1'\}$ is nonempty. Also, since $d_{v_\Delta}, d_{u_1'} \geq 2$, it follows that $M_2(T_1) - M_2(T) < 0$.

If $z \neq u_1$ then $d_{u_1} = 2$ and we obtain

$$M_2(T_1) - M_2(T) = 2\Delta + 2 - 2d_z + d_{v_\Delta}(2-\Delta) + \sum_{y \in N_z \setminus \{z_1\}} \Big(d_y(d_z - 1) - d_y d_z \Big).$$

Since $N_z \setminus \{z_1\}$ is nonempty, $d_{v_\Delta} \geq 2$ and $d_z \geq 3$, it follows that $M_2(T_1) - M_2(T) < 0$. Thus, in either case, we get a contradiction.

Case 2. When there is no vertex of degree between 3 to $\Delta - 1$ on u, v_Δ-path: Since $k \geq 2$, there is at least one neighbor of v other than v_Δ with degree greater than 1. In this case $d_{u_1} = 2$. Without loss of generality, assume that $d_{v_1} \geq 2$. We construct a tree $T_2 \in \mathcal{T}_{n,\Delta,k}$ from T as follows:

$$T_2 = T - \{uu_1, vv_1\} + \{vu, v_1u_1\}.$$

Then, $d_w(T_2) = d_w(T)$ for all $w \in V(T)$. We have

$$M_2(T_2) - M_2(T) = \Delta + 2d_{v_1} - \Delta d_{v_1} - 2 = (\Delta - 2)(1 - d_{v_1}) < 0,$$

as $d_{v_1} \geq 2$ and $\Delta \geq 3$. This is a contradiction to the choice of T.

In each case, we get a contradiction. Hence $n_1 = m_{1,\Delta}$. ■

Observe that when $k = 1$ and $n = \Delta + 1$, we have $\mathcal{T}_{\Delta+1,1} = \{S_{\Delta+1}\}$; for $k = 1$ and $n = \Delta + 2$ we have $\mathcal{T}_{\Delta+2,1} = \{DS_{\Delta,2}\}$; and for $k = 2$ and $n = 2\Delta$ we have $\mathcal{T}_{2\Delta,2} = \{DS_{\Delta-1,\Delta-1}\}$. We now prove the following result:

Theorem 6. *Let $T \in \mathcal{T}_{n,\Delta,k}$ be a tree, where $k \in \{1, 2\}$.*

(i) If $k = 1$ and $n \geq \Delta + 3$, then

$$M_2(T) \geq 4n - 6 + \Delta(\Delta - 3).$$

The equality holds if and only if $T \cong B_{n,\Delta}$.

(ii) If $k = 2$ and $n \geq 2\Delta + 1$, then

$$M_2(T) \geq 4n + 2\Delta(\Delta - 3) - 4.$$

The equality holds if and only if $T \cong (r, \Delta, \Delta)$-dumbbell.

Proof. Let $T' \in \mathcal{T}_{n,\Delta,k}$ be a tree with the minimal second Zagreb index.

(i) To obtain the desired result, we prove two claims.

Claim 3. *If $\Delta \geq 4$, then $n_i(T') = 0$ for each $i \in [3, \Delta - 1]$.*

Proof of Claim 3. On the contrary, assume that T' contains a vertex w such that $3 \leq d_w = t \leq \Delta - 1$, where $N_w = \{w_1, w_2, \ldots, w_t\}$. Since $k = 1$, there exists a unique vertex u such that $d_u = \Delta$. Let w_t lie on the u, w-path, that is, $d_{w_t} \geq 2$. Also, assume that w maximizes $d(u, w)$ among all vertices of degree between 3 and $\Delta - 1$. This implies that there are $t - 1$ pendant paths, each with one end vertex w. Therefore $d_{w_i} \in \{1, 2\}$, for $i = 1, 2, \ldots, t - 1$. Let v be the pendant vertex connected to w via the path that includes w_1. We construct a new tree T_1 from T as follows:

$$T_1 = T' - ww_2 + vw_2.$$

Then $d_v(T_1) = 2$, $d_w(T_1) = t - 1$ and $d_x(T_1) = d_x(T')$ for all $x \in V(T') \backslash \{w, v\}$. We now consider two cases:

Case 1. When $w_1 = v$, we obtain

$$\begin{aligned} M_2(T_1) - M_2(T') &= d_{w_2}(2 - t) + (t - 2) + (d_{w_t}(t - 1) - d_{w_t} \times t) \\ &\quad + \sum_{w_j \in N_w \backslash \{w_2, w_t\}} \Big(d_{w_j}(t - 1) - d_{w_j} \times t\Big), \\ &< (t - 2)(1 - d_{w_2}) - d_{w_t}. \end{aligned}$$

Since $d_{w_2} \geq 1$ and $d_{w_t} \geq 2$, we have $M_2(T_1) - M_2(T') < 0$. This is a contradiction to the choice of T'.

Case 2. When $w_1 \neq v$, we obtain

$$\begin{aligned} M_2(T_1) - M_2(T') &= (d_{w_t}(t - 1) - d_{w_t} \times t) + 2 + d_{w_2}(2 - t) \\ &\quad + \sum_{w_j \in N_w \backslash \{w_2, w_t\}} \Big(d_{w_j}(t - 1) - d_{w_j} \times t\Big), \\ &< d_{w_2}(2 - t) - d_{w_t} + 2. \end{aligned}$$

Since $d_{w_t} \geq 2$, $d_{w_2} \leq 2$ and $t \geq 3$, it follows that $M_2(T_1) < M_2(T')0$. This is a contradiction to the choice of T'. This proves the **Claim 3**.

Claim 4. *The tree T' has exactly one pendant path of length at least 2.*

Proof of Claim 4. On the contrary, assume that T' contains two pendant paths P_1 and P_2 of lengths $l_1, l_2 \geq 2$, respectively. We construct a tree T_2 from T' by detaching the subpath of length $l_2 - 1$ from P_2 and attaching it to the pendant vertex of P_1. Then

$$M_2(T_2) - M_2(T') = \Delta - 2\Delta + 4 - 2 = 2 - \Delta < 0,$$

as $\Delta \geq 3$. This is a contradiction to the choice of T'. Therefore, T' has exactly one pendant path of length at least 2. This completes the proof of **Claim 4**.

From **Claim 3**, the vertex degree sequence of T' is $(\Delta, \underbrace{2, \ldots, 2}_{n-\Delta-1}, \underbrace{1, \ldots, 1}_{\Delta})$, and **Claim 4** implies that $m_{1,2} = 1$ and $m_{2,\Delta} = 1$. From (2), we obtain $m_{2,2} = n - \Delta - 2$ and $m_{1,\Delta} = \Delta - 1$. Hence $T' \cong B_{n,\Delta}$. Thus

$$M_2(T') = \Delta(\Delta - 1) + 2\Delta + 2 + 4(n - \Delta - 2).$$

(ii) To obtain the required result, we prove two claims.

Claim 5. *If $\Delta \geq 4$, then $n_i(T') = 0$ for each $i \in [3, \Delta - 1]$.*

Proof of Claim 5. Assume to the contrary, there exists $u \in V(T')$ such that $d_u \in [3, \Delta - 1]$. Since $k = 2$ and $d_u(T') > k$, it follows that T' contains at least a pendant vertex z such that $z_1 \in N_z$ with $d_{z_1} \neq \Delta$. This contradicts Lemma 7. Therefore $n_i(T') = 0$ for each $i \in [3, \Delta - 1]$. This completes the proof of **Claim 5**.

Claim 6. $n_1(T') = m_{1,\Delta}$.

Proof of Claim 6. The proof directly follows from Lemma 7.

From **Claim 5** and (1), the degree sequence of T' is $(\underbrace{\Delta,\Delta}_{2},\underbrace{2,\ldots,2}_{n-2\Delta},\underbrace{1,\ldots,1}_{2(\Delta-1)})$. By **Claim 6**, we obtain $m_{1,\Delta}=n_1=2(\Delta-1)$. This implies $m_{1,2}=0$. Since $n>2\Delta$, it follows that $n_2>0$ and $m_{\Delta,\Delta}=0$ (as $m_{1,2}=0$). By using $m_{1,\Delta}=2(\Delta-1)$, $m_{1,2}=0$ and $m_{\Delta,\Delta}=0$ in (2), we obtain $m_{2,2}=n-2\Delta-1$ and $m_{2,\Delta}=2$. Hence $T'\cong(r,\Delta,\Delta)$-dumbbell. Therefore

$$M_2(T')=4(n-2\Delta-1)+2\Delta(\Delta-1)+4\Delta.$$

This completes the proof. ■

Applying Lemmas 3 and 7, we draw some graphs that provide information on the minimal second Zagreb index in $\mathcal{T}_{n,\Delta,k}$, as illustrated in Figure 2. From Figure 2, we observe that for $4\le\Delta\le5$, trees with the minimal second Zagreb index do not contain any vertex of degree 3, whereas this is not the case for $\Delta\ge6$ (for example, see the trees in Figure 2 when $\Delta=6$ and $n=22$, and when $\Delta=7$ and $n=25$).

In the next lemma, we find the degree sequence of the minimal trees in $\mathcal{T}_{n,\Delta,k}$ when $\Delta\ge4$ and $k\ge3$. Specifically, when $\Delta\in\{4,5\}$, the degree sequence of minimal trees differs from that of minimal trees with $\Delta\ge6$. Moreover, for graphs with $\Delta\ge6$, the degree sequence changes after every group of four consecutive values of Δ. In particular, for $\max\{4i+2,4\}\le\Delta\le4i+5$, where $i\ge0$, the degree sequence of minimal trees remains the same for these four consecutive values but changes after each such group. Therefore, the structure of minimal trees with respect to second Zagreb index varies after every set of four consecutive values of Δ, when $\Delta\ge6$ and $k\ge3$. We define a subset $\mathcal{T}'_{n,\Delta,k}\subseteq\mathcal{T}_{n,\Delta,k}$ of trees as follows:

$$\mathcal{T}'_{n,\Delta,k}=\{T\in\mathcal{T}_{n,\Delta,k}\mid n\ge(\Delta-1)k+2,\ \Delta\ge4\text{ and }k\ge3\}.$$

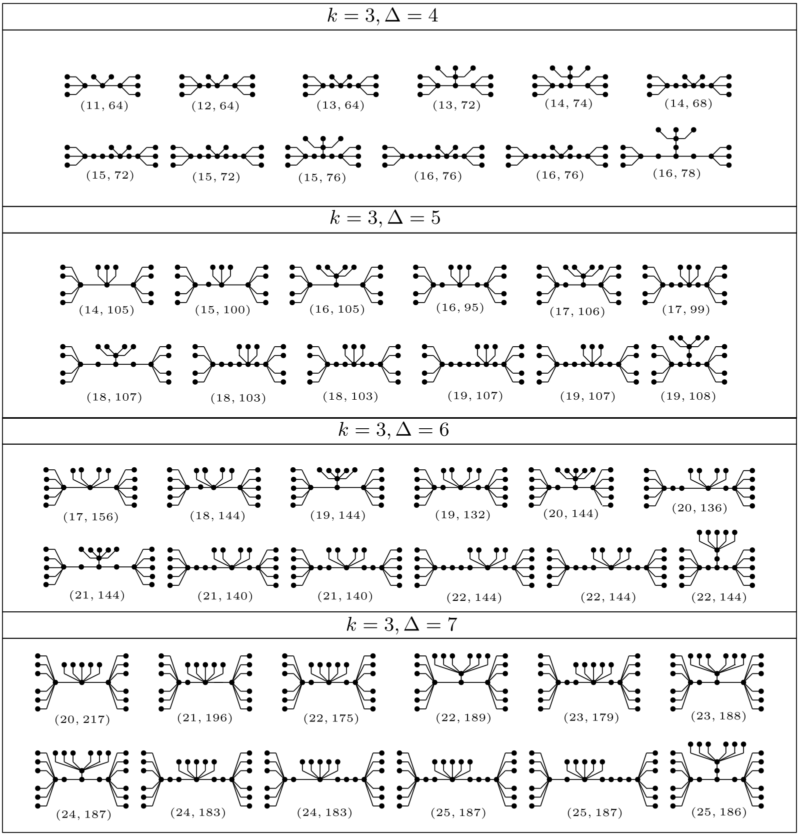

Figure 2. Based on Lemmas 3 and 7, all possible non-isomorphic trees in $\mathcal{T}_{n,\Delta,k}$ for $k(\Delta-1)+2 \leq n \leq k(\Delta-1)+7$, $k = 3$ and $4 \leq \Delta \leq 7$ are shown. In the labels (x, y) beneath the graphs, x represents the order of the graph, while y denotes the second Zagreb index.

Lemma 8. *Let $T \in \mathcal{T}'_{n,\Delta,k}$ be a tree with the minimal second Zagreb index and* $\max\{4i+2, 4\} \leq \Delta \leq 4i+5$*, where $i \geq 0$. Then $n_q(T) = 0$ for each $q \in [i+3, \Delta-1]$.*

Proof. On the contrary, assume that there exists $u \in V(T)$ such that $3 + i \leq d_u \leq \Delta - 1$. Let $N_u = \{u_1, u_2 \cdots, u_t\}$, where $t = d_u$. By Lemma 7, we have $d_{u_j} \geq 2$ for each $j \in \{1, 2, \ldots, t\}$. Then there are t paths, each having one endpoint u and the other endpoint as a pendant vertex. Thus, by Lemma 7, there are atleast t vertices with degree Δ, that is, $k \geq t$.

Let v be a pendant vertex such that there is a u,v-path and without loss of generality assume that u_1 does not lie on this u,v-path. We construct a new tree T_1 from T as follows:

$$T_1 = T - uu_1 + vu_1.$$

Then $T_1 \in \mathcal{T}_{n,\Delta,k}$. Also, $d_v(T_1) = 2$, $d_u(T_1) = t - 1$ and $d_w(T_1) = d_w(T)$ for all $w \in V(T)\backslash\{v,u\}$. We obtain

$$M_2(T_1) - M_2(T) = \Delta - d_{u_1}(t-2) - \sum_{j=2}^{t} d_{u_j}.$$

Since $d_{u_j} \geq 2$ for each $j \in \{1, 2, \ldots, t\}$, $t \geq 3+i$ and $\Delta \leq 4i+5$, we obtain

$$M_2(T_1) - M_2(T) \leq \Delta - 2(t-1) - 2(t-2) = 4(1-t) + \Delta + 2 \leq -1 < 0.$$

This gives a contradiction to the fact that T has minimal second Zagreb index. Thus, $n_q(T) = 0$ for each $q \in [i+3, \Delta-1]$. ■

From Lemma 8, we observe that fully characterizing trees having the minimal second Zagreb index is challenging due to changes in the degree sequence after every group of four consecutive values of Δ. However, we explicitly characterize the trees with the minimal second Zagreb index for $3 \leq \Delta \leq 5$. We define a set $\mathcal{T}''_{n,\Delta,k}$ as follows:

$$\mathcal{T}''_{n,\Delta,k} = \{T \in \mathcal{T}_{n,\Delta,k} : n \geq (\Delta-1)k + 2,\ 3 \leq \Delta \leq 5 \text{ and } k \geq 3\}.$$

Next, we define a class $\mathcal{T}^2_{n,\Delta,k} \subseteq \mathcal{T}''_{n,\Delta,k}$ of trees that satisfy the following conditions:

(i) Every tree in $\mathcal{T}^2_{n,\Delta,k}$ has the degree sequence $\pi_4 = (\underbrace{\Delta,\ldots,\Delta}_{k}, \underbrace{2,\ldots,2}_{n-2-k(\Delta-1)}, \underbrace{1,\ldots,1}_{2+k(\Delta-2)})$.

(ii) If $n \leq \Delta k$, then $m_{1,\Delta} = k(\Delta-2)+2, m_{2,\Delta} = 2n - 2k(\Delta-1) - 4$ and $m_{\Delta,\Delta} = \Delta k - n + 1$.

(iii) If $n \geq \Delta k + 1$, then $m_{1,\Delta} = k(\Delta - 2) + 2, m_{2,\Delta} = 2k - 2$ and $m_{2,2} = n - \Delta k - 1$.

In the next theorem, we characterize minimal trees in $\mathcal{T}''_{n,\Delta,k}$ with respect to second Zagreb index and find lower bounds.

Theorem 7. *Let $T \in \mathcal{T}''_{n,\Delta,k}$ be a tree. Then*

$$M_2(T) \geq \begin{cases} k\Delta^3 - \Delta^2(3k + n - 1) + 2\Delta(2n + k - 3) & \text{if } n \leq \Delta k, \\ 4n - 4 + \Delta(\Delta k - 2k - 2) & \text{if } n \geq \Delta k + 1. \end{cases}$$

The equality holds if and only if $T \in \mathcal{T}^2_{n,\Delta,k}$.

Proof. Let $T' \in \mathcal{T}''_{n,\Delta,k}$ be a tree with the minimal second Zagreb index. From Lemmas 1 ($\Delta = 3$) and 8 ($\Delta \geq 4$), and (1), the tree T' has the degree sequence

$$\pi_4 = (\underbrace{\Delta, \ldots, \Delta}_{k}, \underbrace{2, \ldots, 2}_{n-2-k(\Delta-1)}, \underbrace{1, \ldots, 1}_{2+k(\Delta-2)}).$$

By Lemma 7, we have $m_{1,2} = 0$. Combining this with the above degree sequence π_4 and (2) implies

$$\left.\begin{aligned} &m_{1,\Delta} = n_1 = k(\Delta - 2) + 2, \\ &2m_{2,2} + m_{2,\Delta} = 2(n - 2 - k(\Delta - 1)), \\ &m_{2,\Delta} + 2m_{\Delta,\Delta} = 2(k - 1). \end{aligned}\right\} \tag{17}$$

Claim 7. *$m_{2,2}$ and $m_{\Delta,\Delta}$ cannot be simultaneously positive.*

Proof of Claim 7. To the contrary, assume $m_{2,2} > 0$ and $m_{\Delta,\Delta} > 0$. Let $uv, xy \in E(T')$ such that $d_x = d_y = \Delta$, $d_u = d_v = 2$ and $u_1 \in N_u(T')\backslash\{v\}$. Then by Lemma 3, we obtain a contradiction to the choice of T'. Thus, $m_{2,2}$ and $m_{\Delta,\Delta}$ cannot be simultaneously positive. This completes the proof of **Claim 7**.

We now consider the following two cases.

Case 1. When $n \leq \Delta k$. In this case, we claim that $m_{2,2} = 0$. Otherwise, $m_{2,2} > 0$. From π_4, we have $n_2 = n - k(\Delta - 1) - 2 \leq \Delta k - k(\Delta - 1) - 2 = k - 2$. This, along with $m_{1,2} = 0$, $m_{2,2} > 0$ and the fact that T' contains exactly $k - 1$ internal paths with end vertices of degree Δ, implies that $m_{\Delta,\Delta} > 0$. Now, by applying **Claim 7**, we have $m_{2,2} = 0$. Using this in (17), we obtain $m_{2,\Delta} = 2n - 4 - 2k(\Delta - 1)$ and $m_{\Delta,\Delta} = \Delta k - n + 1$. Thus $T' \in \mathcal{T}^2_{n,\Delta,k}$. Consequently

$$M_2(T') = \Delta(k(\Delta - 2) + 2) + \Delta^2(\Delta k - n + 1) + 2\Delta(2n - 4 - 2k(\Delta - 1)).$$

Case 2. When $n \geq \Delta k + 1$. In this case, we claim that $m_{\Delta,\Delta} = 0$. Contrarily, assume that $m_{\Delta,\Delta} > 0$. From π_4, we have $n_2 = n - k(\Delta - 1) - 2 \geq \Delta k + 1 - k(\Delta - 1) - 2 = k - 1$. This along with $m_{1,2} = 0$, $m_{\Delta,\Delta} > 0$ and the fact that T' contains exactly $k - 1$ internal paths with end vertices of degree Δ, implies that $m_{2,2} > 0$. By **Claim 7**, this is not possible. Thus, $m_{\Delta,\Delta} = 0$. This, with (17) implies that $m_{2,\Delta} = 2k - 2$ and $m_{2,2} = n - \Delta k - 1$. Thus, $T' \in \mathcal{T}^2_{n,\Delta,k}$. Hence

$$M_2(T') = \Delta(k(\Delta - 2) + 2) + 2\Delta(2k - 2) + 4(n - k\Delta - 1).$$

This completes the proof. ■

4 Concluding remarks

In this paper, we provide a complete characterization of the trees with maximal and minimal first Zagreb index in the class $\mathcal{T}_{n,\Delta,k}$, as well as the maximal second Zagreb index in the same class. Additionally, we characterize the trees with minimal second Zagreb index for $\Delta \geq 3$ and $k \in \{1, 2\}$, and for $3 \leq \Delta \leq 5$ with $k \geq 3$.

We defined the subset $\mathcal{T}'_{n,\Delta,k} \subseteq \mathcal{T}_{n,\Delta,k}$ for $\Delta \geq 4$ and $k \geq 3$ and provided a complete solution for the minimal second Zagreb index when $4 \leq \Delta \leq 5$ and $k \geq 3$. Additionally, we presented partial results and observations on trees in $\mathcal{T}'_{n,\Delta,k}$ with the minimal second Zagreb index for $\Delta \geq 6$ and $k \geq 3$. However, completely characterizing the minimal second

Zagreb index in $\mathcal{T}'_{n,\Delta,k}$ for $\Delta \geq 6$ and $k \geq 3$, remains an open problem. Based on Lemmas 3, 7, and 8, such trees satisfy the following constraints:

(*i*) The tree T does not contain internal path of length 1 and length greater than 2 simultaneously.

(*ii*) All the pendant vertices are adjacent to the vertices of degree Δ only.

(*iii*) The tree T with $\max\{4i+2, 4\} \leq \Delta \leq 4i+5$ holds $n_q = 0$ for $i+3 \leq q \leq \Delta - 1$, where $i \geq 0$.

Despite these structural constraints, the complete classification of such trees in $\mathcal{T}'_{n,\Delta,k}$ for $\Delta \geq 6$ and $k \geq 3$ remains unresolved. Thus, we pose the following problem:

Problem 2. *Characterize all n-vertex trees in* $\mathcal{T}'_{n,\Delta,k}$ $(\Delta \geq 6, k \geq 3)$ *with minimal second Zagreb index.*

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