On Bond Incident Degree Indices of Connected Graphs with Fixed Order and Number of Pendent Vertices

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Abstract

The graphs having the maximum value of certain bond incident degree indices (including the second Zagreb index, general sum-connectivity index, and general zeroth-order Randić index) in the class of all connected graphs with fixed order and number of pendent vertices are characterized in this paper. The problem of finding graphs having the minimum values of the second Zagreb index and general zeroth-order Randić index from the aforementioned class of connected graphs is also addressed. One of the obtained results

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1 Introduction and statements of the main results

Throughout this paper, we consider only simple connected graphs. The edge set and vertex set of a graph $G$ are denoted by $E(G)$ and $V(G)$, respectively. Let $d_G(u)$ denote the degree of a vertex $u$ of $G$. We write $d(u)$ instead of $d_G(u)$ whenever there is no confusion about the graph under consideration. Those (chemical) graph theoretical terminology and notation that are used in this paper, but not defined here, can be found in some relevant books, like [5,6,24,26].

A graph invariant is a function $\Phi$ defined on the set of all graphs such that the equation $\Phi(G) = \Phi(G')$ holds whenever the graphs $G$ and $G'$ are isomorphic. A graph invariant may be a numerical value (for example, size of a graph), a polynomial (for example, the matching polynomial of a graph), set of numbers (for example, the spectrum of a graph), etc. In chemical graph theory, a graph invariant assuming a single number for a graph is known as a topological index [26]. In the present paper, we are concerned with the topological indices defined in the following way [9,13] for a graph $G$:

$$BID_\varphi(G) = \sum_{uv \in E(G)} \varphi(d(u), d(v)), \tag{1}$$

where $\varphi$ is a real-valued symmetric function. Following Vukičević and Đurićević [25], we call the topological indices of the form (1) as bond incident degree (BID) indices. These indices are sometimes referred to as the connectivity functions [27] of $G$. If $f$ is a real-valued function
such that $\varphi(d(u), d(v)) = f(d(u))/d(u) + f(d(v))/d(v)$, then Equation (1) yields
\[
BID_\varphi(G) = \sum_{uv \in E(G)} \left[ \frac{f(d(u))}{d(u)} + \frac{f(d(v))}{d(v)} \right] = \sum_{v \in V(G)} f(d(v)). \tag{2}
\]

We remark here that the right equality of Equation (2) follows from a more general result reported in [7]. Following Yao et al. [29], we denote the rightmost expression of (2) by $H_f(G)$ and refer to such indices as the **vertex-degree-function indices** of $G$. It seems that these indices were first considered by Linial and Rozenman [18]. The vertex-degree-function indices $H_f$, being simple types of BID indices, have attracted considerable attention from researchers recently; for example, see the recent papers [1, 3, 14, 15, 22, 23, 29], recent review [16], and the related references listed therein.

The first and second Zagreb indices of a graph $G$, usually denoted by $M_1(G)$ and $M_2(G)$, respectively, are defined as
\[
M_1(G) = \sum_{u \in V(G)} [d(u)]^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).
\]

The first Zagreb index was appeared almost fifty years ago in [12] while the second Zagreb index was introduced in [11]. They were extended to **zeroth-order general Randić index** $R_0^\alpha(G)$ and **general Randić index** $R_\alpha(G)$ of $G$, respectively, where
\[
R_0^\alpha(G) = \sum_{u \in V(G)} [d(u)]^\alpha \quad \text{and} \quad R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha,
\]

where $\alpha$ is a real number. Denote by $\chi_\alpha(G)$ and $Pl_\alpha(G)$ the **general sum-connectivity index** and **general Platt index** of $G$, respectively, where
\[
\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha \quad \text{and} \quad Pl_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v) - 2)^\alpha.
\]

The concept of general Randić index was firstly proposed by Bollobás and
Erdős [4], the zeroth-order general Randić index was firstly put forward by Li and Zheng [17], the general sum-connectivity index was introduced by Zhou and Trinajstić [31], and the general Platt index of $G$ was firstly studied by Ali and Dimitrov [2]. Actually, the topological indices $R_\alpha(G)$, $R_0^\alpha(G)$, $\chi_\alpha(G)$, and $Pl_\alpha(G)$ are special cases of (2) and general cases of many famous topological indices. For instance, $M_1(G) = R_0^0(G)$ is the first Zagreb index, $M_2(G) = R_1(G)$ is the second Zagreb index, $R_{1/2}(G)$ is called the inverse degree $ID(G)$ of $G$ (see [28]), $R_{-1/2}(G)$ is mostly referred to as the Randić index of $G$ [21], $\chi_{-1/2}(G)$ is famous with the name sum-connectivity index of $G$ [30], and $Pl_2(G)$ is known as the reformulated first Zagreb index of $G$ [20].

As usual, the path, star, and complete graphs with $n$ vertices are denoted by $P_n$, $K_{1,n-1}$, and $K_n$, respectively. As in [8], let $D_{n;s,t}$ be the tree obtained from the path graph $P_{n-s-t}$ by attaching $s$ pendant vertices to one of its end vertices and $t$ pendant vertices to the other end vertex. Let $K^{(p)}_{n-p}$ be the graph obtained from the complete graph $K_{n-p}$ by attaching $p$ pendant vertices to one vertex of $K_{n-p}$. Denote by $C^{(p)}_n$ the class of all connected graphs with $n$ vertices and $p$ pendant vertices. Let

$$G_0 = \begin{cases} 
D_{n;n-3,1} & \text{if } p = n - 2, \\
K^{(p)}_{n-p} & \text{if } 0 \leq p \leq n - 3. 
\end{cases}$$

(3)

**Theorem 1.** In the class $C^{(p)}_n$ with $0 \leq p \leq n - 2$ and $n \geq 4$, the graph $G_0$ uniquely attains the maximum values of $\chi_\alpha$, $Pl_\alpha$ and $R_0^\alpha$ for $\alpha > 1$ and maximum value of $M_2$.

We note that each of the BID indices considered in Theorem 1 satisfies the inequality $BID_\varphi(G + uv) > BID_\varphi(G)$ for every pair of non-adjacent vertices $u$ and $v$ of a graph $G$. This observation implies that a graph attaining the minimum value of any of the aforementioned BID indices in the class $C^{(p)}_n$, with $2 \leq p \leq n - 2$ and $n \geq 4$, must be a tree. Denote by $T^{(p)}_n$ the class of trees with $n$ vertices and $p$ pendant vertices, where $2 \leq p \leq n - 2$.

**Theorem 2.** Let $F_0$ be a tree having the minimum value of $R_0^\alpha$ in the
class $\mathbb{T}_n^{(p)}$. If $\alpha > 1$ and $s_0 = \left\lceil \frac{p-2}{n-p} \right\rceil + 2$, then $F_0$ has the degree sequence

$$\pi_0 = (s_0, \ldots, s_0, s_0 - 1, \ldots, s_0 - 1, 1, \ldots, 1),$$

(4)

where $t_0 = p(s_0 - 2) - n(s_0 - 3) - 2$.

The following result has been proved by Gutman and Kamran Jamil (see Theorem 4.1 of [10]) and Enteshari and Taeri [8] gave another proof using different method. Actually, it follows immediately from Theorem 2.

**Corollary.** [8, 10] If $T^*$ is a tree with the minimum first Zagreb index in the class $\mathbb{T}_n^{(p)}$, then $T^*$ has the degree sequence $\pi_0$, where $\pi_0$ is as defined in (4)

In [8], it has been shown that $D_{n;\lceil \frac{p}{2} \rceil, \lfloor \frac{p}{2} \rfloor}$ uniquely attains the minimum second Zagreb index among all trees of $\mathbb{T}_n^{(p)}$ for $p \in \{2, 3, 4, n - 3, n - 2\}$. Here, we extend this result to the case when $n \geq 3p - 5$ and $p \geq 4$ (by finding a lower bound on $M_2$ for nontrivial trees in terms of $n$ and $p$ for any $n$ and $p$). By a branching vertex of a graph, we mean a vertex with degree at least three. Let $\mathcal{T}_0(n, p)$ be the class of all trees with $n$ vertices, maximum degree 3 and $p$ pendent vertices such that every pendent vertex is adjacent to a branching vertex and no two branching vertices are adjacent.

**Theorem 3.** If $T$ is a tree with $n$ vertices and $p$ pendent vertices, then

$$M_2(T) \geq 4n + 3p - 16,$$

with equality if and only if $T \in \mathcal{T}_0(n, p) \cup \{K_{1,3}, K_{1,4}\}$.

For $n \geq 3p - 5$ and $p \geq 4$, we can construct a tree $T$ belonging to $\mathcal{T}_0(n, p)$ explained as follows: If $p = 4$ then $n \geq 7$ and hence $D_{n;2,2} \in \mathcal{T}_0(n, 4)$. If $p \geq 5$ then we obtain $T \in \mathcal{T}_0(n, p)$ by adding one edge between a pendent vertex pertaining to a tree of $\mathcal{T}_0(n - 3, p - 1)$ and the center of the star $K_{1,2}$. This observation leads to the next corollary of Theorem 3.

**Corollary.** If $4 \leq p \leq \frac{n+5}{3}$, then the member(s) of $\mathcal{T}_0(n, p)$ is/are the only tree(s) with the minimum second Zagreb index in the class of trees with $n$ vertices and $p$ pendent vertices.
2 Proofs of Theorems 1 and 2

We start this section with some definitions that are needed in the remaining part of this paper. A \( k \)-vertex of \( G \) is a vertex with degree \( k \). A vertex adjacent to at least one pendent vertex is called a quasi-pendent vertex. Let \( N_G(u) \) denote the set of neighbors of a vertex \( u \) of a graph \( G \). Hereafter, let \( G \) be a connected graph, and let \( u \) and \( v \) be two vertices of \( G \) such that \( \{w_1, w_2, \ldots, w_s\} \subseteq N_G(v) \setminus (N_G(u) \cup \{u\}) \), where \( 1 \leq s \leq d(v) \). Denote by

\[
G^* = G - vw_1 - vw_2 - \cdots - vw_s + uw_1 + uw_2 + \cdots + uw_s.
\]

**Lemma 1.** [19] If \( f(x) \) is a strictly convex and strictly increasing function, then \( H_f(G^*) > H_f(G) \) when \( d_G(u) \geq d_G(v) \) and \( H_f(G) > H_f(F) \) when \( F \) is a proper subgraph of \( G \).

**Proposition 4.** Let \( G \) be a graph with the maximum \( H_f(G) \) in \( C^{(p)}_n \), where \( 0 \leq p \leq n - 2 \) and \( n \geq 4 \). If \( f(x) \) is a strictly convex and strictly increasing function, then \( G = G_0 \), where \( G_0 \) is as defined in (3).

**Proof.** By Lemma 1, \( H_f(G) > H_f(F) \) holds for any proper subgraph \( F \) of \( G \), which implies that \( G \) is obtained from \( K_{n-p} \) by adding \( p \) pendent vertices to some vertices of \( K_{n-p} \).

The cases \( p = 0, 1 \), are trivial. When \( 2 \leq p \leq n - 2 \), we only prove the case of \( p = n - 2 \), as the remaining cases can be proved similarly. Since \( p = n - 2 \), \( G = D_{n;s,n-2-s} \), where \( n - s - 2 \geq s \geq 1 \). If \( s \geq 2 \), then \( G^* = G - vw_1 + uw_1 \) is also a tree with \( n - 2 \) pendent vertices, where \( d_G(v) = s + 1 \), \( d_G(u) = n - s - 1 \), and \( w_1 \) is a pendent neighbor of \( v \). By Lemma 1, we have \( H_f(G^*) > H_f(G) \), a contradiction. \( \blacksquare \)

A symmetric bivariate non-negative function \( f(x, y) \) defined on positive real numbers is called a **special function** if the inequalities \( \frac{\partial \varphi(x, y)}{\partial x} > 0 \), \( \varphi(x+1, z) + \varphi(y-1, z) \geq \varphi(x, z) + \varphi(y, z) \) and \( \varphi(x+1, y-1) + \varphi(x+1, 1) \geq \varphi(x, y) + \varphi(y, 1) \) hold for any \( x \geq y > 1 \) and \( z \geq 1 \). Note that if \( \varphi(x, y) \) is a special function and if \( G \) is a connected graph with \( uv \notin E(G) \), then \( BID_\varphi(G + uv) > BID_\varphi(G) \).
Proposition 5. Let $G$ be a graph with the maximum $BID_{\varphi}(G)$ in $C_n^{(p)}$, where $0 \leq p \leq n-2$ and $n \geq 4$. If $\varphi(x,y)$ is a special function, then $G = G_0$, where $G_0$ is defined in (3).

Proof. Since $\varphi(x,y)$ is a special function, $G$ is obtained from $K_{n-p}$ by adding $p$ pendent vertices to some vertices of $K_{n-p}$. If $0 \leq p \leq 1$ then the result trivially holds. In what follows, we assume that $2 \leq p \leq n-2$.

Case 1. $p = n-2$.
Since $p = n-2$, $G = D_{n:s,n-2-s}$, where $n-s-2 \geq s \geq 1$. Contrarily, assume that $s \geq 2$. Note that $G^* = G - vw_1 + uw_1$ is also a tree with $n-2$ pendent vertices, where $d_G(v) = s + 1$, $d_G(u) = n - s - 1$, and $w_1$ is a pendent neighbor of $v \in V(G)$. Since $n \geq 2s + 2$ and $\frac{\partial \varphi(x,y)}{\partial x} > 0$, we have

\[
BID_{\varphi}(G^*) - BID_{\varphi}(G)
= \varphi(n-s,s) + (s-1)\varphi(s,1) + (n-s-1)\varphi(n-s,1)
- \varphi(n-1-s,s+1) - s\varphi(s+1,1) - (n-s-2)\varphi(n-s-1,1)
= s(\varphi(s,1) + \varphi(n-s,1) - \varphi(n-1-s,1) - \varphi(s+1,1))
+ (n-2s-2)(\varphi(n-s,1) - \varphi(n-1-s,1))
+ \varphi(n-s,s) + \varphi(n-s,1) - \varphi(n-s-1,s+1) - \varphi(s,1)
\geq \varphi(n-s,s) + \varphi(n-s,1) - \varphi(n-1-s,s+1) - \varphi(s,1)
\geq \varphi(s+1,1) - \varphi(s,1) > 0,
\]

contrary with the choice of $G$.

Case 2. $2 \leq p \leq n-3$.
Recall that $G$ is obtained from $K_{n-p}$ by adding $p$ pendent vertices to some vertices of $K_{n-p}$. It suffices to show that all of these $p$ pendent vertices are adjacent to the same vertex of $K_{n-p}$. Suppose to the contrary that $u$ and $v$ are two quasi-pendent vertices of $K_{n-p}$ adjacent to $t$ and $s$ pendent vertices, respectively, where $t \geq s \geq 1$. This implies that $d_G(u) = n - p - 1 + t \geq n-p-1+s = d_G(v) \geq 3$. Let $u_1, u_2, \ldots, u_{n-p-2}$ be the non-pendent vertices of $G$ different from $u$ and $v$. Let $G^* = G - vw_1 + uw_1$, where $w_1$ is
a pendent vertex adjacent to \( v \). From the definition of \( BID_\varphi(G) \), we have

\[
BID_\varphi(G^*) - BID_\varphi(G) = \varphi(d_G(u) + 1, d_G(v) - 1) + (s - 1)\varphi(d_G(v) - 1, 1) \\
+ (t + 1)\varphi(d_G(u) + 1, 1) - \varphi(d_G(u), d_G(v)) - s\varphi(d_G(v), 1) \\
- t\varphi(d_G(u), 1) + \sum_{i=1}^{n-p-2} \left[ \varphi(d_G(u) + 1, d_G(u_i)) + \varphi(d_G(v) - 1, d_G(u_i)) \\
- \varphi(d_G(u), d_G(u_i)) - \varphi(d_G(v), d_G(u_i)) \right] \\
\geq (s - 1)\left[ \varphi(d_G(v) - 1, 1) + \varphi(d_G(u) + 1, 1) - \varphi(d_G(u), 1) - \varphi(d_G(v), 1) \right] \\
+ (t + 1 - s)\varphi(d_G(u) + 1, 1) - \varphi(d_G(u), d_G(v)) - \varphi(d_G(v), 1) \\
\geq (t + 1 - s)\left[ \varphi(d_G(u) + 1, 1) - \varphi(d_G(u), 1) \right] > 0,
\]
a contradiction. \( \Box \)

**Proof of Theorem 1.** Let \( f(x) = x^\alpha, \varphi_0(x, y) = (x + y - 2)^\alpha, \varphi_1(x, y) = (x + y)^\alpha, \) and \( \varphi_2(x, y) = xy, \) where \( \alpha > 1. \) The function \( f \) is strictly convex as well as strictly increasing because \( f''(x) = \alpha(\alpha - 1)x^{\alpha - 2} > 0 \) and \( f'(x) = \alpha x^{\alpha - 1} > 0. \) By Proposition 4, \( G_0 \) uniquely attains the maximum value of \( R_0^{(\alpha)} \) among all the members of \( \mathbb{C}_n^{(p)} \) for \( \alpha > 1. \)

In what follows, we prove that each of the functions \( \varphi_0, \varphi_1, \varphi_2, \) is a special function and hence by using Proposition 5 we arrive at the desired conclusion.

Since \( \alpha > 1, \) we conclude that \( \varphi_1(x + 1, z) + \varphi_1(y - 1, z) = (x + 1 + z)^\alpha + (y + z - 1)^\alpha \geq (x + z)^\alpha + (y + z)^\alpha = \varphi_1(x, z) + \varphi_1(y, z), \) \( \frac{\partial \varphi_1(x, y)}{\partial x} = \alpha(x + y)^{\alpha - 1} > 0, \varphi_1(x + 1, y - 1) + \varphi_1(x + 1, 1) = (x + y)^\alpha + (x + 2)^\alpha > (x + y)^\alpha + (y + 1)^\alpha = \varphi_1(x, y) + \varphi_1(y, 1) \) hold for \( x \geq y > 1 \) and \( z \geq 1. \) Thus, \( \varphi_1 \) is a special function. In a similar way, we can verify that \( \varphi_0 \) is also a special function.

Finally, we note that \( \varphi_2(x + 1, z) + \varphi_2(y - 1, z) = z(x + y) = \varphi_2(x, z) + \varphi_2(y, z), \frac{\partial \varphi_2(x, y)}{\partial x} = y > 0, \) and \( \varphi_2(x + 1, y - 1) + \varphi_2(x + 1, 1) = \varphi_2(x, y) + \varphi_2(y, 1) \) hold for \( x \geq y > 1 \) and \( z \geq 1. \) Thus, \( \varphi_2 \) is also a special function. \( \Box \)
Let $D = (d_1, d_2, \ldots, d_n)$ and $D^* = (d_1^*, d_2^*, \ldots, d_n^*)$ be two different degree sequences of two graphs where $d_i \geq d_j$ and $d_i^* \geq d_j^*$ whenever $i \leq j$. We write $D \prec D^*$ if and only if $\sum_{i=1}^n d_i = \sum_{i=1}^n d_i^*$, and $\sum_{i=1}^j d_i \leq \sum_{i=1}^j d_i^*$ for all $j = 1, 2, \ldots, n$, provided that the inequality $\sum_{i=1}^j d_i < \sum_{i=1}^j d_i^*$ holds for at least one $j \in \{1, 2, \ldots, n\}$. In [19], the next lemma has been proven.

**Lemma 2.** [19] Let $G$ and $G^*$ be two graphs with the degree sequences $D$ and $D^*$, respectively. If $D \prec D^*$ and $f(x)$ is a strictly convex function on $x \geq 1$, then $H_f(G) < H_f(G^*)$.

As shown in Theorem 4.2 of [29], if $f(x)$ is a strictly convex function defined on $x \geq 1$, then the trees with the degree sequence

$$(p, 2, \ldots, 2, 1, \ldots, 1)_{n-p-1 \atop p}$$

has the maximum value of $H_f$ among all trees of $T_n^{(p)}$; the following theorem can be considered as the minimal version of this result.

**Theorem 6.** Let $T^*$ be a tree having the minimum value of $H_f$ in $T_n^{(p)}$. If $s_0 = \left\lceil \frac{p-2}{n-p} \right\rceil + 2$ and $f(x)$ is a strictly convex function on $x \geq 1$, then $T^*$ is a tree with the degree sequence $\pi_0$, where $\pi_0$ is defined in (4).

**Proof.** Because of Lemma 2, it suffices to show that $\pi_0$ is minimum with respect to the relation ‘$\prec$’. Let $D^* = (d_1^*, d_2^*, \ldots, d_n^*)$ be the degree sequence of a tree belonging to the class $T_n^{(p)}$ such that $D^* \neq \pi_0$. Denote by $t_0 = p(s_0 - 2) - n(s_0 - 3) - 2$ and $\pi_0 = (d_1, d_2, \ldots, d_n)$, that is, $d_1 = d_2 = \cdots = d_{t_0} = s_0$ and $d_{t_0+1} = d_{t_0+2} = \cdots = d_{n-p} = s_0 - 1$. To complete the proof, it suffices to show that

$$\sum_{i=1}^j d_i \leq \sum_{i=1}^j d_i^*$$

for all $1 \leq j \leq n-p$. 
If \( d_1^* \leq s_0 - 1 \), then

\[
2(n-1) = d_1^* + d_2^* + \cdots + d_n^*
\]

\[
\leq (n-p)(s_0 - 1) + p = (n-p) \left( \left\lfloor \frac{p-2}{n-p} \right\rfloor + 1 \right) + p
\]

\[
< (n-p) \left( \frac{p-2}{n-p} + 2 \right) + p = 2(n-1),
\]

a contradiction. Thus, \( d_1^* \geq s_0 \). If \( d_{n-p}^* \geq s_0 \), then (5) holds and we are done. In what follows, we suppose that there exists \( k \) with \( 1 \leq k \leq n-p-1 \) such that \( d_1^* \geq \cdots \geq d_k^* \geq s_0 \) and \( d_{k+1}^* \leq s_0 - 1 \).

Since (5) already holds for \( 1 \leq j \leq k \), we take \( j \) satisfying \( k+1 \leq j \leq n-p \). Since \( d_{n-p}^* \leq d_{n-p-1}^* \leq \cdots \leq d_{j+1}^* \leq d_j^* \leq \cdots \leq d_{k+1}^* \leq s_0 - 1 = d_{n-p} = d_{n-p-1} = \cdots = d_{t_0+1} < s_0 = d_{t_0} = d_{t_0-1} = \cdots = d_1 \) and \( k+1 \leq j \leq n-p \), we have

\[
d_1^* + d_2^* + \cdots + d_j^* = 2(n-1) - p - d_{n-p}^* - \cdots - d_{j+1}^*
\]

\[
\geq 2(n-1) - p - (n-p - j)(s_0 - 1)
\]

\[
\geq 2(n-1) - d_{j+1} - d_{j+2} - \cdots - d_n
\]

\[
= d_1 + d_2 + \cdots + d_j,
\]

which implies that (5) holds. This completes the proof. \( \blacksquare \)

One can easily checked that Theorem 2 follows from Theorem 6, as \( f(x) = x^\alpha \) is a strictly convex function defined on \( x \geq 1 \) for \( \alpha > 1 \).

### 3 Proof of Theorem 3

This section is dedicated to the proof of Theorem 3. Recall that a **branching vertex** of \( G \) is a vertex with degree at least three. Let \( q(G) \) be the **branching number**, that is, the number of branching vertices of \( G \).

**Lemma 3.** [8] *Let \( T \) be a tree of \( T_n^{(p)} \), where \( 2 \leq p \leq n-2 \). If \( 1 \leq q(T) \leq 2 \) and \( T \not= D_{n;\lfloor \frac{p}{2} \rfloor,\lfloor \frac{p}{2} \rfloor} \), then \( M_2(T) > M_2(D_{n;\lfloor \frac{p}{2} \rfloor,\lfloor \frac{p}{2} \rfloor}) \).*

A **special vertex** is a quasi-pendent vertex having at most one non-pendent neighbor. For any two vertices \( x \) and \( y \) of a tree \( T \), let \( P_{xy} \) be the
Lemma 4. Let $x, y$ be two non-pendent vertices of a tree $T$ such that $x$ is a quasi-pendent vertex of $T$. If $y$ is not a special vertex and $d_T(y) > d_T(x)$, then there exists another tree $T'$ such that $M_2(T') < M_2(T)$, where $T$ and $T'$ have the same degree sequence.

Proof. Suppose that $w_1$ is a pendent vertex adjacent to $x$. Since $y$ is not a special vertex, $y$ is adjacent to some non-pendent vertex $y_1$ such that $y_1 \notin P_{xy}$. Let $T' = T + xy_1 + yw_1 - xw_1 - yy_1$. Since $d_T(y_1) > 1 = d_T(w_1)$ and $d_T(x) < d_T(y)$, we have $M_2(T') - M_2(T) = (d_T(y) - d_T(x))(d_T(w_1) - d_T(y_1)) < 0$. Now, it is easily checked that $T'$ is a tree containing the same degree sequence as $T$. \[\blacksquare\]

Recall that $T_0(n, p)$ is the class of trees with $n$ vertices, maximum degree 3 and $p$ pendent vertices such that every pendent vertex is adjacent to a branching vertex and no two branching vertices are adjacent. If $T \in T_0(n, p)$, then let $n_i$ be the number of vertices of degree $i$ of $T$ and let $m_{i,j}(T)$ be the number of those edges of $T$ whose one end-vertex is an $i$-vertex and the other one is a $j$-vertex. By a fact reported in [8], it holds that

$$\sum_{i=3}^{p} (i-2)n_i = p - 2,$$

which gives $n_3 = p - 2$. Since $m_{1,3}(T) = p$, we have $m_{2,3}(T) = 3n_3 - m_{1,3}(T) = 2(p - 3)$. Combining this with $|E(T)| = n - 1$, we can conclude that

$$m_{1,3}(T) = p, \quad m_{2,2}(T) = n - 3p + 5, \quad \text{and} \quad m_{2,3}(T) = 2(p - 3),$$

which implies that

$$M_2(T) = 4n + 3p - 16.$$

Proof of Theorem 3. For $n = 1, 2, 3$, the result trivially holds, as $T$ must be a star. If $p = n - 1 \geq 3$, then $T = K_{1, n-1}$ and thus $M_2(T) = (n-1)^2 \geq 4n + 3(n-1) - 16 = 4n + 3p - 16$, with equality if and only if $T \in \{K_{1,3}, K_{1,4}\}$. Next, we prove the theorem by induction on $p$, where $2 \leq p \leq n - 2$. The result is trivial for $p = 2$, because $n \geq 4$ and
\[ M_2(P_n) = 4n - 8 > 4n - 10. \] Also, if \( p = 3 \) and \( n \geq 5 \), then from Lemma 3 it follows that \( M_2(T) \geq M_2(D_n; [\frac{p}{2}], [\frac{p}{2}]) = 4n - 6 > 4n - 7. \) Hence, the induction starts. Assume that \( p \geq 4 \). Then, \( n \geq p + 2 \geq 6 \). Take \( T \) as a tree belonging to \( T^{(p)}_n \) such that \( M_2(T) \) is as small as possible. To complete the proof, it suffices to show that \( M_2(T) \geq 4n + 3p - 16 \) with equality if and only if \( T \in T_0(n, p) \).

We first suppose that at least one quasi-pendent vertex, say \( x_0 \), of \( T \) is a 2-vertex. Since \( p \geq 4 \), \( T \) contains at least one branching vertex. By Lemma 4, we can conclude that each branching vertex of \( T \) must be a special vertex. Now, let \( y_0 \) be a branching vertex of \( T \) such that the distance between \( x_0 \) and \( y_0 \) is as small as possible. Since each branching vertex of \( T \) must be a special vertex, \( y_0 \) is a special vertex and it is the unique branching vertex of \( T \). Now, we can conclude that \( T = D_{n:p-1,1} \). Combining this with \( p \geq 4 \), it follows that \( M_2(T) = p(p - 1) + 2p + 2 + 4(n - 2 - p) = p(p - 3) + 4n - 6 > 4n + 3p - 16 \), as required.

Next, we suppose that each quasi-pendent vertex of \( T \) is a branching vertex.

**Case 1.** \( T \) contains at least one quasi-pendent vertex with degree greater than 3.

Let \( u_0 \in V(T) \) be a pendent vertex adjacent to an \( s \)-vertex \( u \), where \( s \geq 4 \). Take \( N_T(u) = \{u_0, u_1, \ldots, u_{r-1}, u_r, u_{r+1}, \ldots, u_{s-1}\} \) where \( d_T(u_i) = 1 \) for all \( i \in \{0, 1, \ldots, r - 1\} \) and \( d_T(u_j) \geq 2 \) for all \( j \in \{r, r + 1, \ldots, s - 1\} \), with \( r \geq 1 \). Certainly, \( T - u_0 \) is a tree with \( n - 1 \) vertices and \( p - 1 \) pendent vertices. By using the inductive hypothesis, we have \( M_2(T - u_0) \geq 4(n - 1) + 3(p - 1) - 16 \). Combining this with \( s > r \) and \( s \geq 4 \), we have

\[
M_2(T) = M_2(T - u_0) + s + r - 1 + \sum_{j=r}^{s-1} d_T(u_j)
\geq 4(n - 1) + 3(p - 1) - 16 + s + r - 1 + 2(s - r)
= (4n + 3p - 16) + (s - r) + (2s - 8)
> 4n + 3p - 16,
\]

as desired.
Case 2. Every quasi-pendent vertex of $T$ is a 3-vertex and $T$ contains at least one quasi-pendent vertex having only one pendent neighbor.

Let $u \in V(T)$ such that $N_T(u) = \{u_0, u_1, u_2\}$ where $d_T(u_0) = 1$ and $2 \leq d_T(u_1) \leq d_T(u_2)$. Certainly, $T - u_0$ is also a tree with $n - 1$ vertices and $p - 1$ pendent vertices. By using the inductive hypothesis, we have

$$M_2(T) = M_2(T - u_0) + d_T(u_1) + d_T(u_2) + 3 \geq (4n + 3p - 16) + d_T(u_1) + d_T(u_2) - 4 \geq 4n + 3p - 16,$$

where the equation $M_2(T - u_0) = 4(n - 1) + 3(p - 1) - 16$ holds if and only if $T - u_0 \in \mathcal{T}_0(n - 1, p - 1)$ and $d_T(u_1) = d_T(u_2) = 2$; that is, if and only if $T \in \mathcal{T}_0(n, p)$.

Case 3. Every quasi-pendent vertex of $T$ is a 3-vertex and $T$ contains at least one quasi-pendent vertex having two pendent neighbors and a neighbor of degree greater than 2.

Let $u \in V(T)$ such that $N_T(u) = \{u_0, u_1, u_2\}$ where $d_T(u_0) = d_T(u_1) = 1$ and $d_T(u_2) \geq 3$. Let $T_1$ be the tree formed from $T$ by deleting the vertices $u_0$ and $u_1$. Then, $T_1$ is a tree with $n - 2$ vertices and $p - 1$ pendent vertices. Since $n - 2 \geq 4$, by using the inductive hypothesis, we have

$$M_2(T) = M_2(T_1) + 2d_T(u_2) + 6 \geq (4n + 3p - 16) + 2d_T(u_2) - 5 \quad > 4n + 3p - 16,$$

as desired.

Case 4. Every quasi-pendent vertex of $T$ is a 3-vertex, which has two pendent neighbors and a neighbor of degree 2.

We first assume that the maximum degree of $T$ is at least 4. By our hypothesis, the vertex with maximum degree of $T$ is not a quasi-pendent vertex and thus it is not a special vertex, which is contrary with the choice of $T$ and Lemma 4. Next, we suppose that the maximum degree of $T$ is
equal to 3.

If the maximum degree of $T$ is 3 and no two branching vertices of $T$ are adjacent, then $T \in \mathcal{T}_0(n, p)$ and hence $M_2(T) = 4n + 3p - 16$.

Next, we suppose that the maximum degree of $T$ is 3 and it contains at least one pair of adjacent branching vertices. Let $u_0v_0$ be an edge of $T$ with $d_T(u_0) = d_T(v_0) = 3$. Let $w_0$ be a pendent vertex of $T$ such that $w_0$ is connected with $v_0$ in $T - u_0v_0$. Let $T_2$ be the tree formed from $T$ by deleting the edge $u_0v_0$ and then adding the edge $u_0w_0$. Then, $T_2$ is a tree with $n$ vertices and $p - 1$ pendent vertices. Suppose that $N_T(v_0) = \{u_0, u_1, u_2\}$. Since every quasi-pendent vertex of $T$ is a 3-vertex, which has two pendent neighbors and a neighbor of degree 2, $d_T(u_1) \geq d_T(u_2) \geq 2$. By using the inductive hypothesis, we have

$$M_2(T) = M_2(T_2) + d_T(u_1) + d_T(u_2) \geq 4n + 3(p - 1) - 16 + 4$$
$$> 4n + 3p - 16,$$

as desired.

4 Further discussion

As indicated in Corollary 1, the bound on $M_2$ for trees of $\mathbb{T}_n^{(p)}$ given in Theorem 3 is best possible when $4 \leq p \leq \frac{n+5}{3}$. The following result gives the best possible bound on $M_2$ for members of $\mathbb{T}_n^{(p)}$ when $p \in \{2, 3, 4, n - 3, n - 2\}$.

**Lemma 5.** [8] If $p \in \{2, 3, 4, n - 3, n - 2\}$, then $D_{n;\lceil \frac{p}{2}\rceil,\lfloor \frac{p}{2}\rfloor}$ uniquely attains the minimum second Zagreb index among all trees in the class $\mathbb{T}_n^{(p)}$.

Thus, it seems to be an interesting problem to characterize the trees having minimum value of $M_2$ in the class $\mathbb{T}_n^{(p)}$ when $\frac{n+5}{3} < p \leq n - 4$.

In what follows, we take $T_0 \in \mathbb{T}_n^{(p)}$ such that $M_2(T_0)$ is as small as possible. We may suppose that $q(T_0) \geq 3$ by Lemma 3. With the similar argument as Lemma 4, we have

**Lemma 6.** Let $x_0, y_0$ be two non-pendent vertices of $T_0$ such that $x_0$ is a quasi-pendent vertex. If $y_0$ is not a special vertex, then $d_{T_0}(y_0) \leq d_{T_0}(x_0)$.
In what follows, we give more properties of $T_0$. Firstly, from Lemma 6, we conclude that the following claim holds.

**Claim 1.** Let $x_0$ and $y_0$ be two non-pendent vertices of $T_0$.

(i) If they are quasi-pendent vertices and they are not special vertices, then $d_{T_0}(x_0) = d_{T_0}(y_0)$;

(ii) If $x_0$ is a special vertex and $y_0$ is not a special vertex, then $d_{T_0}(x_0) \geq d_{T_0}(y_0)$;

(iii) If $x_0$ is a quasi-pendent vertex and $y_0$ is not a quasi-pendent vertex, then $d_{T_0}(x_0) \geq d_{T_0}(y_0)$;

(iv) $T_0$ must contain a special vertex with maximum degree $\Delta$.

**Claim 2.** Let $x_0$ and $y_0$ be two branching vertices of $T_0$. If $x_0y_0 \in E(T_0)$, then $T_0$ contains no edge $u_0v_0$ with $d_{T_0}(u_0) = d_{T_0}(v_0) = 2$.

**Proof.** By contradiction, we assume that $u_0v_0 \in E(T_0)$ with $d_{T_0}(u_0) = d_{T_0}(v_0) = 2$. We may suppose that $v_0, x_0 \notin P_{y_0u_0}$. Let $T_2 = T_0 + x_0u_0 + y_0v_0 - x_0y_0 - u_0v_0$. Then, $T_2$ is also a tree with $n$ vertices and $p$ pendent vertices such that $M_2(T_2) - M_2(T_0) = (d_{T_0}(x_0) - 2)(2 - d_{T_0}(y_0)) < 0$, contrary with the choice of $T_0$. ■

**Claim 3.** Let $x_0$ and $y_0$ be two special vertices of $T_0$ and $x, y$ be two non-pendent vertices adjacent to $x_0$ and $y_0$, respectively. Then, $d_{T_0}(x_0) \geq d_{T_0}(y)$. Furthermore, if $d_{T_0}(x_0) < d_{T_0}(y_0)$ and $yx_0 \notin E(T_0)$, then $d_{T_0}(x) \geq d_{T_0}(y)$.

**Proof.** Let $x_1$ be a pendent vertex adjacent to $x_0$ and $T_3 = T_0 + x_0y_0 + yx_1 - yy_0 - x_0x_1$. Then,

$$M_2(T_3) - M_2(T_0) = d_{T_0}(x_0)d_{T_0}(y_0) + d_{T_0}(y) - d_{T_0}(x_0) - d_{T_0}(y)d_{T_0}(y_0)$$

$$= (d_{T_0}(y_0) - 1)(d_{T_0}(x_0) - d_{T_0}(y)) \geq 0$$

and thus $d_{T_0}(x_0) \geq d_{T_0}(y)$.

Let $T_4 = T_0 + x_0y + y_0x - yy_0 - x_0x$. Then, $M_2(T_4) - M_2(T_0) = (d_{T_0}(y_0) - d_{T_0}(x_0))(d_{T_0}(x) - d_{T_0}(y))$. By the choice of $T_0$, we have $d_{T_0}(x) \geq d_{T_0}(y)$ when $d_{T_0}(x_0) < d_{T_0}(y_0)$. ■
Claim 4. Let \( x_0 \) and \( y_0 \) be two special vertices of \( T_0 \) and \( x, y \) be two non-pendent vertices adjacent to \( x_0 \) and \( y_0 \), respectively. If \( d_{T_0}(x) \geq d_{T_0}(y) \), then \( d_{T_0}(y_0) \geq d_{T_0}(x_0) - 1 \). Furthermore, if \( d_{T_0}(x) > d_{T_0}(y) \), then \( d_{T_0}(y_0) \geq d_{T_0}(x_0) \).

Proof. Since \( x_0 \) and \( y_0 \) are two special vertices of \( T_0 \), \( x_0 \) and \( y_0 \) are adjacent to exactly \( d_{T_0}(x_0) - 1 \) and \( d_{T_0}(y_0) - 1 \) pendent vertices, respectively. Assume that \( d_{T_0}(x_0) - 2 \geq d_{T_0}(y_0) \geq 2 \). Denote by \( T_5 = T_0 + y_0x_1 - x_0x_1 \), where \( x_1 \) is a pendent vertex adjacent to \( x_0 \). Then,

\[
M_2(T_5) - M_2(T_0) = (d_{T_0}(x_0) - 1)(d_{T_0}(x) + d_{T_0}(x_0) - 2) + (d_{T_0}(y_0) + 1)(d_{T_0}(y) + d_{T_0}(y_0))
- d_{T_0}(x_0)(d_{T_0}(x) + d_{T_0}(x_0) - 1) - d_{T_0}(y_0)(d_{T_0}(y) + d_{T_0}(y_0) - 1)
= d_{T_0}(y) - d_{T_0}(x) + 2(d_{T_0}(y_0) - d_{T_0}(x_0)) + 2 < 0, \tag{6}
\]

contrary with the choice of \( T_0 \). By (6), with the similar reason, we can show the Furthermore part. \( \square \)

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