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NEIGHBORHOOD VERSION OF THIRD ZAGREB INDEX OF TREES

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Abstract. For a graph G, the third neighborhood degree index of G is defined as:

$$ND_3(G) = \sum_{ab \in E(G)} \delta_G(a)\delta_G(b)\Big(\delta_G(a) + \delta_G(b)\Big),$$

where $\delta_G(a)$ represents the sum of degrees of all neighboring vertices of vertex a. In this short paper, we establish a new lower bound on the third neighborhood degree index of trees and characterize the extremal trees achieving this bound.

Keywords: Third neighborhood degree index, trees, lower bound.
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1. Introduction

Let G be an undirected simple connected graph whose vertex and edge sets are $V(G)$ and $E(G)$, respectively. For a vertex $a \in V(G)$, the open neighborhood of a is written as $N_G(a) = \{b \in V(G) \mid ab \in E(G)\}$. The degree of a vertex a in G is the cardinality of $N_G(a)$, and will be denoted by $\deg_G(a)$. Let $\Delta(G) = \Delta$ be the maximum degree of G. The distance between two vertices a and b in $V(G)$, denoted by $d(a, b)$, is the length of the shortest (a, b)-path in G.

Graph invariants have been a prolific thread in graph theory due to their wide applications and connections in different areas of mathematics and sciences. The Zagreb indices are one of the most prominent and widely studied vertex-degree-based graph invariants. The Zagreb indices were introduced in the 1970s [7,8]. The wide range of theoretical and applicable fields, mostly in chemistry, can be found in the surveys [2,6]. In the last two decades, several modifications of the Zagreb indices have been put forward. They include Zagreb coindices [5,23], entire Zagreb indices [1,11], multiplicative Zagreb indices [10,26], leap Zagreb indices [3,20,22,24], Lanzhou index [4,25], reformulated Zagreb indices [9,12], etc.

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Among them, Mondal et al. introduced several new indices [13,14] based on neighborhood degree sum of vertices, which received increasing research attention. Here, we consider a variant of these indices named the third neighborhood degree index. The third neighborhood degree index defined in [15] as:

$$ND_3(G) = \sum_{ab\in E(G)} \delta_G(a)\delta_G(b)\Big(\delta_G(a) + \delta_G(b)\Big),$$

where $\delta_G(a) = \sum_{b\in N_G(a)} \deg_G(b)$. For more information see [16–19, 21].

In this short paper, we present a new lower bound on the third neighborhood degree index of trees with n vertices and given maximum degree. We further determine the extremal trees achieve this bound.

2. Trees

A tree together with a special vertex chosen as the *root* of the tree is a *rooted tree.* A vertex of a tree of degree one is said to be a *leaf.* A *branching vertex* of a tree is each vertex of degree greater than two.

A tree with exactly one branching vertex is called a *spider.* The branching vertex of a spider T is its *center.* A *leg* of a spider is a path from its center to a leaf. A star is a spider whose all legs have length one. Also, a path can be considered to be a *spider* with one or two legs.

A spanning tree of an undirected connected graph G is a subgraph that is a tree which includes all of the vertices of G.

In this section, we let T be a rooted tree with root a where $\deg_T(a) = \Delta$ and $N_T(a) = \{a_1, a_2, \ldots, a_\Delta\}$. Let $\mathcal{T}(n, \Delta)$, be the set of all trees with n vertices and maximum degree Δ.

Lemma 2.1. *Let $T \in \mathcal{T}(n, \Delta)$ and let b be a branching vertex of T with maximum distance to a. If vertex b is adjacent to at least two leaves, then there is a tree $T_1 \in \mathcal{T}(n, \Delta)$ such that $ND_3(T_1) < ND_3(T)$.*

Proof. Assume that $\deg_T(b) = \rho$ and $N_T(b) = \{b_1, \ldots, b_\rho\}$, where b_ρ lies on the path from b to a. By our assumption, for $1 \le i \le \rho - 1$, $\deg_T(b_i) = 1$ or $\deg_T(b_i) = 2$. Since b is adjacent to at least two leaves, we let b_1 and b_2 be leaves. Let T_1 be the tree obtained from T by removing the edge bb_1 and adding the edge b_1b_2. If $3 \le i \le \rho$, then

$$\begin{aligned}\delta_{T_1}(b_i) &= \deg_{T_1}(b) + \sum_{x\in N_{T_1}(b_i)-\{b\}} \deg_{T_1}(x)\\ &= \deg_T(b) - 1 + \sum_{x\in N_T(b_i)-\{b\}} \deg_T(x) = \delta_T(b_i) - 1.\end{aligned}$$

Therefore,

$$\begin{aligned}\alpha =&\sum_{i=3}^{\rho}\delta_T(b)\delta_T(b_i)[\delta_T(b)+\delta_T(b_i)]-\sum_{i=3}^{\rho}\delta_{T_1}(b)\delta_{T_1}(b_i)[\delta_{T_1}(b)+\delta_{T_1}(b_i)]\\ =&\sum_{i=3}^{\rho}\delta_T(b)\delta_T(b_i)[\delta_T(b)+\delta_T(b_i)]\\ &-\sum_{i=3}^{\rho}\delta_T(b)(\delta_T(b_i)-1)[\delta_T(b)+\delta_T(b_i)-1]>0.\end{aligned}$$

Since $\rho \geq 3$, we have

$$\begin{aligned}ND_3(T)-ND_3(T_1)\geq&\alpha+\delta_T(b)\delta_T(b_1)[\delta_T(b)+\delta_T(b_1)]\\ &+\delta_T(b)\delta_T(b_2)[\delta_T(b)+\delta_T(b_2)]\\ &-\delta_{T_1}(b_1)\delta_{T_1}(b_2)[\delta_{T_1}(b_1)+\delta_{T_1}(b_2)]\\ &-\delta_{T_1}(b)\delta_{T_1}(b_2)[\delta_{T_1}(b)+\delta_{T_1}(b_2)]\\ =&\alpha+2\rho\delta_T(b)[\delta_T(b)+\rho]-2\rho(\rho+2)-\rho\delta_T(b)[\delta_T(b)+\rho]\\ >&\rho\delta_T(b)[\delta_T(b)+\rho]-2\rho(\rho+2)>0.\end{aligned}$$

□

Lemma 2.2. *Let $T \in \mathcal{T}(n,\Delta)$ and let b be a branching vertex of T with maximum distance to a. If vertex b is adjacent to a leaf, then there is a tree $T_1 \in \mathcal{T}(n,\Delta)$ such that $ND_3(T_1) < ND_3(T)$.*

Proof. Assume that $\deg_T(b)=\rho$ and $N_T(b)=\{b_1,\dots,b_\rho\}$, where b_ρ lies on the path from b to a. Then, we let b_1 be a leaf and $\deg_T(b_i)=2$ for $2\leq i\leq \rho-1$. Let $bc_1\dots c_l$ be a path in T with $b_2=c_1$ and $l\geq 2$. Let T_1 be the tree derived from T by removing the edge bb_1 and adding the edge c_lb_1. Then

$$\begin{aligned}\alpha =&\sum_{i=3}^{\rho}\delta_T(b)\delta_T(b_i)[\delta_T(b)+\delta_T(b_i)]-\sum_{i=3}^{\rho}\delta_{T_1}(b)\delta_{T_1}(b_i)[\delta_{T_1}(b)+\delta_{T_1}(b_i)]\\ =&\sum_{i=3}^{\rho}\delta_T(b)\delta_T(b_i)[\delta_T(b)+\delta_T(b_i)]\\ &-\sum_{i=3}^{\rho}(\delta_T(b)-1)(\delta_T(b_i)-1)[\delta_T(b)+\delta_T(b_i)-2]>0.\end{aligned}$$

If $l = 2$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) \geq & \alpha + \delta_T(b)\delta_T(b_1)[\delta_T(b) + \delta_T(b_1)] \\
& + \delta_T(b)\delta_T(c_1)[\delta_T(b) + \delta_T(c_1)] \\
& + \delta_T(c_1)\delta_T(c_2)[\delta_T(c_1) + \delta_T(c_2)] \\
& - \delta_{T_1}(b_1)\delta_{T_1}(c_2)[\delta_{T_1}(b_1) + \delta_{T_1}(c_2)] \\
& - \delta_{T_1}(c_1)\delta_{T_1}(c_2)[\delta_{T_1}(c_1) + \delta_{T_1}(c_2)] \\
& - \delta_{T_1}(b)\delta_{T_1}(c_1)[\delta_{T_1}(b) + \delta_{T_1}(c_1)] \\
= & \alpha + \rho\delta_T(b)[\rho + \delta_T(b)] + (\rho+1)\delta_T(b)[\rho + \delta_T(b) + 1] \\
& + 2(\rho+1)(\rho+3) - 30 - 3(\rho+1)(\rho+4) \\
& - (\rho+1)(\delta_T(b) - 1)[\rho + \delta_T(b)] \\
> & [\rho\delta_T(b) + \rho + 1][\rho + \delta_T(b)] + (\rho+1)\delta_T(b) \\
& - \rho^2 - 7\rho - 36 > 0.
\end{aligned}$$

If $l = 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) \geq & \alpha + \delta_T(b)\delta_T(b_1)[\delta_T(b) + \delta_T(b_1)] \\
& + \delta_T(b)\delta_T(c_1)[\delta_T(b) + \delta_T(c_1)] \\
& + \delta_T(c_1)\delta_T(c_2)[\delta_T(c_1) + \delta_T(c_2)] \\
& + \delta_T(c_2)\delta_T(c_3)[\delta_T(c_2) + \delta_T(c_3)] \\
& - \delta_{T_1}(b)\delta_{T_1}(c_1)[\delta_{T_1}(b) + \delta_{T_1}(c_1)] \\
& - \delta_{T_1}(b_1)\delta_{T_1}(c_3)[\delta_{T_1}(b_1) + \delta_{T_1}(c_3)] \\
& - \delta_{T_1}(c_3)\delta_{T_1}(c_2)[\delta_{T_1}(c_3) + \delta_{T_1}(c_2)] \\
& - \delta_{T_1}(c_2)\delta_{T_1}(c_1)[\delta_{T_1}(c_2)\delta_{T_1}(c_1)] \\
= & \alpha + \rho\delta_T(b)[\rho + \delta_T(b)] + 30 + 3(\rho+2)(\rho+5) \\
& + (\rho+2)\delta_T(b)[\rho + \delta_T(b) + 2] - 30 - 84 \\
& - 4(\rho+1)(\rho+5) - (\rho+1)(\delta_T(b) - 1)[\rho + \delta_T(b)] \\
> & [\rho\delta_T(b) + \delta_T(b) + \rho + 1][\rho + \delta_T(b)] + 2(\rho+2)\delta_T(b) \\
& - \rho^2 - 3\rho - 84 > 0.
\end{aligned}$$

Now if $l > 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) \geq& \alpha + \delta_T(b)\delta_T(b_1)[\delta_T(b) + \delta_T(b_1)] \\
&+ \delta_T(b)\delta_T(c_1)[\delta_T(b) + \delta_T(c_1)] \\
&+ \delta_T(c_l)\delta_T(c_{l-1})[\delta_T(c_l) + \delta_T(c_{l-1})] \\
&+ \delta_T(c_{l-1})\delta_T(c_{l-2})[\delta_T(c_{l-1}) + \delta_T(c_{l-2})] \\
&- \delta_{T_1}(b_1)\delta_{T_1}(c_l)[\delta_{T_1}(b_1) + \delta_{T_1}(c_l)] \\
&- \delta_{T_1}(b)\delta_{T_1}(c_1)[\delta_{T_1}(b) + \delta_{T_1}(c_1)] \\
&- \delta_{T_1}(c_l)\delta_{T_1}(c_{l-1})[\delta_{T_1}(c_l) + \delta_{T_1}(c_{l-1})] \\
&- \delta_{T_1}(c_{l-1})\delta_{T_1}(c_{l-2})[\delta_{T_1}(c_{l-1})\delta_{T_1}(c_{l-2})] \\
=& \alpha + \rho\delta_T(b)[\rho + \delta_T(b)] + 30 + 84 \\
&+ (\rho + 2)\delta_T(b)[\rho + \delta_T(b) + 2] \\
&- 30 - 84 - 128 - (\rho + 1)(\delta_T(b) - 1)[\rho + \delta_T(b)] \\
>& [\rho\delta_T(b) + \rho + \delta_T(b) + 1][\rho + \delta_T(b)] + 2\delta_T(b) - 128 > 0.
\end{aligned}$$

□

Lemma 2.3. *Let $T \in \mathcal{T}(n, \Delta)$ and let b be a branching vertex of T with maximum distance to a. Then there is a tree $T_1 \in \mathcal{T}(n, \Delta)$ such that $ND_3(T_1) < ND_3(T)$.*

Proof. Assume that $\deg_T(b) = \rho$ and $N_T(b) = \{b_1, \ldots, b_\rho\}$, where b_ρ lies on the path from b to a. By Lemmas 2.1 and 2.2, we may assume that $\deg_T(b_i) = 2$ for $1 \leq i \leq \rho - 1$. Let $bc_1 \ldots c_l$ and $bd_1 \ldots d_s$, $l, s \geq 2$, be two paths in T with $b_1 = c_1$ and $b_2 = d_1$. Let T_1 be the tree derived from $T - \{bb_1\}$ by attaching the path $d_s b_1$. Then

$$\begin{aligned}
\alpha_1 =& \sum_{i=3}^{\rho} \delta_T(b)\delta_T(b_i)[\delta_T(b) + \delta_T(b_i)] - \sum_{i=3}^{\rho} \delta_{T_1}(b)\delta_{T_1}(b_i)[\delta_{T_1}(b) + \delta_{T_1}(b_i)] \\
=& \sum_{i=3}^{\rho} \delta_T(b)\delta_T(b_i)[\delta_T(b) + \delta_T(b_i)] \\
&- \sum_{i=3}^{\rho}(\delta_T(b) - 2)(\delta_T(b_i) - 1)[\delta_T(b) + \delta_T(b_i) - 3] > 0,
\end{aligned}$$

and

$$\begin{aligned}\alpha_2 =&\sum_{i=2}^{\rho}\delta_T(b)\delta_T(b_i)[\delta_T(b)+\delta_T(b_i)]-\sum_{i=2}^{\rho}\delta_{T_1}(b)\delta_{T_1}(b_i)[\delta_{T_1}(b)+\delta_{T_1}(b_i)]\\ =&\sum_{i=2}^{\rho}\delta_T(b)\delta_T(b_i)[\delta_T(b)+\delta_T(b_i)]\\ &-\sum_{i=2}^{\rho}(\delta_T(b)-2)(\delta_T(b_i)-1)[\delta_T(b)+\delta_T(b_i)-3]>0.\end{aligned}$$

If $l=s=2$, then

$$\begin{aligned}ND_3(T)-ND_3(T_1)\geq&\alpha_1+\delta_T(b)\delta_T(c_1)[\delta_T(b)+\delta_T(c_1)]\\ &+\delta_T(c_1)\delta_T(c_2)[\delta_T(c_1)+\delta_T(c_2)]\\ &+\delta_T(b)\delta_T(d_1)[\delta_T(b)+\delta_T(d_1)]\\ &+\delta_T(d_1)\delta_T(d_2)[\delta_T(d_1)+\delta_T(d_2)]\\ &-\delta_{T_1}(c_2)\delta_{T_1}(c_1)[\delta_{T_1}(c_2)+\delta_{T_1}(c_1)]\\ &-\delta_{T_1}(c_1)\delta_{T_1}(d_2)[\delta_{T_1}(c_1)+\delta_{T_1}(d_2)]\\ &-\delta_{T_1}(d_2)\delta_{T_1}(d_1)[\delta_{T_1}(d_1)+\delta_{T_1}(d_2)]\\ &-\delta_{T_1}(b)\delta_{T_1}(d_1)[\delta_{T_1}(b)+\delta_{T_1}(d_1)]\\ =&\alpha_1+4(\rho+1)(\rho+3)+2(\rho+1)\delta_T(b)[\rho+1+\delta_T(b)]\\ &-30-84-4(\rho+1)(\rho+5)\\ &-(\rho+1)(\delta_T(b)-2)[\rho+\delta_T(b)-1]\\ >&4(\rho+1)(\rho+3)+2(\rho+1)[\rho+\delta_T(b)-1]-114>0.\end{aligned}$$

If $l = 2$ and $s = 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) \geq & \alpha_1 + \delta_T(b)\delta_T(c_1)[\delta_T(b) + \delta_T(c_1)] \\
& + \delta_T(c_1)\delta_T(c_2)[\delta_T(c_1) + \delta_T(c_2)] \\
& + \delta_T(b)\delta_T(d_1)[\delta_T(b) + \delta_T(d_1)] \\
& + \delta_T(d_1)\delta_T(d_2)[\delta_T(d_1) + \delta_T(d_2)] \\
& + \delta_T(d_2)\delta_T(d_3)[\delta_T(d_2) + \delta_T(d_3)] \\
& - \delta_{T_1}(c_2)\delta_{T_1}(c_1)[\delta_{T_1}(c_2) + \delta_{T_1}(c_1)] \\
& - \delta_{T_1}(c_1)\delta_{T_1}(d_3)[\delta_{T_1}(c_1) + \delta_{T_1}(d_3)] \\
& - \delta_{T_1}(d_3)\delta_{T_1}(d_2)[\delta_{T_1}(d_3) + \delta_{T_1}(d_2)] \\
& - \delta_{T_1}(d_2)\delta_{T_1}(d_1)[\delta_{T_1}(d_2) + \delta_{T_1}(d_1)] \\
& - \delta_{T_1}(b)\delta_{T_1}(d_1)[\delta_{T_1}(b) + \delta_{T_1}(d_1)] \\
= & \alpha_1 + 2(\rho+1)(\rho+3) + (\rho+1)\delta_T(b)[\rho + 1 + \delta_T(b)] \\
& + 30 + 3(\rho+2)(\rho+5) + (\rho+2)\delta_T(b)[\rho + 2 + \delta_T(b)] \\
& - 30 - 84 - 128 - 4(\rho+1)(\rho+5) \\
& - (\rho+1)(\delta_T(b) - 2)[\rho + \delta_T(b) - 1] \\
> & 6\rho^3 + 21\rho^2 + 17\rho - 220 > 0.
\end{aligned}$$

If $l = 2$ and $s > 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) \geq & \alpha_2 + \delta_T(b)\delta_T(c_1)[\delta_T(b) + \delta_T(c_1)] \\
& + \delta_T(c_1)\delta_T(c_2)[\delta_T(c_1) + \delta_T(c_2)] \\
& + \delta_T(d_s)\delta_T(d_{s-1})[\delta_T(d_s) + \delta_T(d_{s-1})] \\
& + \delta_T(d_{s-1})\delta_T(d_{s-2})[\delta_T(d_{s-1}) + \delta_T(d_{s-2})] \\
& - \delta_{T_1}(c_2)\delta_{T_1}(c_1)[\delta_{T_1}(c_2) + \delta_{T_1}(c_1)] \\
& - \delta_{T_1}(c_1)\delta_{T_1}(d_s)[\delta_{T_1}(c_1) + \delta_{T_1}(d_s)] \\
& - \delta_{T_1}(d_{s-1})\delta_{T_1}(d_s)[\delta_{T_1}(d_s) + \delta_{T_1}(d_{s-1})] \\
& - \delta_{T_1}(d_{s-1})\delta_{T_1}(d_{s-2})[\delta_{T_1}(d_{s-1}) + \delta_{T_1}(d_{s-2})] \\
= & \alpha_2 + 2(\rho+1)(\rho+3) + (\rho+1)\delta_T(b)[\rho + 1 + \delta_T(b)] \\
& + 30 + 84 + (\rho+2)\delta_T(b)[\rho + 2 + \delta_T(b)] \\
& - 30 - 84 - 128 - 128 \\
& - (\rho+1)(\delta_T(b) - 2)[\rho + \delta_T(b) - 1] \\
> & 6\rho^3 + 10\rho^2 + 10\rho - 250 > 0.
\end{aligned}$$

If $l = s = 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) \geq& \alpha_2 + \delta_T(b)\delta_T(c_1)[\delta_T(b) + \delta_T(c_1)] \\
&+ \delta_T(c_1)\delta_T(c_2)[\delta_T(c_1) + \delta_T(c_2)] \\
&+ \delta_T(c_2)\delta_T(c_3)[\delta_T(c_2) + \delta_T(c_3)] \\
&+ \delta_T(d_1)\delta_T(d_2)[\delta_T(d_1) + \delta_T(d_2)] \\
&+ \delta_T(d_2)\delta_T(d_3)[\delta_T(d_2) + \delta_T(d_3)] \\
&- \delta_{T_1}(c_3)\delta_{T_1}(c_2)[\delta_{T_1}(c_3) + \delta_{T_1}(c_2)] \\
&- \delta_{T_1}(c_2)\delta_{T_1}(c_1)[\delta_{T_1}(c_1) + \delta_{T_1}(c_2)] \\
&- \delta_{T_1}(c_1)\delta_{T_1}(d_3)[\delta_{T_1}(c_1) + \delta_{T_1}(d_3)] \\
&- \delta_{T_1}(d_3)\delta_{T_1}(d_2)[\delta_{T_1}(d_3) + \delta_{T_1}(d_2)] \\
&- \delta_{T_1}(d_2)\delta_{T_1}(d_1)[\delta_{T_1}(d_2) + \delta_{T_1}(d_1)] \\
=& \alpha_2 + 60 + 6(\rho+2)(\rho+5) + (\rho+2)\delta_T(b)[\rho + 2 + \delta_T(b)] \\
&- 30 - 84 - 128 - 128 - 4(\rho+1)(\rho+5) \\
>& 6\rho^3 + 22\rho^2 + 26\rho - 260 > 0.
\end{aligned}$$

If $l = 3$ and $s > 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) \geq& \alpha_2 + \delta_T(b)\delta_T(c_1)[\delta_T(b) + \delta_T(c_1)] \\
&+ \delta_T(c_1)\delta_T(c_2)[\delta_T(c_1) + \delta_T(c_2)] \\
&+ \delta_T(c_2)\delta_T(c_3)[\delta_T(c_2) + \delta_T(c_3)] \\
&+ \delta_T(d_s)\delta_T(d_{s-1})[\delta_T(d_s) + \delta_T(d_{s-1})] \\
&+ \delta_T(d_{s-1})\delta_T(d_{s-2})[\delta_T(d_{s-1}) + \delta_T(d_{s-2})] \\
&- \delta_{T_1}(c_3)\delta_{T_1}(c_2)[\delta_{T_1}(c_3) + \delta_{T_1}(c_2)] \\
&- \delta_{T_1}(c_2)\delta_{T_1}(c_1)[\delta_{T_1}(c_1) + \delta_{T_1}(c_2)] \\
&- \delta_{T_1}(c_1)\delta_{T_1}(d_s)[\delta_{T_1}(c_1) + \delta_{T_1}(d_s)] \\
&- \delta_{T_1}(d_s)\delta_{T_1}(d_{s-1})[\delta_{T_1}(d_s) + \delta_{T_1}(d_{s-1})] \\
&- \delta_{T_1}(d_{s-1})\delta_{T_1}(d_{s-2})[\delta_{T_1}(d_{s-1}) + \delta_{T_1}(d_{s-2})] \\
=& \alpha_2 + 30 + 3(\rho+2)(\rho+5) \\
&+ (\rho+2)\delta_T(b)[\rho + 2 + \delta_T(b)] + 30 + 84 \\
&- 30 - 84 - 128 - 128 - 128 \\
>& 6\rho^3 + 21\rho^2 + 29\rho - 294 > 0.
\end{aligned}$$

If $l, s > 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) \geq & \alpha_2 + \delta_T(b)\delta_T(c_1)[\delta_T(b) + \delta_T(c_1)] \\
& + \delta_T(c_1)\delta_T(c_2)[\delta_T(c_1) + \delta_T(c_2)] \\
& + \delta_T(d_s)\delta_T(d_{s-1})[\delta_T(d_s) + \delta_T(d_{s-1})] \\
& + \delta_T(d_{s-1})\delta_T(d_{s-2})[\delta_T(d_{s-1}) + \delta_T(d_{s-2})] \\
& - \delta_{T_1}(c_2)\delta_{T_1}(c_1)[\delta_{T_1}(c_1) + \delta_{T_1}(c_2)] \\
& - \delta_{T_1}(c_1)\delta_{T_1}(d_s)[\delta_{T_1}(c_1) + \delta_{T_1}(d_s)] \\
& - \delta_{T_1}(d_s)\delta_{T_1}(d_{s-1})[\delta_{T_1}(d_s) + \delta_{T_1}(d_{s-1})] \\
& - \delta_{T_1}(d_{s-1})\delta_{T_1}(d_{s-2})[\delta_{T_1}(d_{s-1}) + \delta_{T_1}(d_{s-2})] \\
= & \alpha_2 + 4(\rho+2)(\rho+6) \\
& + (\rho+2)\delta_T(b)[\rho + 2 + \delta_T(b)] + 30 + 84 \\
& - 128 - 128 - 128 - 128 \\
> & 6\rho^3 + 20\rho^2 + 40\rho - 350 > 0.
\end{aligned}$$

□

Proposition 2.4. *Let $T \in \mathcal{T}(n, \Delta)$ be a spider with $\Delta \geq 3$ such that T has two legs of length more than one. Then there exists a spider $T_1 \in \mathcal{T}(n, \Delta)$ with $ND_3(T_1) < ND_3(T)$.*

Proof. Assume that a is the center of T and $ab_1 \ldots b_l$ and $ac_1 \ldots c_s$ are two legs of length more than one in T. Let T_1 be the tree deduced from $T - \{b_1 b_2\}$ by attaching the path $c_s b_2$. If $l = s = 2$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) > & \delta_T(a)\delta_T(b_1)[\delta_T(a) + \delta_T(b_1)] \\
& + \delta_T(b_1)\delta_T(b_2)[\delta_T(b_1) + \delta_T(b_2)] \\
& + \delta_T(a)\delta_T(c_1)[\delta_T(a) + \delta_T(c_1)] \\
& + \delta_T(c_1)\delta_T(c_2)[\delta_T(c_1) + \delta_T(c_2)] \\
& - \delta_{T_1}(a)\delta_{T_1}(b_1)[\delta_{T_1}(a) + \delta_{T_1}(b_1)] \\
& - \delta_{T_1}(b_2)\delta_{T_1}(c_2)[\delta_{T_1}(b_2) + \delta_{T_1}(c_2)] \\
& - \delta_{T_1}(c_2)\delta_{T_1}(c_1)[\delta_{T_1}(c_1) + \delta_{T_1}(c_2)] \\
& - \delta_{T_1}(a)\delta_{T_1}(c_1)[\delta_{T_1}(a) + \delta_{T_1}(c_1)] \\
= & 4(\Delta+1)(\Delta+3) + 2(\Delta+1)\delta_T(a)[\Delta + 1 + \delta_T(a)] \\
& - 30 - 3(\Delta+2)(\Delta+5) \\
& - \Delta(\delta_T(a) - 1)[\Delta + \delta_T(a) - 1] \\
& - (\Delta+2)(\delta_T(a) - 1)[\Delta + \delta_T(a) + 1] \\
> & 3\Delta^2 + 6\Delta\delta_T(a) + 6\delta_T(a) - 3\Delta - 46 > 0.
\end{aligned}$$

If $l = 2$ and $s = 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) >& \delta_T(a)\delta_T(b_1)[\delta_T(a) + \delta_T(b_1)] \\
&+ \delta_T(b_1)\delta_T(b_2)[\delta_T(b_1) + \delta_T(b_2)] \\
&+ \delta_T(a)\delta_T(c_1)[\delta_T(a) + \delta_T(c_1)] \\
&+ \delta_T(c_1)\delta_T(c_2)[\delta_T(c_1) + \delta_T(c_2)] \\
&+ \delta_T(c_2)\delta_T(c_3)[\delta_T(c_2) + \delta_T(c_3)] \\
&- \delta_{T_1}(a)\delta_{T_1}(b_1)[\delta_{T_1}(a) + \delta_{T_1}(b_1)] \\
&- \delta_{T_1}(b_2)\delta_{T_1}(c_3)[\delta_{T_1}(b_2) + \delta_{T_1}(c_3)] \\
&- \delta_{T_1}(c_2)\delta_{T_1}(c_1)[\delta_{T_1}(c_1) + \delta_{T_1}(c_2)] \\
&- \delta_{T_1}(a)\delta_{T_1}(c_1)[\delta_{T_1}(a) + \delta_{T_1}(c_1)] \\
&- \delta_{T_1}(c_2)\delta_{T_1}(c_3)[\delta_{T_1}(c_2) + \delta_{T_1}(c_3)] \\
=& 2(\Delta + 1)(\Delta + 3) + (\Delta + 1)\delta_T(a)[\Delta + 1 + \delta_T(a)] \\
&+ 30 + 3(\Delta + 2)(\Delta + 5) \\
&+ (\Delta + 2)\delta_T(a)[\Delta + 2 + \delta_T(a)] \\
&- 30 - 84 - 4(\Delta + 2)(\Delta + 6) \\
&- \Delta(\delta_T(a) - 1)[\Delta + \delta_T(a) - 1] \\
&- (\Delta + 2)(\delta_T(a) - 1)[\Delta + \delta_T(a) + 1] \\
>& 3\Delta^2 + 7\Delta\delta_T(a) + \delta_T^2(a) + 5\delta_T(a) - \Delta - 94 > 0.
\end{aligned}$$

If $l = 2$ and $s > 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) >& \delta_T(a)\delta_T(b_1)[\delta_T(a) + \delta_T(b_1)] \\
&+ \delta_T(b_1)\delta_T(b_2)[\delta_T(b_1) + \delta_T(b_2)] \\
&+ \delta_T(c_s)\delta_T(c_{s-1})[\delta_T(c_s) + \delta_T(c_{s-1})] \\
&+ \delta_T(c_{s-1})\delta_T(c_{s-2})[\delta_T(c_{s-1}) + \delta_T(c_{s-2})] \\
&- \delta_{T_1}(a)\delta_{T_1}(b_1)[\delta_{T_1}(a) + \delta_{T_1}(b_1)] \\
&- \delta_{T_1}(b_2)\delta_{T_1}(c_s)[\delta_{T_1}(b_2) + \delta_{T_1}(c_s)] \\
&- \delta_{T_1}(c_s)\delta_{T_1}(c_{s-1})[\delta_{T_1}(c_s) + \delta_{T_1}(c_{s-1})] \\
&- \delta_{T_1}(c_{s-1})\delta_{T_1}(c_{s-2})[\delta_{T_1}(c_{s-1}) + \delta_{T_1}(c_{s-2})] \\
=& 2(\Delta + 1)(\Delta + 3) + 30 + 84 \\
&+ (\Delta + 1)\delta_T(a)[\Delta + 1 + \delta_T(a)] \\
&- 30 - 84 - 128 - \Delta(\delta_T(a) - 1)[\Delta + \delta_T(a) - 1] \\
>& 3\Delta^2 + 4\Delta\delta_T(a) + \delta_T^2(a) + \delta_T(a) + 7\Delta - 122 > 0.
\end{aligned}$$

If $l = s = 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) >& \delta_T(a)\delta_T(b_1)[\delta_T(a) + \delta_T(b_1)] \\
&+ \delta_T(b_1)\delta_T(b_2)[\delta_T(b_1) + \delta_T(b_2)] \\
&+ \delta_T(b_2)\delta_T(b_3)[\delta_T(b_2) + \delta_T(b_3)] \\
&+ \delta_T(c_1)\delta_T(c_2)[\delta_T(c_1) + \delta_T(c_2)] \\
&+ \delta_T(c_2)\delta_T(c_3)[\delta_T(c_2) + \delta_T(c_3)] \\
&- \delta_{T_1}(a)\delta_{T_1}(b_1)[\delta_{T_1}(a) + \delta_{T_1}(b_1)] \\
&- \delta_{T_1}(b_2)\delta_{T_1}(b_3)[\delta_{T_1}(b_2) + \delta_{T_1}(b_3)] \\
&- \delta_{T_1}(b_2)\delta_{T_1}(c_3)[\delta_{T_1}(b_2) + \delta_{T_1}(c_3)] \\
&- \delta_{T_1}(c_2)\delta_{T_1}(c_1)[\delta_{T_1}(c_1) + \delta_{T_1}(c_2)] \\
&- \delta_{T_1}(c_2)\delta_{T_1}(c_3)[\delta_{T_1}(c_2) + \delta_{T_1}(c_3)] \\
=& 30 + 3(\Delta + 2)(\Delta + 5) + (\Delta + 2)\delta_T(a)[\Delta + 2 + \delta_T(a)] \\
&+ 30 + 3(\Delta + 2)(\Delta + 5) - 30 - 84 - 128 \\
&- 4(\Delta + 2)(\Delta + 6) - \Delta(\delta_T(a) - 1)[\Delta + \delta_T(a) - 1] \\
>& 3\Delta^2 + 8\Delta\delta_T(a) + 2\delta_T^2(a) + 4\delta_T(a) + 9\Delta - 166 > 0.
\end{aligned}$$

If $l = 3$ and $s > 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) >& \delta_T(a)\delta_T(b_1)[\delta_T(a) + \delta_T(b_1)] \\
&+ \delta_T(b_1)\delta_T(b_2)[\delta_T(b_1) + \delta_T(b_2)] \\
&+ \delta_T(b_2)\delta_T(b_3)[\delta_T(b_2) + \delta_T(b_3)] \\
&+ \delta_T(c_s)\delta_T(c_{s-1})[\delta_T(c_s) + \delta_T(c_{s-1})] \\
&+ \delta_T(c_{s-1})\delta_T(c_{s-2})[\delta_T(c_{s-1}) + \delta_T(c_{s-2})] \\
&- \delta_{T_1}(a)\delta_{T_1}(b_1)[\delta_{T_1}(a) + \delta_{T_1}(b_1)] \\
&- \delta_{T_1}(b_2)\delta_{T_1}(b_3)[\delta_{T_1}(b_2) + \delta_{T_1}(b_3)] \\
&- \delta_{T_1}(b_2)\delta_{T_1}(c_s)[\delta_{T_1}(b_2) + \delta_{T_1}(c_s)] \\
&- \delta_{T_1}(c_s)\delta_{T_1}(c_{s-1})[\delta_{T_1}(c_s) + \delta_{T_1}(c_{s-1})] \\
&- \delta_{T_1}(c_{s-1})\delta_{T_1}(c_{s-2})[\delta_{T_1}(c_{s-1}) + \delta_{T_1}(c_{s-2})] \\
=& 30 + 3(\Delta + 2)(\Delta + 5) \\
&+ (\Delta + 2)\delta_T(a)[\Delta + 2 + \delta_T(a)] + 30 + 84 \\
&- 30 - 84 - 128 - 128 \\
&- \Delta(\delta_T(a) - 1)[\Delta + \delta_T(a) - 1] \\
>& 4\Delta^2 + 8\Delta\delta_T(a) + 2\delta_T^2(a) \\
&+ 4\delta_T(a) + 20\Delta - 196 > 0.
\end{aligned}$$

If $l, s > 3$, then

$$\begin{aligned}
ND_3(T) - ND_3(T_1) >&\delta_T(a)\delta_T(b_1)[\delta_T(a) + \delta_T(b_1)]\\
&+ \delta_T(b_1)\delta_T(b_2)[\delta_T(b_1) + \delta_T(b_2)]\\
&+ \delta_T(c_s)\delta_T(c_{s-1})[\delta_T(c_s) + \delta_T(c_{s-1})]\\
&+ \delta_T(c_{s-1})\delta_T(c_{s-2})[\delta_T(c_{s-1}) + \delta_T(c_{s-2})]\\
&- \delta_{T_1}(a)\delta_{T_1}(b_1)[\delta_{T_1}(a) + \delta_{T_1}(b_1)]\\
&- \delta_{T_1}(b_2)\delta_{T_1}(c_s)[\delta_{T_1}(b_2) + \delta_{T_1}(c_s)]\\
&- \delta_{T_1}(c_s)\delta_{T_1}(c_{s-1})[\delta_{T_1}(c_s) + \delta_{T_1}(c_{s-1})]\\
&- \delta_{T_1}(c_{s-1})\delta_{T_1}(c_{s-2})[\delta_{T_1}(c_{s-1}) + \delta_{T_1}(c_{s-2})]\\
=&4(\Delta + 2)(\Delta + 6) + (\Delta + 2)\delta_T(a)[\Delta + 2 + \delta_T(a)]\\
&+ 30 + 84 - 128 - 128 - 128\\
&- \Delta(\delta_T(a) - 1)[\Delta + \delta_T(a) - 1]\\
>&5\Delta^2 + 6\Delta\delta_T(a) + 2\delta_T^2(a) + 4\delta_T(a) + 31\Delta - 222 > 0.
\end{aligned}$$

This completes the proof. □

Theorem 2.5. *If $T \in \mathcal{T}(n, \Delta)$, then*

$$ND_3(T) = 2\Delta^4,$$

when $\Delta = n - 1$,

$$ND_3(T) = 2(\Delta + 1)(\Delta + 3) + 2(\Delta + 1)^3 + (\Delta^3 - \Delta)(2\Delta + 1),$$

when $\Delta = n - 2$,

$$ND_3(T) \geq (\Delta + 2)(2\Delta^2 + 8\Delta + 18) + (\Delta^3 - \Delta)(2\Delta + 1) + 30,$$

when $\Delta = n - 3$, *and*

$$ND_3(T) \geq 128(n - \Delta) + (\Delta + 2)(2\Delta^2 + 9\Delta + 27) + (\Delta^3 - \Delta)(2\Delta + 1) - 398,$$

when $\Delta < n - 3$. *The equality holds if and only if T is a spider with at most one leg of length more than one.*

Proof. Assume that $T^* \in \mathcal{T}(n, \Delta)$ with $ND_3(T^*) \leq ND_3(T)$ for all $T \in \mathcal{T}(n, \Delta)$. Rooted T^* at a such that $\deg_{T^*}(a) = \Delta$. First let $\Delta = 2$. Hence T^* is a path and the result is immediate. Now let $\Delta \geq 3$. Then by Lemmas 2.1, 2.2 and 2.3, T^* is a spider with center a and by Proposition 2.4, T^* has at most one leg of length more than one. If T^* is a star, then $ND_3(T^*) = 2\Delta^4$. Hence, assume that T^* is not a star and T^* has only one leg of length more than one. If $\Delta = n - 2$, then

$$ND_3(T^*) = 2(\Delta + 1)(\Delta + 3) + 2(\Delta + 1)^3 + (\Delta^3 - \Delta)(2\Delta + 1),$$

now if $\Delta = n - 3$, then

$$ND_3(T^*) = (\Delta + 2)(2\Delta^2 + 8\Delta + 18) + (\Delta^3 - \Delta)(2\Delta + 1) + 30.$$

Finally, let $\Delta < n-3$. Then

$$\begin{aligned}ND_3(T^*) =&\Delta(\Delta-1)(\Delta+1)(2\Delta+1)+(\Delta+1)(\Delta+2)(2\Delta+3)\\ &+4(\Delta+2)(\Delta+6)+128(n-\Delta-4)+84+30\\ =&128(n-\Delta)+(\Delta+2)(2\Delta^2+9\Delta+27)+(\Delta^3-\Delta)(2\Delta+1)-398.\end{aligned}$$

Then the proof is complete. □

Corollary 2.6. *For every tree T with n vertices, $ND_3(T) \geq ND_3(P_n)$.*

Proof. It is easy to see that for path graph P_n,

$$ND_3(P_n) = \begin{cases} 2, & \text{if } n=2 \\ 32, & \text{if } n=3 \\ 114, & \text{if } n=4 \\ 228, & \text{if } n=5 \\ 128n-412, & \text{if } n \geq 6. \end{cases}$$

If $\Delta \geq 2$, then $2\Delta^4 \geq 32 = ND_3(P_3)$,

$$2(\Delta+1)(\Delta+3)+2(\Delta+1)^3+(\Delta^3-\Delta)(2\Delta+1) \geq 114 = ND_3(P_4),$$

and

$$(\Delta+2)(2\Delta^2+8\Delta+18)+(\Delta^3-\Delta)(2\Delta+1)+30 \geq 228 = ND_3(P_5).$$

Also if $\Delta \geq 2$ and $n > 5$,

$$\begin{aligned}128(n-\Delta)+(\Delta+2)(2\Delta^2+9\Delta+27)+(\Delta^3-\Delta)(2\Delta+1)-398\\ \geq 128n-412 = ND_3(P_n).\end{aligned}$$

Therefore by Theorem 2.5, the result is obtained. □

The following observation is immediately achieved from the definition of ND_3 index.

Observation 2.7. *Let G be a graph and $e \notin E(G)$. Then $ND_3(G+e) > ND_3(G)$.*

Corollary 2.8. *If G is a simple connected graph with n vertices and maximum degree Δ, then*

$$ND_3(G) \geq 2\Delta^4,$$

when $\Delta = n-1$,

$$ND_3(G) \geq 2(\Delta+1)(\Delta+3)+2(\Delta+1)^3+(\Delta^3-\Delta)(2\Delta+1),$$

when $\Delta = n-2$,

$$ND_3(T) \geq (\Delta+2)(2\Delta^2+8\Delta+18)+(\Delta^3-\Delta)(2\Delta+1)+30,$$

when $\Delta = n-3$, *and*

$$ND_3(G) \geq 128(n-\Delta) + (\Delta+2)(2\Delta^2+9\Delta+27) + (\Delta^3-\Delta)(2\Delta+1) - 398,$$

when $\Delta < n-3$. *The equality holds if and only if* G *is a spider with at most one leg of length more than one.*

Proof. By our assumption, G is a simple connected graph with n vertices and maximum degree Δ. It is a well known fact that, there is a spanning tree T of G with n vertices and maximum degree Δ. Since $E(T) \subseteq E(G)$, then by Observation 2.7, $ND_3(G) \geq ND_3(T)$ and by Theorem 2.5,

$$ND_3(G) \geq 2\Delta^4,$$

when $\Delta = n-1$,

$$ND_3(G) \geq 2(\Delta+1)(\Delta+3) + 2(\Delta+1)^3 + (\Delta^3-\Delta)(2\Delta+1),$$

when $\Delta = n-2$,

$$ND_3(T) \geq (\Delta+2)(2\Delta^2+8\Delta+18) + (\Delta^3-\Delta)(2\Delta+1) + 30,$$

when $\Delta = n-3$, and

$$ND_3(G) \geq 128(n-\Delta) + (\Delta+2)(2\Delta^2+9\Delta+27) + (\Delta^3-\Delta)(2\Delta+1) - 398,$$

when $\Delta < n-3$. By Observation 2.7, if G is not a tree, then the equality does not hold. Therefore by Theorem 2.5, the equality holds if and only if G is a spider with at most one leg of length more than one. □

3. Data Availability Statement

The paper does not include or use any datasets.

4. Conflict of interest

The authors declare no conflict of interest.

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