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Short Note

A note on the re-defined third Zagreb index of trees

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Abstract: For a graph Γ, the re-defined third Zagreb index is defined as

$$ReZG_3(\Gamma) = \sum_{ab \in E(\Gamma)} \deg_\Gamma(a) \deg_\Gamma(b) \Big(\deg_\Gamma(a) + \deg_\Gamma(b) \Big),$$

where $\deg_\Gamma(a)$ is the degree of vertex a. We prove for any tree T with n vertices and maximum degree Δ, $ReZG_3(T) \geq 16n + \Delta^3 + 2\Delta^2 - 13\Delta - 26$ when $\Delta < n-1$ and $ReZG_3(T) = n\Delta^2 + n\Delta - \Delta^2 - \Delta$ when $\Delta = n-1$. Also we determine the corresponding extremal trees.

Keywords: Zagreb indices, re-defined third Zagreb index, trees

AMS Subject classification: 05C07

1. Introduction

Consider a simple graph Γ, such that $V(\Gamma)$ and $E(\Gamma)$ are the vertex and edge sets of Γ respectively. Let $n = |V(\Gamma)|$ is the order of Γ. For $a \in V(\Gamma)$ the open neighborhood of a is the set $N_\Gamma(a) = \{b \mid ab \in E(\Gamma)\}$. $\deg_\Gamma(a) = |N_\Gamma(a)|$ is the degree of a in Γ and $\Delta(\Gamma) = \Delta$ is the maximum degree of Γ. The distance between two vertices of Γ is the length of any shortest path in Γ connecting them.

Zagreb indices [12, 14] are the oldest members of degree-based topological indices which are defined as:

$$M_1(\Gamma) = \sum_{a \in V(\Gamma)} \deg_\Gamma(a)^2, \quad M_2(\Gamma) = \sum_{ab \in E(\Gamma)} \deg_\Gamma(a) \deg_\Gamma(b).$$

Other information on these indices can be seen in [1, 2, 5, 11].

Recently, some variants of Zagreb indices introduced, such as multiplicative Zagreb indices, Zagreb coindices, augmented Zagreb index, re-defined Zagreb indices, Lanzhou

index, leap Zagreb indices, entire Zagreb indices, irregularity, etc. For more information about these variants see [3, 4, 6–10, 13, 15–21] and the references therein.
Here, we consider re-defined third Zagreb index. The re-defined third Zagreb index defined in [17] as:

$$ReZG_3(\Gamma) = \sum_{ab\in E(\Gamma)} \deg_\Gamma(a)\deg_\Gamma(b)\Big(\deg_\Gamma(a)+\deg_\Gamma(b)\Big).$$

We give a lower bound on the re-defined third Zagreb index of a tree in terms of its order and maximum degree. Finally we determine the extremal trees achieve this bound.

2. Trees

A *tree* is a connected acyclic graph. A *leaf* is a vertex of degree one. A rooted tree is a tree with a special vertex chosen as the *root* of the tree.
A *spider* is a tree with one vertex of degree at least three. The vertex with degree at least three in a spider is called the *center*. A *leg* of a spider is a path from the center to a leaf. A star is a spider with all legs of length one, and also a path is a spider with one or two leg.
We let $\mathcal{T}(n,\Delta)$ be the trees of order n and maximum degree Δ.

Lemma 1. *Let $T\in\mathcal{T}(n,\Delta)$ be rooted at a such that $\deg_T(a)=\Delta$. If T contains the vertex $b\neq a$ with $\deg_T(b)\geq 3$, then there is $T_1\in\mathcal{T}(n,\Delta)$ with $ReZG_3(T_1)<ReZG_3(T)$.*

Proof. Assume that b be a vertex with maximum distance from a and $\deg_T(b)=\rho$. Suppose that $N_T(b)=\{b_1,b_2,\ldots,b_\rho\}$, where b_ρ lies on the path from b to a. By our assumption, for $1\leq i\leq\rho-1$, $\deg_T(b_i)=1$ or $\deg_T(b_i)=2$. Consider the following cases.

Case 1. b is adjacent to at least two leaves.
We may assume that, b_1 and b_2 be leaves. Denote by T_1 the tree achieved by attaching the edge b_1b_2 to $T-\{bb_1\}$. Since $\rho\geq 3$, then

$$\begin{aligned}
ReZG_3(T)-ReZG_3(T_1) =& \deg_T(b)\deg_T(b_1)\Big(\deg_T(b)+\deg_T(b_1)\Big)\\
&+\deg_T(b)\deg_T(b_2)\Big(\deg_T(b)+\deg_T(b_2)\Big)\\
&+\sum_{i=3}^{\rho}\deg_T(b)\deg_T(b_i)\Big(\deg_T(b)+\deg_T(b_i)\Big)\\
&-\deg_{T_1}(b_1)\deg_{T_1}(b_2)\Big(\deg_{T_1}(b_1)+\deg_{T_1}(b_2)\Big)\\
&-\deg_{T_1}(b)\deg_{T_1}(b_2)\Big(\deg_{T_1}(b)+\deg_{T_1}(b_2)\Big)
\end{aligned}$$

$$
\begin{aligned}
&- \sum_{i=3}^{\rho} \deg_{T_1}(b)\deg_{T_1}(b_i)\Big(\deg_{T_1}(b)+\deg_{T_1}(b_i)\Big)\\
&= 2\rho(\rho+1) + \sum_{i=3}^{\rho} \rho\deg_{T}(b_i)\Big(\rho+\deg_{T}(b_i)\Big)\\
&- 6 - 2(\rho-1)(\rho+1) - (\rho-1)\sum_{i=3}^{\rho} \deg_{T}(b_i)\Big(\rho+\deg_{T}(b_i)-1\Big)\\
&= 2(\rho+1) - 6 + \sum_{i=3}^{\rho} \deg_{T}(b_i)\Big(2\rho+\deg_{T}(b_i)-1\Big)\\
&> 2(\rho+1) - 6 > 0.
\end{aligned}
$$

Case 2. b is adjacent to exactly one leaf.

We may assume that, b_1 be a leaf and $bc_1c_2\dots c_l$ 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. Since $\rho \geq 3$, then

$$
\begin{aligned}
ReZG_3(T) - ReZG_3(T_1) =& \deg_T(b)\deg_T(b_1)\Big(\deg_T(b)+\deg_T(b_1)\Big)\\
&+ \deg_T(b)\deg_T(b_2)\Big(\deg_T(b)+\deg_T(b_2)\Big)\\
&+ \deg_T(c_l)\deg_T(c_{l-1})\Big(\deg_T(c_l)+\deg_T(c_{l-1})\Big)\\
&+ \sum_{i=3}^{\rho} \deg_T(b)\deg_T(b_i)\Big(\deg_T(b)+\deg_T(b_i)\Big)\\
&- \deg_{T_1}(b_1)\deg_{T_1}(c_l)\Big(\deg_{T_1}(b_1)+\deg_{T_1}(c_l)\Big)\\
&- \deg_{T_1}(b)\deg_{T_1}(b_2)\Big(\deg_{T_1}(b)+\deg_{T_1}(b_2)\Big)\\
&- \deg_{T_1}(c_l)\deg_{T_1}(c_{l-1})\Big(\deg_{T_1}(c_l)+\deg_{T_1}(c_{l-1})\Big)\\
&- \sum_{i=3}^{\rho} \deg_{T_1}(b)\deg_{T_1}(b_i)\Big(\deg_{T_1}(b)+\deg_{T_1}(b_i)\Big)\\
=&\rho(\rho+1) + 2\rho(\rho+2) + 6 + \sum_{i=3}^{\rho} \rho\deg_T(b_i)\Big(\rho+\deg_T(b_i)\Big)\\
&- 6 - 16 - 2(\rho-1)(\rho+1)\\
&- (\rho-1)\sum_{i=3}^{\rho} \deg_T(b_i)\Big(\rho+\deg_T(b_i)-1\Big)\\
=&\rho^2 + 5\rho - 14 + \sum_{i=3}^{\rho} \deg_T(b_i)\Big(2\rho+\deg_T(b_i)-1\Big)\\
>&\rho^2 + 5\rho - 14 > 0.
\end{aligned}
$$

Case 3. None of the vertices adjacent to b are leaves.

Let $bc_1c_2\dots c_l$ and $bd_1d_2\dots d_s$, $l, s \geq 2$, 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_sb_1. Since $\rho \geq 3$, then

$$\begin{aligned}
ReZG_3(T) - ReZG_3(T_1) = & \deg_T(b)\deg_T(b_1)\Big(\deg_T(b)+\deg_T(b_1)\Big) \\
& + \deg_T(b)\deg_T(b_2)\Big(\deg_T(b)+\deg_T(b_2)\Big) \\
& + \deg_T(d_s)\deg_T(d_{s-1})\Big(\deg_T(d_s)+\deg_T(d_{s-1})\Big) \\
& + \sum_{i=3}^{\rho}\deg_T(b)\deg_T(b_i)\Big(\deg_T(b)+\deg_T(b_i)\Big) \\
& - \deg_{T_1}(b_1)\deg_{T_1}(d_s)\Big(\deg_{T_1}(b_1)+\deg_{T_1}(d_s)\Big) \\
& - \deg_{T_1}(b)\deg_{T_1}(b_2)\Big(\deg_{T_1}(b)+\deg_{T_1}(b_2)\Big) \\
& - \deg_{T_1}(d_s)\deg_{T_1}(d_{s-1})\Big(\deg_{T_1}(d_s)+\deg_{T_1}(d_{s-1})\Big) \\
& - \sum_{i=3}^{\rho}\deg_{T_1}(b)\deg_{T_1}(b_i)\Big(\deg_{T_1}(b)+\deg_{T_1}(b_i)\Big) \\
= & 4\rho(\rho+2)+6+\sum_{i=3}^{\rho}\rho\deg_T(b_i)\Big(\rho+\deg_T(b_i)\Big) \\
& - 16 - 16 - 2(\rho-1)(\rho+1) \\
& - (\rho-1)\sum_{i=3}^{\rho}\deg_T(b_i)\Big(\rho+\deg_T(b_i)-1\Big) \\
= & 2\rho^2+8\rho-24+\sum_{i=3}^{\rho}\deg_T(b_i)\Big(2\rho+\deg_T(b_i)-1\Big) \\
> & 2\rho^2+8\rho-24>0.
\end{aligned}$$

□

Proposition 1. *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 $ReZG_3(T_1) < ReZG_3(T)$.*

Proof. Assume that a be the center of T and $ab_1b_2\ldots b_t$, $ac_1c_2\ldots c_l$ be two legs of length more than one in T. Let T_1 be the tree deduced from $T-\{b_1b_2\}$ by attaching the path c_lb_2. By definition we have,

$$\begin{aligned}
ReZG_3(T) - ReZG_3(T_1) = & \deg_T(a)\deg_T(b_1)\Big(\deg_T(a)+\deg_T(b_1)\Big) \\
& + \deg_T(b_1)\deg_T(b_2)\Big(\deg_T(b_1)+\deg_T(b_2)\Big) \\
& + \deg_T(c_l)\deg_T(c_{l-1})\Big(\deg_T(c_l)+\deg_T(c_{l-1})\Big) \\
& - \deg_{T_1}(a)\deg_{T_1}(b_1)\Big(\deg_{T_1}(a)+\deg_{T_1}(b_1)\Big) \\
& - \deg_{T_1}(b_2)\deg_{T_1}(c_l)\Big(\deg_{T_1}(b_2)+\deg_{T_1}(c_l)\Big) \\
& - \deg_{T_1}(c_l)\deg_{T_1}(c_{l-1})\Big(\deg_{T_1}(c_l)+\deg_{T_1}(c_{l-1})\Big)
\end{aligned}$$

$$
\begin{aligned}
=&2\Delta(\Delta+2)+2\deg_T(b_2)\Big(\deg_T(b_2)+2\Big)+6\\
&-\Delta(\Delta+1)-2\deg_T(b_2)\Big(\deg_T(b_2)+2\Big)-16\\
=&\Delta^2+3\Delta-10>0.
\end{aligned}
$$

This complete the proof. □

Now we prove the main theorems of this paper.

Theorem 1. *Let $T \in \mathcal{T}(n,\Delta)$. Then $ReZG_3(T) \geq 16n+\Delta^3+2\Delta^2-13\Delta-26$ when $\Delta < n-1$ and $ReZG_3(T) = n\Delta^2+n\Delta-\Delta^2-\Delta$ when $\Delta = n-1$. 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 $ReZG_3(T^*) \leq ReZG_3(T)$ 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 Lemma 1, T^* is a spider with center a and by Proposition 1, T^* has at most one leg of length more than one. If T^* is a star, then $ReZG_3(T^*) = n\Delta^2+n\Delta-\Delta^2-\Delta$. Hence let T^* is not a star and T^* have only one leg of length more than one. Then

$$ReZG_3(T^*) = 16n+\Delta^3+2\Delta^2-13\Delta-26,$$

and the proof is complete. □

By defination of re-defined third Zagreb index, we have the next result.

Lemma 2. *Let Γ be a graph and $e \notin E(\Gamma)$. Then $ReZG_3(\Gamma+e) > ReZG_3(\Gamma)$.*

By Theorem 1 and Lemma 2, we obtain the next theorem.

Theorem 2. *Let Γ be a graph with n vertices and maximum degree Δ. Then*

$$ReZG_3(\Gamma) \geq \begin{cases} 16n+\Delta^3+2\Delta^2-13\Delta-26, & \text{if } \Delta < n-1 \\ n\Delta^2+n\Delta-\Delta^2-\Delta, & \text{if } \Delta = n-1. \end{cases}$$

The equality holds if and only if Γ is a spider with at most one leg of length more than one.

Conflict of interest. The author declares that there is no competing interest related to this paper.

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