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A Unified Approach to Extremal Trees with Respect to Geometric–Arithmetic, Szeged and Edge Szeged Indices *

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Abstract

The second and third geometric-arithmetic indices $GA_2(G)$ and $GA_3(G)$ of a graph G are defined, respectively, as $\sum\limits_{uv\in E(G)} \frac{\sqrt{n_u(e,G)n_v(e,G)}}{\frac{1}{2}[n_u(e,G)+n_v(e,G)]}$ and $\sum\limits_{uv\in E(G)} \frac{\sqrt{m_u(e,G)m_v(e,G)}}{\frac{1}{2}[m_u(e,G)+m_v(e,G)]}$, where $e = uv$ is one edge in G, $n_u(e,G)$ denotes the number of vertices in G lying closer to u than to v and $m_u(e,G)$ denotes the number of edges in G lying closer to u than to v. The Szeged and edge Szeged indices are defined, respectively, as $Sz(G) = \sum\limits_{uv\in E(G)} n_u(e,G)\cdot n_v(e,G)$ and $Sz_e(G) = \sum\limits_{uv\in E(G)} m_u(e,G)\cdot m_v(e,G)$. In this paper, we provide a unified approach to characterize the tree with the minimum and maximum GA_2, GA_3, Sz and Sz_e indices among the set of trees with given order and pendent vertices, respectively. As applications, we deduce a result of [2] concerning tree with the maximum GA_2 index and a result of [3] concerning tree with the maximum GA_3 index.

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1. Introduction

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Recently, a class of geometric-arithmetic topological indices indices were raised [2]

$$GA = GA_{general}(G) = \sum_{uv \in E(G)} \frac{\sqrt{\mathcal{Q}_u \mathcal{Q}_v}}{\frac{1}{2}(\mathcal{Q}_u + \mathcal{Q}_v)}$$

where $\mathcal{Q}_u$ is some quantity that in a unique manner can be associated with the vertex u of the graph G.

The reason why this class of topological indices is called 'geometric-arithmetic index' is that $\sqrt{\mathcal{Q}_u \mathcal{Q}_v}$ and $\mathcal{Q}_u + \mathcal{Q}_v$ are the geometric and arithmetic means, respectively, of the numbers $\mathcal{Q}_u$ and $\mathcal{Q}_v$.

The first member of geometric-arithmetic topological indices was conceived [1] by setting $\mathcal{Q}_u$ to be the degree d_u of the vertex u of the graph G, namely,

$$GA = GA(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} \,.$$

The second member of geometric-arithmetic topological indices, called GA_2 index, was recently studied [2–6] and defined by setting $\mathcal{Q}_u$ to be $n_u(e, G)$, the number of vertices in G lying closer to u than to v in the graph G, namely,

$$GA_2 = GA_2(G) = \sum_{uv \in E(G)} \frac{\sqrt{n_u(e,G) n_v(e,G)}}{\frac{1}{2}[n_u(e,G) + n_v(e,G)]} \tag{1}$$

where $e = uv$ is an edge of G.

The third member of geometric-arithmetic topological indices, called GA_3 index, was recently studied [3] and defined by setting $\mathcal{Q}_u$ to be $m_u(e, G)$, the number of edges in G lying closer to u than to v in the graph G, namely,

$$GA_3 = GA_3(G) = \sum_{uv \in E(G)} \frac{\sqrt{m_u(e,G) m_v(e,G)}}{\frac{1}{2}[m_u(e,G) + m_v(e,G)]} \tag{2}$$

where $e = uv$ is an edge of G.

The other two previously established molecular structure descriptors are, respectively, the *Szeged index* [7–12]), defined as

$$Sz(G) = \sum_{uv \in E(G)} n_u(e,G) \cdot n_v(e,G) \tag{3}$$

and the *edge Szeged index* [13–17], defined as

$$Sz_e(G) = \sum_{uv\in E(G)} m_u(e,G)\cdot m_v(e,G)\ . \tag{4}$$

More recently, Fath-Tabar et al. [2] obtained various lower and upper bounds of GA_2 index for a connected graph in terms of $Sz(G)$ and Zhou et al. [3] obtained various lower and upper bounds of GA_3 index for a connected graph in terms of $Sz_e(G)$. In particular, they proved [2, 3] that the $n-$vertex path is the unique tree with the maximum GA_2 and GA_3 indices and the $n-$vertex star is the unique tree with the minimum GA_2 and GA_3 indices, respectively. Other papers concerning GA indices can be found in [4–6].

In this paper, we shall provide a unified approach to characterize the tree with the minimum and maximum GA_2, GA_3, Sz and Sz_e indices among the set of trees with given order and pendent vertices, respectively. As applications, we obtain a result of [2] concerning tree with the maximum GA_2 index and a result of [3] concerning tree with the maximum GA_3 index.

For any edge $e = uv$ in a tree T of n vertices, we always have $n_u(e,T)+n_v(e,T) = n$, $m_u(e,T)+m_v(e,T) = n-2$, $m_u(e,T) = n_u(e,T)-1$ and $m_v(e,T) = n_v(e,T)-1$. In particular, if $e = uv$ is a pendent edge with pendent vertex u, then $m_u(e,T) = 0$. So, for a $n-$vertex tree T, Eqs. (1) and (2) are simplified as

$$GA_2 = GA_2(T) = \sum_{uv\in E(T)} \frac{2}{n}\sqrt{n_u(e,T)n_v(e,T)} \tag{5}$$

$$GA_3 = GA_3(T) = \sum_{uv\in E(T)} \frac{2}{n-2}\sqrt{m_u(e,T)\,m_v(e,T)} \tag{6}$$

respectively.

Thus, the above Eq. s (3)–(6) provide us a unified way of comparing the GA_2, GA_3, Sz and Sz_e indices of two trees of the same order.

Given two trees T_1, T_2 of n vertices. Let f be a one to one map from $E(T_1)$ to $E(T_2)$ such that for any $e_i = u_iv_i$ in T_1, there exists a unique edge $e_i^{'} = u_i^{'}v_i^{'}$ in T_2 corresponding to it. Under the map f, e_i and its image $e_i^{'}$ constitute an edge pair $\{e_i,\ e_i^{'}\}$. Then $\{\{e_1,\ e_1^{'}\},\ \{e_2,\ e_2^{'}\},\ \cdots,\ \{e_{n-1},\ e_{n-1}^{'}\}\}$ is called to be an edge partition of $E(T_1)$ and $E(T_2)$. By the definition of edge partition, there exists $(n-1)!$ edge partition of $E(T_1)$ and $E(T_2)$. If there exists an edge partition of $E(T_1)$ and $E(T_2)$ such that $n_{u_i}(e_i,T_1)\cdot n_{v_i}(e_i,T_1) \geq n_{u_i^{'}}(e_i^{'},T_2)\cdot n_{v_i^{'}}(e_i^{'},T_2)(i = 1,\ \cdots,\ n-1)$, and there exists an edge pair $\{e_j, e_j^{'}\}$ such that

$n_{u_j}(e_j, T_1) \cdot n_{v_j}(e_j, T_1) > n_{u'_j}(e'_j, T_2) \cdot n_{v'_j}(e'_j, T_2)$, then $GA_2(T_1) > GA_2(T_2)$. Similarly, we have $GA_3(T_1) > GA_3(T_2)$, $Sz(T_1) > Sz(T_2)$, $Sz_e(T_1) > Sz_e(T_2)$.

2. Main results

Let $d_u(T)$, or simply d_u, denote the degree of the vertex u in a tree T. If $d_u(T) \geq 3$, then u is said to be a *branch vertex*, and if $d_u(T) = 1$, then u is said to be a *pendent vertex*. An internal path $P = v_1 v_2 \cdots v_t (t \geq 2)$ in a tree T is said to be a *pendent path starting with* v_1, or simply, *pendent path*, if $d_{v_1}(T) \geq 3$, $d_{v_t}(T) = 1$ and $d_{v_i}(T) = 2 (1 < i < t)$. In particular, if $t = 2$, then P is said to be a *pendent edge*.

If a tree T has exactly one branch vertex, say u, with $d_u(T) = k$, then we call T a *star-like tree*. A *double star tree* $S_{a,b}$ is defined to be the tree obtained from the path P_2 by attaching to its two end-vertices a and b pendent edges, respectively. If we insert new vertices into pendent edges of a double star $S_{a,b}$, we obtain the so-called *double star-like tree*, and if we insert new vertices into edges of a double star $S_{a,b}$, we obtain the so-called *generalized double star-like tree*.

Denote by $GDSL(n; a, b)$ a special generalized double star-like tree obtained from the path P_{n-a-b} by attaching to its two end-vertices a and b pendent edges, respectively.

Let $\mathcal{B}(T)$ and $\mathcal{P}(T)$ denote the number of branch vertices and pendent vertices in a tree T, respectively. Denote by $\mathcal{T}_{n,k}$ the set of trees of with n vertices and k pendent vertices.

In the following, we will always use $n(T_x)$ to denote the number of vertices in a subtree T_x rooted at x of T.

Our starting point is a simple, but useful elementary result.

Lemma 1. *Let x_i, y_i be positive integers satisfying $x_i + y_i = n$. If $|x_k - y_k| > |x_j - y_j|$, then $x_k y_k < x_j y_j$.*

Next, we shall give some graph transformations that decrease or increase the GA_2, GA_3, Sz and Sz_e indices of graphs under consideration.

Lemma 2. *Let T^1, T^2 and T^3 be trees shown as in Fig. 1. Then*

(a) $GA_2(T^1) > GA_2(T^2)$ *or* $GA_2(T^1) > GA_2(T^3)$

(b) $GA_3(T^1) > GA_3(T^2)$ *or* $GA_3(T^1) > GA_3(T^3)$

(c) $Sz(T^1) > Sz(T^2)$ *or* $Sz(T^1) > Sz(T^3)$

(d) $Sz_e(T^1) > Sz_e(T^2)$ *or* $Sz_e(T^1) > Sz_e(T^3)$

where $n(T_i) \geq 2 (i = 1, 2)$, T_l(resp., T_r) may be a single vertex x(resp., y).

Proof. Here, we only check the validity of (a). It is not difficult to see from Fig. 1 that $\mathcal{P}(T^1) = \mathcal{P}(T^2) = \mathcal{P}(T^3)$.

First, we assume that $n(T_1) + n(T_l) \geq n(T_2) + n(T_r)$. We consider the graph transformation I: $T^1 \longrightarrow T^3$. For one edge $e = zw$ in $E(T_1) \cup E(T_2) \cup E(T_l) \cup E(T_r) \cup \{ux, vy\}$, we clearly have $n_z(e, T^1) \cdot n_w(e, T^1) = n_z(e, T^3) \cdot n_w(e, T^3)$. For the edge $e = uv$, we have $n_u(e, T^1) \cdot n_v(e, T^1) = [n(T_1) + n(T_l)] \cdot [n(T_2) + n(T_r)]$ and $n_u(e, T^3) \cdot n_v(e, T^3) = [n(T_1)+n(T_l)+n(T_2)-1] \cdot [1+n(T_r)]$. By Lemma 1 and the assumption that $n(T_1)+n(T_l) \geq n(T_2) + n(T_r)$, we have $GA_2(T^1) > GA_2(T^3)$.

Similarly, if $n(T_1) + n(T_l) < n(T_2) + n(T_r)$, we consider the graph transformation I: $T^1 \longrightarrow T^2$, and we obtain $GA_2(T^1) > GA_2(T^2)$.

This completes the proof. □

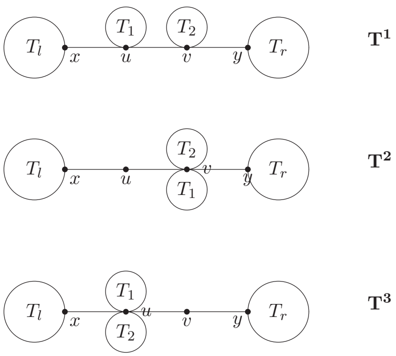

Fig. 1. Graph transformation I: $T^1 \longrightarrow T^2$ or $T^1 \longrightarrow T^3$ that decreases the value of $GA_2(T^1)$.

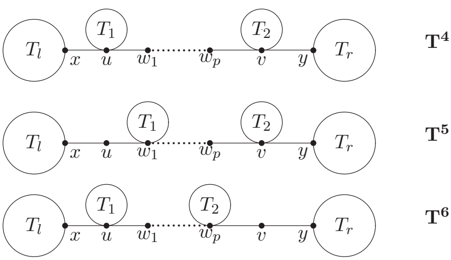

Fig. 2. Graph transformation II: $T^4 \longrightarrow T^5$ or $T^4 \longrightarrow T^6$ that decreases the value of $GA_2(T^4)$.

Lemma 3. *Let T^4, T^5 and T^6 be trees shown as in Fig. 2. Then*

(*a*) $GA_2(T^4) > GA_2(T^5)$ *or* $GA_2(T^4) > GA_2(T^6)$

(*b*) $GA_3(T^4) > GA_3(T^5)$ *or* $GA_3(T^4) > GA_3(T^6)$

(*c*) $Sz(T^4) > Sz(T^5)$ *or* $Sz(T^4) > Sz(T^6)$

(*d*) $Sz_e(T^4) > Sz_e(T^5)$ *or* $Sz_e(T^4) > Sz_e(T^6)$

where $p \geq 1$, $n(T_j) \geq 2(j = 1, 2)$, *and* T_l(*resp.*, T_r) *may be a single vertex* x *(resp.,* y*).*

Proof. We only consider the GA_2 index here. It can be seen from Fig. 2 that $\mathcal{P}(T^4) = \mathcal{P}(T^5) = \mathcal{P}(T^6)$.

If $n(T_l)+n(T_1) < p+n(T_2)+n(T_r)$, we consider the graph transformation II: $T^4 \longrightarrow T^5$. Obviously, for any edge $e = x_1x_2$ in $E(T_1) \cup E(T_2) \cup E(T_l) \cup E(T_r) \cup \{xu,\ w_1w_2, \ldots, w_{p-1}w_p,\ w_pv,\ vy\}$, we have $n_{x_1}(e, T^4) \cdot n_{x_2}(e, T^4) = n_{x_1}(e, T^5) \cdot n_{x_2}(e, T^5)$. For the edge uw_1, $n_u(e, T^4) \cdot n_{w_1}(e, T^4) = [n(T_l) + n(T_1)] \cdot [p + n(T_2) + n(T_r)] > [n(T_l) + 1] \cdot [p - 1 + n(T_1) + n(T_2) + n(T_r)] = n_u(e, T^5) \cdot n_{w_1}(e, T^5)$ by Lemma 1. So we have $GA_2(T^4) > GA_2(T^5)$.

If $n(T_l) + n(T_1) \geq p + n(T_2) + n(T_r)$, then $n(T_l) + n(T_1) + p > n(T_2) + n(T_r)$. We consider the graph transformation II: $T^4 \longrightarrow T^6$. By the same reasoning as above, we obtain $GA_2(T^4) > GA_2(T^6)$.

This completes the proof. □

The following theorem shall determine the unique tree with the minimum GA_2, GA_3, Sz and Sz_e indices within all trees in $\mathcal{T}_{n,k}$.

Theorem 1. *Among all trees in* $\mathcal{T}_{n,k}$, $2 \leq k \leq n-1$, *the unique tree with the minimum* GA_2, GA_3, Sz *and* Sz_e *indices is a star-like tree, in which the length of all pendent paths are almost equal.*

Proof. We only consider the GA_2 index here.

If $k = n - 1$ or $k = 2$, then $T \cong S_n$ or P_n, the theorem is obvious. So we may suppose that $3 \leq k \leq n - 2$. Thus T has at least one branch vertex.

Let T be a tree chosen in $\mathcal{T}_{n,k}$ such that $GA_2(T)$ attains the minimum value. By Lemmas 2 and 3, we claim that T has exactly one branch vertex, that is, T is a star-like tree with k pendent vertices. Suppose, to the contrary that, T has $t(\geq 2)$ branch vertices.

Let $\mathbb{P}$ be a path in T with two pendent vertices of T being its two ends such that there exist two branch vertices u and v along $\mathbb{P}$. Obviously, such a path $\mathbb{P}$ does exist.

If u is adjacent to v, then we can view T the graph T^1 shown as in Fig. 1. Then we can employ the graph transformation I on T, and we shall obtain a new tree $\overline{T} \in \mathcal{T}_{n,k}$ with $GA_2(T) > GA_2(\overline{T})$, a contradiction to our choice of T.

Suppose now that u is not adjacent to v, and that no other branch vertices lying along the $u - v$ path. If it is not so, then we can choose new branch vertices u and v satisfying the above requirement. Denote the $u - v$ path as $uw_1 \cdots w_p v (p \geq 1)$. Now, T can be viewed the graph T^4 shown as in Fig. 2. So, we can employ the graph transformation II on T, and we shall obtain a new tree $\widehat{T} \in \mathcal{T}_{n,k}$ with $GA_2(T) > GA_2(\widehat{T})$, a contradiction once again.

From above arguments, we know that T has exactly one branch vertex, namely, T is a star-like tree. We further claim that the length of all pendent paths in T are almost equal.

Suppose, to the contrary, that there are two pendent paths in T of length x and y such that $x - y \geq 2$. Now, let $x = a + 1$ and $y = b - 1$. Then T can be viewed the graph $T_{a+1,b-1}$ shown as in Fig. 3. Now, we employ the reverse graph transformation III: $T_{a+1,b-1} \longrightarrow T_{a,b}$ on T, and we obtain a new graph $\widetilde{T} \in \mathcal{T}_{n,k}$ with $GA_2(T) > GA_2(\widetilde{T})$, a contradiction.

This contradiction leads to our desired result. □

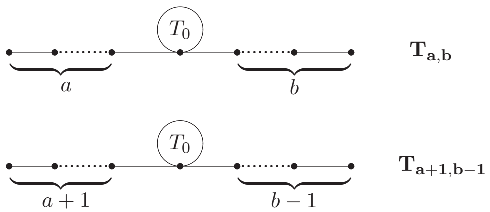

Fig. 3. Graph transformation III: $T_{a,b} \longrightarrow T_{a+1,b-1}$ that increases the value of $GA_2(T_{a,b})$ for $a \geq b \geq 1$.

Fath-Tabar et al. [2] prove that (a) in Lemma 4 holds. In fact, we can deduce $(b) - (d)$ by the same way.

Lemma 4. *Let $T_{a,b}$ and $T_{a+1,b-1}$ be trees shown as in Fig. 3. If $a \geq b \geq 1$, then*

(a) ([2]) $GA_2(T_{a+1,b-1}) > GA_2(T_{a,b})$

(b) $GA_3(T_{a+1,b-1}) > GA_3(T_{a,b})$

(c) $Sz(T_{a+1,b-1}) > Sz(T_{a,b})$

(d) $Sz_e(T_{a+1,b-1}) > Sz_e(T_{a,b})$

where $n(T_0) \geq 2$.

Now, we generalize the above graph transformation III to a more general form, that is, the following transformation III$'$, shown as in Fig. 4.

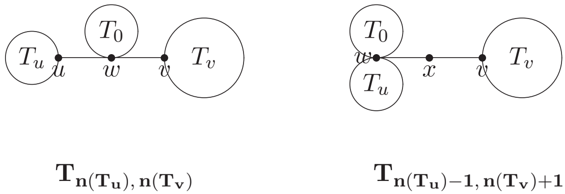

Fig. 4. Graph transformation III$'$: $T_{n(T_u),\,n(T_v)} \longrightarrow T_{n(T_u)-1,\,n(T_v)+1}$ that increases the value of $GA_2(T_{n(T_u),\,n(T_v)})$ for $n(T_v) \geq n(T_u) \geq 1$.

Lemma 5. *Let* $T_{n(T_u),\,n(T_v)}$ *and* $T_{n(T_u)-1,\,n(T_v)+1}$ *be trees shown as in Fig. 4. If* $n(T_v) \geq n(T_u) \geq 1$, *then*

(a) $GA_2(T_{n(T_u)-1,\,n(T_v)+1}) > GA_2(T_{n(T_u),\,n(T_v)})$

(b) $GA_3(T_{n(T_u)-1,\,n(T_v)+1}) > GA_3(T_{n(T_u),\,n(T_v)})$

(c) $Sz(T_{n(T_u)-1,\,n(T_v)+1}) > Sz(T_{n(T_u),\,n(T_v)})$

(d) $Sz_e(T_{n(T_u)-1,\,n(T_v)+1}) > Sz_e(T_{n(T_u),\,n(T_v)})$

where $n(T_0) \geq 2$.

Proof. We only prove that the statement (a) is true. Obviously, for any edge $e = x_1x_2$ in $E(T_0) \cup E(T_u) \cup E(T_v) \cup \{xv\}$, we have

$$n_{x_1}(e, T_{n(T_u)-1,\,n(T_v)+1}) \cdot n_{x_2}(e, T_{n(T_u)-1,\,n(T_v)+1}) = n_{x_1}(e, T_{n(T_u),\,n(T_v)}) \cdot n_{x_2}(e, T_{n(T_u),\,n(T_v)}).$$

For the edge $e_1 = xw$ in $T_{n(T_u)-1,\,n(T_v)+1}$ and $e_2 = uw$ in $T_{n(T_u),\,n(T_v)}$, we have

$n_x(e, T_{n(T_u)-1,\,n(T_v)+1}) \cdot n_w(e, T_{n(T_u)-1,\,n(T_v)+1}) = [n(T_v)+1)] \cdot [n(T_0)+n(T_u)-1] > n(T_u) \cdot [n(T_v) + n(T_0)]$(by Lemma 1) $= n_u(e_2, T_{n(T_u),\,n(T_v)}) \cdot n_w(e_2, T_{n(T_u),\,n(T_v)})$.

So we have $GA_2(T_{n(T_u)-1,\,n(T_v)+1}) > GA_2(T_{n(T_u),\,n(T_v)})$, completing the proof. □

Remark 1. In order to keep the statement of Lemmas 4 and 5 valid, we need only to set $a \geq b \geq 1$ and $n(T_v) \geq n(T_u) \geq 1$. But, we should note that all trees under consideration must be members of $\mathcal{T}_{n,k}$ according to the study goal of this paper. So, in order to keep the number of pendent vertices unchanged through graph transformation III or III$'$, we actually require that $a \geq b \geq 2$ and $n(T_v) \geq n(T_u) \geq 2$ in the following proof of Theorem 2.

Lemma 6. *Let a and b be positive integers with $a \geq b+2$. Then*

(a) $GA_2(GDSL(n; a-1, b+1)) > GA_2(GDSL(n; a, b))$

(b) $GA_3(GDSL(n; a-1, b+1)) > GA_3(GDSL(n; a, b))$

(c) $Sz(GDSL(n; a-1, b+1)) > Sz(GDSL(n; a, b))$

(d) $Sz_e(GDSL(n; a-1, b+1)) > Sz_e(GDSL(n; a, b))$

Proof. We only prove that the statement (a) is true.

Since $a \geq b+2$, then $GDSL(n; a-1, b+1) \ncong GDSL(n; a, b)$. Suppose that u and v are two branch vertices in $GA_2(GDSL(n; a, b))$ with $d_u(T) = a, d_v(T) = b$. Let pendent vertices adjacent to u be $u_1, \cdots, u_a$, and the internal vertex adjacent to u be w. Let pendent vertices adjacent to v be $v_1, \cdots, v_b$, and the internal vertex adjacent to v be z.

Firstly, we delete the edge uu_1 and insert u_1 to the edge uw, we obtain a new tree, denoted by $\tilde{T}$. Secondly, we contract the edge vz in $\tilde{T}$ and add one additional pendent edge vz, then we obtain the tree $GA_2(GDSL(n; a-1, b+1))$.

During the first step: $GDSL(n; a, b) \longrightarrow \tilde{T}$, the value of $n_x(e) \cdot n_y(e)$ remains unchanged except for the edge $e = uu_1$.

Thus,

$$\begin{aligned} GA_2(\tilde{T}) - GA_2(GDSL(n; a, b)) &= n_u(uu_1, \tilde{T}) \cdot n_{u_1}(uu_1, \tilde{T}) \\ &- n_u(uu_1, GDSL(n; a, b)) \cdot n_{u_1}(uu_1, GDSL(n; a, b)) \\ &= a \cdot (n-a) - 1 \cdot (n-1) \end{aligned}$$

During the second step: $\tilde{T} \longrightarrow GDSL(n; a-1, b+1)$, the value of $n_x(e) \cdot n_y(e)$ remains unchanged except for the edge $e = vz$.

Thus, $GA_2(GDSL(n; a-1, b+1)) - GA_2(\tilde{T}) = n_v(vz, GDSL(n; a-1, b+1)) \cdot n_z(vz, GDSL(n; a-1, b+1)) - n_v(vz, \tilde{T}) \cdot n_z(vz, \tilde{T}) = 1 \cdot (n-1) - (b+1) \cdot (n-b-1)$.

So, $GA_2(GDSL(n; a-1, b+1)) - GA_2(GDSL(n; a, b)) = a \cdot (n-a) - (b+1) \cdot (n-b-1)$.

Obviously, $n-b-1 > b+1$, since $n \geq a+b+2$ and $a-b \geq 2$.

If $a \geq n-a$, then $a-(n-a) = 2a-n < n-2b-2 = (n-b-1)-(b+1)$. Thus, by Lemma 1, $GA_2(GDSL(n; a-1, b+1)) - GA_2(GDSL(n; a, b)) = a \cdot (n-a) - (b+1) \cdot (n-b-1) > 0$.

Suppose now that $a < n-a$. Then $(n-a)-a = n-2a < n-2b-2 = (n-b-1)-(b+1)$, since $a \geq b+2$. So, $GA_2(GDSL(n; a-1, b+1)) - GA_2(GDSL(n; a, b)) = a \cdot (n-a) - (b+1) \cdot (n-b-1) > 0$.

This completes the proof. □

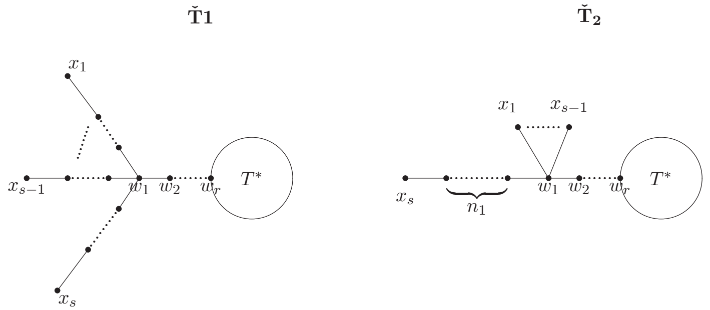

Fig. 5. The graphs occurred in the proof of Theorem 2, where $s \geq 2$, $d_{w_r}(\check{T}_i) \geq 3 (i = 1, 2)$, n_1 is equal to the total number of vertices in all $w_1 - x_j (j = 1, \cdots, s)$ paths, not including pendent vertices $x_1, \cdots, x_s$, and there exists at least two pendent paths of length ≥ 2 starting with w_1.

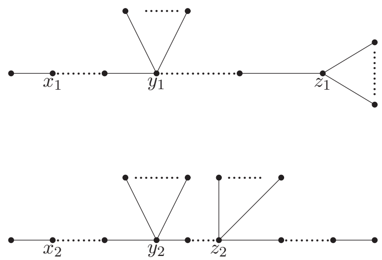

Fig. 6. The graphs occurred in the proof of Theorem 2.

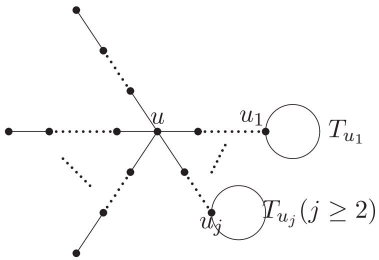

Fig. 7. The graph occurred in the proof of Theorem 2, where u is the branch vertex, $d_{u_i} \geq 3$, $j \geq 2$, and $u_i(i = 1, \cdots, j)$ is the branch vertex nearest to u among branch vertices in component containing u_i of $T - \{u\}$.

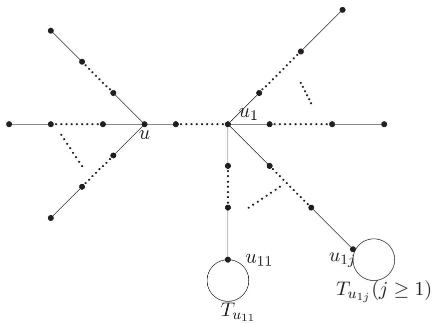

Fig. 8. The graph occurred in the proof of Theorem 2, where u and u_1 are branch vertices, $u_{1i}(i = 1, \cdots, j)$ is the branch vertex nearest to u_1 among branch vertices in component containing u_{1i} of $T - \{u_1\}$.

The following theorem shall determine the unique tree with the maximum GA_2, GA_3, Sz and Sz_e indices within all trees in $\mathcal{T}_{n,k}$.

Theorem 2. *Among all trees in $\mathcal{T}_{n,k}$, $2 \leq k \leq n-1$, the tree with the maximum GA_2, GA_3, Sz and Sz_e indices is $GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor)$ or S_n, the star graph of n vertices.*

Proof. We need only to check the validity of theorem for the GA_2 index.

If $k = 2$ or $n - 1$, the result is obvious. Suppose now that $3 \leq k \leq n - 2$. So, T has at least one branch vertex, that is, $\mathcal{B}(T) \geq 1$.

Let T be a tree chosen in $\mathcal{T}_{n,k}$ such that it has the maximum GA_2 index. Next, we shall prove that $T \cong GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor)$.

If $\mathcal{B}(T) = 1$, then T is a star-like tree. If $T \ncong GDSL(n;1,k-1)$, then we can apply graph transformation III on T many times to obtain $GDSL(n;1,k-1)$. But then, $GA_2(T) < GA_2(GDSL(n;1,k-1))$ by Lemma 4, a contradiction to the choice of T. So $T \cong GDSL(n;1,k-1)$. If $k \geq 4$, then by Lemma 6, we have $GA_2(T) = GA_2(GDSL(n;1,k-1)) < GA_2(GDSL(n;2,k-2))$, a contradiction to the choice of T. So, we have $k = 3$, and the result holds readily.

Now, suppose that $\mathcal{B}(T) \geq 2$, and we shall prove the theorem by induction on $\mathcal{B}(T)$.

First, we check the validity of the statement of theorem for $\mathcal{B}(T) = 2$. In this case, T is a generalized double star-like tree.

If T has two pendent paths of length ≥ 2 pasting to the same branch vertex, then it can be viewed the tree $\check{T}_1$, shown as in Fig. 5. Now, we can repeatedly use graph transformation III on it, and in the end, we obtain $\check{T}_2$, shown as in Fig. 5. By Lemma 5, we have $GA_2(\check{T}_2) > GA_2(\check{T}_1) = GA_2(T)$, contradicting the choice of T.

So, T has at most one pendent path of length ≥ 2 pasting to each of two branch vertices. Now, T must be isomorphic to one of the two graphs shown as in Fig. 6 and $GDSL(n;a,b)(a+b=k)$, since $\mathcal{B}(T) = 2$.

If T is isomorphic to the first graph in Fig. 6, then we can repeatedly use graph transformation III$'$ on it until we get $x_1 = y_1$ or $z_1 = y_1$. If T is isomorphic to the second graph in Fig. 6, then we can repeatedly use graph transformation III$'$ on it until we get $x_2 = y_2$ or $z_2 = y_2$. In either case, by Lemma 5, we shall get a new tree with greater GA_2 index than that of T, a contradiction. So we have $T \cong GDSL(n;a,b)(a+b=k)$.

If $T \ncong GDSL(n;\lceil k/2\rceil,\lfloor k/2\rfloor)$, then $|a-b| \geq 2$. Suppose, without loss of generality, that $a - b \geq 2$. It then follows from Lemma 6 that $GA_2(GDSL(n;a-1,b+1)) > GA_2(GDSL(n;a,b)) = GA_2(T)$, a contradiction once again.

So, we have $T \cong GDSL(n;\lceil k/2\rceil,\lfloor k/2\rfloor)$ for the case of $\mathcal{B}(T) = 2$.

Suppose now that $\mathcal{B}(T) \geq 3$ and the theorem is true for smaller values of $\mathcal{B}(T)$.

Now, T must be a tree shown as in Fig. 7 or Fig. 8. If T is a tree shown as in Fig. 7, then we can repeatedly use graph transformation III$'$ on it until $u_1 = u$ or $u_j = u$. If T is a tree shown as in Fig. 8, then we may assume that $d_{u_{11}} \geq 3$ and repeatedly use graph transformation III$'$ on it until $u = u_1$ or $u_{11} = u_1$.

In either case, we finally get a new tree $\vec{T} \in \mathcal{T}_{n,k}$ with $\mathcal{B}(\vec{T}) = \mathcal{B}(T) - 1$, $GA_2(T) <$

$GA_2(\vec{T})$ by Lemma 5. By induction assumption, we have

$$GA_2(\vec{T}) < GA_2\left(GDSL\left(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor\right)\right) \ .$$

So,

$$GA_2(T) < GA_2(GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor))$$

a contradiction.

Thus, the desired result follows as expected. □

By the same reasoning as that used in the proof of Lemma 6, we can obtain

Lemma 7. *For $3 \leq k \leq n-2$, we have*

(*a*) $GA_2(GDSL(n; \lceil (k-1)/2 \rceil, \lfloor (k-1)/2 \rfloor)) > GA_2(GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor))$

(*b*) $GA_3(GDSL(n; \lceil (k-1)/2 \rceil, \lfloor (k-1)/2 \rfloor)) > GA_3(GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor))$

(*c*) $Sz(GDSL(n; \lceil (k-1)/2 \rceil, \lfloor (k-1)/2 \rfloor)) > Sz(GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor))$

(*d*) $Sz_e(GDSL(n; \lceil (k-1)/2 \rceil, \lfloor (k-1)/2 \rfloor)) > Sz_e(GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor))$.

For any tree T in $\mathcal{T}_{n,k}$ with $3 \leq k \leq n-2$, if $T \ncong GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor)$, then $GA_2(T) < GA_2(GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor)$ by Theorem 2. Also, by Lemma 7, we have

$$GA_2(GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor)) < GA_2(GDSL(n; \lceil (k-1)/2 \rceil, \lfloor (k-1)/2 \rfloor)) \ .$$

Thus,

$$\begin{aligned} GA_2(T) &< GA_2(GDSL(n; \lceil k/2 \rceil, \lfloor k/2 \rfloor)) < GA_2(GDSL(n; \lceil (k-1)/2 \rceil, \lfloor (k-1)/2 \rfloor)) \\ &< \cdots < GA_2(GDSL(n; \lceil (3-1)/2 \rceil, \lfloor (3-1)/2 \rfloor)) \ . \end{aligned}$$

Note that $GDSL(n; \lceil (3-1)/2 \rceil, \lfloor (3-1)/2 \rfloor)$ is just the $n-$vertex path P_n. So, we have the following consequence.

Corollary 2([2, 3]). *Among all trees with n vertices, the path P_n has the maximum GA_2, GA_3, Sz and Sz_e indices.*

Remark 2. In [2], Fath-Tabar et al. obtained that the path P_n is the unique tree with maximum GA_2 index and in [3], Zhou et al. proved that the path P_n has the maximum GA_3 index within all trees of n vertices.

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