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Trees with Given Diameter and Minimum Second Geometric–Arithmetic Index*

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Abstract

The second geometric-arithmetic index $GA_2(G)$ of a graph G was introduced recently by Fath-Tabar et al. [2] and is defined to be $\sum\limits_{uv\in E(G)} \frac{\sqrt{n_u(e,G)n_v(e,G)}}{\frac{1}{2}[n_u(e,G)+n_v(e,G)]}$, where $e = uv$ is one edge in G, and $n_u(e,G)$ denotes the number of vertices in G lying closer to u than to v. In this paper, we characterize the tree with the minimum GA_2 index among the set of trees with given order and diameter. As applications, we deduce the trees with the minimum and second-minimum GA_2 index among the set of trees of given order, respectively. In addition, all the trees minimizing the GA_2 index have been shown to have minimum Szeged index and Wiener index, which deduced a result of [7] concerning the Wiener index of trees with given diameter.

1. Introduction

The geometric-arithmetic index GA was conceived [1], defined as

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

where uv is an edge of the graph G, d_u stands for the degree of the vertex u, and the summation goes over all edges of G.

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More recently, another geometric-arithmetic index, which we called GA_2 index, was studied [2] and defined as

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

where $e = uv$ is an edge of the graph G, $n_u(e,G)$ is equal to the number of vertices in G lying closer to u than to v, and the summation goes over all edges of G.

The other two structure descriptors, based on the numbers $n_u(e,G)$ and $n_v(e,G)$, are the so-called *Szeged index* [5, 6], defined as

$$Sz(G) = \sum_{uv \in E(G)} n_u(e,G) \cdot n_v(e,G) \tag{2}$$

and the *vertex PI index* [5, 6], defined as

$$PI_v(G) = \sum_{uv \in E(G)} [n_u(e,G) + n_v(e,G)].$$

Numerical examples and discussion [2] have shown that GA and GA_2 will both be simultaneously applicable in QSPR and QSAR studies. So it make sense for scholars to further investigate these two indices in mathematical chemistry.

Fath-Tabar et al. [2] proposed the GA_2 index and obtained various lower and upper bounds of this index for a connected graph in terms of $PI_v(G)$ or $Sz(G)$. In particular, they determined the $n-$vertex trees with the maximum and minimum GA_2 index, respectively. We encourage the reader to consult [3] and [4], for more information on these two newly defined GA indices.

Note that for any edge $e = uv$ in a tree T, we always have $n_u(e,T) + n_v(e,T) = n$. Thus, for a $n-$vertex tree T, Eq. (1) is simplified as

$$GA_2 = GA_2(T) = \sum_{uv \in E(G)} \frac{2}{n}\sqrt{n_u(e,T)n_v(e,T)}. \tag{3}$$

In this paper, we characterize the tree with the minimum GA_2 index among the set of trees with given order and diameter. As applications, we deduce the trees with the minimum and second-minimum GA_2 index among the set of trees of given order, respectively. In addition, all the trees minimizing the GA_2 index have been shown to have minimum Szeged index and Wiener index, which deduced a result of [7] concerning the Wiener index of trees with given diameter.

2. Main results

A vertex in a tree T is said to be a *branch vertex*, if the degree of this vertex is greater than or equal to 3. The *diameter* of a graph G, denoted by $diam(G)$, is the largest distance between any two vertices in G. Since the diameter of any tree T is not less than 2 and the star S_n is the unique tree with $diam(T) = 2$, we assume that $diam(T) \geq 3$ for any tree T in our following discussions. Denote by $\mathcal{T}_{n,d}$ the set of trees of with n vertices and diameter d.

We first give some graph transformations that decrease the GA_2 index of graphs under consideration.

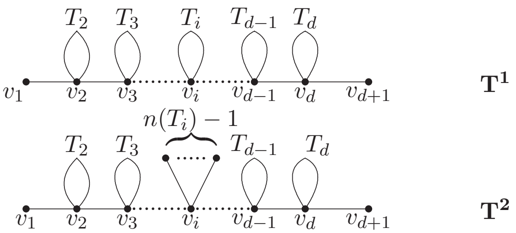

Fig. 1. Graph transformation I: $T^1 \longrightarrow T^2$ that decreases the value of $GA_2(T^1)$.

Lemma 1. *Let T^1 and T^2 be trees shown as in Fig. 1 with $P_{d+1} = v_1 \cdots v_{d+1}$ being diametrical path in both T^1 and T^2. If T_i in T^1 is not isomorphic to a star centered at v_i, then $GA_2(T^1) > GA_2(T^2)$, where T_i is a subtree of T^1 rooted at v_i and $n(T_i)(\geq 3)$ is the number of vertices in T_i.*

Proof. According to Eq.(2), we need only to consider the term $\sqrt{n_u(e) \cdot n_v(e)}$. Consider trees T^1 and T^2. For any edge $e = uv$ not in T_i, we clearly have $n_u(e,T^1) \cdot n_v(e,T^1) = n_u(e,T^2) \cdot n_v(e,T^2)$. Also, for one pendent edge $e = uv$ in any graph G, we have $n_u(e,G) \cdot n_v(e,G) = 1 \times (n-1) = n-1$ attains the minimum value of $n_u(e,G) \cdot n_v(e,G)$. So

$$\begin{aligned}
GA_2(T^1) &= \sum_{e=uv \in E(T^1)} \sqrt{n_u(e,T^1) \cdot n_v(e,T^1)} \\
&= \sum_{e=uv \in E(T_i)} \sqrt{n_u(e,T^1) \cdot n_v(e,T^1)} + \sum_{e=uv \notin E(T_i)} \sqrt{n_u(e,T^1) \cdot n_v(e,T^1)} \\
&> \sum_{e=uv \in E(T_i)} \sqrt{n_u(e,T^2) \cdot n_v(e,T^2)} + \sum_{e=uv \notin E(T_i)} \sqrt{n_u(e,T^2) \cdot n_v(e,T^2)} \\
&= GA_2(T^2).
\end{aligned}$$

This completes the proof. □

Remark 1. Noth that both T^1 and T^2 have $P_{d+1} = v_1 \cdots v_{d+1}$ as a diametrical path. Since all trees we considered in this paper come from $\mathcal{T}_{n,d}$, the graph transformation I: $T^1 \longrightarrow T^2$ that did not change the diameter of T^1 is valid to our proof of main result. So, we have either $n(T_2) = 1(resp., n(T_d))$ or $T_2(resp., n(T_d))$ is a star centered at $v_2(resp., v_d)$.

A simple but useful elementary result is given as follows.

Lemma 2. *Let x_i, y_i be positive integers satisfying $x_i + y_i = n$. If $|x_k - y_k| > |x_j - y_j|$, then $x_k y_k < x_j y_j$.*

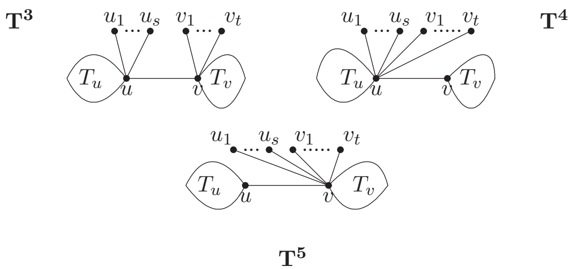

Fig. 2. Graph transformation II: $T^3 \longrightarrow T^4$ or $T^3 \longrightarrow T^5$ that decreases the value of $GA_2(T^3)$.

In the following, we will always use $n(T)$ to denote the number of vertices in a tree T.

Lemma 3. *Let T^3, T^4 and T^5 be trees shown as in Fig. 2. Then $GA_2(T^3) > GA_2(T^4)$ or $GA_2(T^3) > GA_2(T^5)$, where $s, t \geq 1$, and $T_u(resp., T_v)$ may be a single vertex $u(resp., v)$.*

Proof. It is not difficult to see from Fig. 2 that $diam(T^3) = diam(T^4) = diam(T^5)$. First, we assume that $n(T_u) + s \geq n(T_v) + t$. We consider the graph transformation II: $T^3 \longrightarrow T^4$. For one edge $e = xy$ in $E(T_u) \cup E(T_v)$, we clearly have $n_x(e, T^3) \cdot n_y(e, T^3) = n_x(e, T^4) \cdot n_y(e, T^4)$. Also, for any pendent edge $e = uu_i$ or $vv_j(uv_j)$, we have $n_u(e, T^3) \cdot n_{u_i}(e, T^3) = n_u(e, T^4) \cdot n_{u_i}(e, T^4) = n_v(e, T^3) \cdot n_{v_j}(e, T^3) = n_u(e, T^4) \cdot n_{v_j}(e, T^4) = 1 \times (n-1) = n-1$. For the edge $e = uv$, we have $n_u(e, T^3) \cdot n_v(e, T^3) = (n(T_u)+s) \cdot (n(T_v)+t)$ and $n_u(e, T^4) \cdot n_v(e, T^4) = n(T_v) \cdot (n(T_u) + s + t)$. By Lemma 2, we have $GA_2(T^3) > GA_2(T^4)$.

Similarly, if $n(T_u) + s < n(T_v) + t$, then $GA_2(T^3) > GA_2(T^5)$.

This completes the proof. □

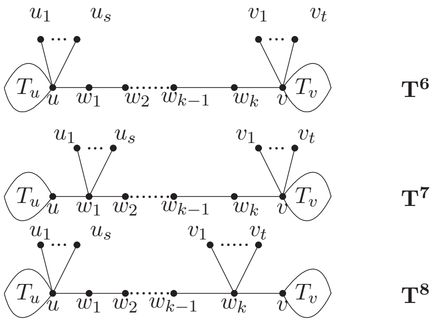

Fig. 3. Graph transformation III: $T^6 \longrightarrow T^7$ or $T^6 \longrightarrow T^8$ that decreases the value of $GA_2(T^6)$.

Remark 2. Since the trees we consider in this paper are members of $\mathcal{T}_{n,d}$, the graph transformation II: $T^3 \longrightarrow T^4$ or II: $T^3 \longrightarrow T^5$ that will not change the diameter of T^3 is valid to our proof of main result. So in our following proof of Theorem 5, we actually require that $n(T_u), n(T_v) \geq 2$.

Lemma 4. *Let T^6, T^7 and T^8 be trees shown as in Fig. 3. Then $GA_2(T^6) > GA_2(T^7)$ or $GA_2(T^6) > GA_2(T^8)$, where $s, t, k \geq 1$, and $T_u(resp., T_v)$ may be a single vertex $u(resp., v)$.*

Proof. From Fig. 3, we know that $diam(T^6) = diam(T^7) = diam(T^8)$. If $n(T_u) + s \geq n(T_v) + t + k$, then $n(T_u) + s + k > n(T_v) + t$. We consider the graph transformation III: $T^6 \longrightarrow T^8$. Obviously, for any edge $e = xy \in E(T^j)\backslash\{w_kv, vv_1, \cdots, vv_t, w_kv_1, \cdots, w_kv_t\}$ $(j = 6, 8)$, we have $n_x(e, T^6) \cdot n_y(e, T^6) = n_x(e, T^8) \cdot n_y(e, T^8)$. Also, $n_v(vv_j, T^6) \cdot n_{v_j}(vv_j, T^6) = n_{w_k}(w_kv_j, T^8) \cdot n_{v_j}(w_kv_j, T^8)(j = 1, \cdots, t) = n - 1$. For the edge w_kv, $n_v(e, T^6) \cdot n_{w_k}(e, T^6) = (n(T_u) + s + k) \cdot (n(T_v) + t) > n(T_v) \cdot (n(T_u) + s + t + k) = n_v(e, T^8) \cdot n_{w_k}(e, T^8)$. So we have $GA_2(T^6) > GA_2(T^8)$.

If $n(T_u) + s < n(T_v) + t + k$, we consider the graph transformation III: $T^6 \longrightarrow T^7$. By the same reasoning as above, we obtain $GA_2(T^6) > GA_2(T^7)$.

This completes the proof. □

Remark 3. As stated in Remark 2, we actually require that $n(T_u), n(T_v) \geq 2$ in the proof of main result.

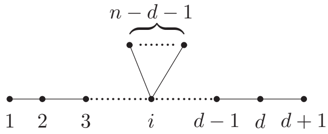

Fig. 4. Graph $P_{d+1}(i, n-d-1)$.

Let $P_{d+1}(i, n-d-1)$ denote the tree in $\mathcal{T}_{n,d}$ obtained from the path $P_{d+1} = v_1 \cdots v_{d+1}$ by attaching to its ith vertex $(2 \leq i \leq d)$ $n-d-1$ leaves.

The following is our main result of this paper.

Theorem 5. *Among all trees in $\mathcal{T}_{n,d}$, the tree $P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)$ has the minimum GA_2 index.*

Proof. Let T be a tree in $\mathcal{T}_{n,d}$ such that $GA_2(T)$ attains the minimum value. By Lemma 1, T must be a caterpillar of diameter d. By Lemmas 3 and 4, we claim that T must be isomorphic to $P_{d+1}(i, n-d-1)$. If not so, T must be a caterpillar with $P_{d+1} = v_0 v_1 \cdots v_d$ as its diametrical path, and there exist at least two branch vertices v_i, v_j $(2 \leq i \leq j \leq d)$.

If v_i is adjacent to v_j, then T can be viewed as the graph T^3 in Fig. 2. So, we can employ the graph transformation II on T and we shall obtain a new tree $\overline{T} \in \mathcal{T}_{n,d}$ with $GA_2(T) > GA_2(\overline{T})$, a contradiction to our choice of T.

Suppose v_i is not adjacent to v_j, but branch vertices v_i, v_j are chosen such that there is no other branch vertices along the path $v_i v_{i+1} \cdots v_j (j \geq i+2)$. Now, T can be viewed as the graph T^6 in Fig. 3. So, we can employ the graph transformation III on T, and we obtain a new tree $\widehat{T} \in \mathcal{T}_{n,d}$ with $GA_2(T) > GA_2(\widehat{T})$, a contradiction once again. Thus, $T \cong P_{d+1}(i, n-d-1)$.

Suppose that $T \ncong P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)$. Denote by $u_1, u_2, \cdots, u_{n-d-1}$ the leaves adjacent to v_i. If $i < d+1-i$, then $GA_2(P_{d+1}(i, n-d-1)) > GA_2(P_{d+1}(i+1, n-d-1))$. If $i > d+1-i$, then $GA_2(P_{d+1}(i, n-d-1)) > GA_2(P_{d+1}(i-1, n-d-1))$. These contradictions give $T \cong P_{d+1}(i, n-d-1)$, completing the proof. $\square$

Remark 4. In the proof of Lemmas 1, 3 and 4, in order to compare the GA_2 index of two trees $T^{'}, T^{''} \in \mathcal{T}_{n,d}$, we actually proved that for each edge–pair $\{e^{'}, e^{''}\}$, $(e^{'} = u^{'}v^{'} \in T^{'}, e^{''} = u^{''}v^{''} \in T^{''})$, if $n_{u^{'}}(e^{'}, T^{'}) \cdot n_{v^{'}}(e^{'}, T^{'}) \geq n_{u^{''}}(e^{''}, T^{''}) \cdot n_{v^{''}}(e^{'}, T^{''})$ and there exists one pair of edges $\{e_0^{'}, e_0^{''}\}$ such that $n_{u_0^{'}}(e_0^{'}, T^{'}) \cdot n_{v_0^{'}}(e_0^{'}, T^{'}) > n_{u_0^{''}}(e_0^{''}, T^{''}) \cdot n_{v_0^{''}}(e_0^{'}, T^{''})$, then

$GA_2(T') > GA_2(T'')$.

By Eq. (2) and Remark 4, the statements of Lemmas 1, 3 and 4 are valid for Szeged index. Recall that for a tree T, its Wiener index, a well-known molecular-structure descriptor, is equal to Szeged index. It then follows immediately the following result, which is a result of [7] concerning the Wiener index of trees with fixed diameter.

Theorem 6. *Among all trees in $\mathcal{T}_{n,d}$, the tree $P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)$ has the minimum Szeged and Wiener indices.*

Lemma 7. *For any $3 \leq d \leq n-2$, $GA_2(P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)) > GA_2(P_d(\lceil \frac{d}{2} \rceil, n-d))$.*

Proof. If $d = 2k$, we contract the edge $v_k v_{k+1}$ in $P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)$ and add one additional pendent edge $v_{k+1}x$ to the resulting graph. Now, we obtain $P_d(\lceil \frac{d}{2} \rceil, n-d)$. During this process, $n_u(e) \cdot n_v(e)$ remains unchanged for any edge $e(= uv) \neq v_k v_{k+1}$. Thus, $GA_2(P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)) - GA_2(P_d(\lceil \frac{d}{2} \rceil, n-d)) = n_{v_k}(v_k v_{k+1}, P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)) \cdot n_{v_{k+1}}(v_k v_{k+1}, P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)) - n_{v_{k+1}}(v_{k+1}x, P_d(\lceil \frac{d}{2} \rceil, n-d)) \cdot n_x(v_{k+1}x, P_d(\lceil \frac{d}{2} \rceil, n-d)) = k \cdot (n-k) - 1 \cdot (n-1) > 0$.

If $d = 2k+1$, we contract the edge $v_{k+1}v_{k+2}$ in $P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)$ and add the pendent edge $v_{k+1}y$ to the resulting graph. Similar to above, we can prove the desired result. This completes the proof. □

For any tree T in $\mathcal{T}_{n,d}$ with a given diameter $d(\geq 3)$, if $T \ncong P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)$, then $GA_2(T) > GA_2(P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1))$ by Theorem 5. Also, by Lemma 7, we have $GA_2(P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)) > GA_2(P_d(\lceil \frac{d}{2} \rceil, n-d))$. Thus, $GA_2(T) > GA_2(P_{d+1}(\lceil \frac{d+1}{2} \rceil, n-d-1)) > GA_2(P_d(\lceil \frac{d}{2} \rceil, n-d)) > \cdots > GA_2(P_3(\lceil \frac{3}{2} \rceil, n-3))$. Note that $P_3(\lceil \frac{3}{2} \rceil, n-3)$ is just the $n-$vertex star S_n. So, we have the following consequence.

Corollary 8([2]). *Among all trees with n vertices, the star S_n has the minimum GA_2 index.*

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. Note that $P_4(\lceil \frac{4}{2} \rceil, n-4)$ is just the double star tree $S_{1,n-3}$. By above discussion, we have

Corollary 9. *Among all trees with n vertices, the double star tree $S_{1,n-3}$ has the second-minimum GA_2 index.*

By means of Corollaries 8 and 9, we thus have

Corollary 10. *Among all trees with n vertices, the star S_n has the minimum Szeged and Wiener indices.*

Corollary 11. *Among all trees with n vertices, the double star tree $S_{1,n-3}$ has the second-minimum Szeged and Wiener indices.*

3. Concluding remarks

In this paper, we have determined the unique tree with the minimum GA_2 index among all trees in $\mathcal{T}_{n,d}$. A related problem arising at this moment is: which tree has the maximum GA_2 index among all trees in $\mathcal{T}_{n,d}$? It seems to be a much more difficult problem than the one we have solved in this paper.

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