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On the Maximum Atom–Bond Sum-Connectivity Index of Trees

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Abstract

The atom-bond sum-connectivity (ABS) index of a graph G, introduced by Ali et al., is defined as

$$ABS(G) = \sum_{uv\in E(G)} \sqrt{1-\frac{2}{d_G(u)+d_G(v)}},$$

where $d_G(u)$ denotes the degree of the vertex u in G. In this paper, we present the extremal trees with the maximum ABS index among all trees of a given order with matching number or diameter, respectively. Moreover, the tree with a perfect matching having the maximum ABS index is also determined.

1 Introduction

All graphs considered in this paper are simple, undirected and finite, and we refer to [7] for undefined terminology and notation.

The vertex and edge sets of G are denoted by $V(G)$ and $E(G)$, respectively. The number of vertices is called the *order* of G, denoted by $n(G)$.

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For a vertex $u \in V(G)$, the *degree* of u, denoted by $d_G(u)$, is the number of edges incident with u in G. If $d_G(u) = 1$, then u is called a *pendant vertex* and the unique edge incident with a pendant vertex v is called a *pendant edge*. Denote by $N_G(u)$ the set of *neighborhood* of a vertex u. For $v \in V(G)$, $G - v$ is the graph obtained from G by deleting v and its incident edges. As usual, the path and the star of order n are denoted by P_n and S_n, respectively. A tree T is called to be a *caterpillar* if it become a path after deleting all pendant vertices.

A *matching* in a graph is a set of pairwise nonadjacent edges. If M is a matching, the two ends of each edge of M are said to be matched under M, and each vertex incident with an edge of M is said to be covered by M. A *perfect matching* is one which covers every vertex of the graph. A matching M is a maximum matching of G if there does not exist a matching M' of G such that $|M'| > |M|$. The cardinality of a maximum matching is called the *matching number* of G, denoted by $\alpha'(G)$. We say that $S \subseteq V(G)$ is a *covering* of a graph G if each edge of G is incident with a vertex of S in G. The *covering number* of G, denoted by $\beta(G)$, is the minimum cardinality of a covering of G. The well-known König's min-max theorem states that

$$\alpha'(G) = \beta(G)$$

for any bipartite graph G.

The distance between the vertices u and v of G is denoted by $d_G(u, v)$, which is defined as the length of a shortest path between u and v in G. The *diameter* of a graph G is defined as $\mathrm{diam}(G) = \max_{\{u,v\} \subseteq V(G)} d_G(u, v)$.

The atom-bond connectivity (ABC) index of a graph G is defined as [12]

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) d_G(v)}}.$$

Based on the Randić index, Zhou and Trinajstić [19] proposed the sum-connectivity (SC) index, defined as

$$SC(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_G(u) + d_G(v)}}.$$

The ABC and SC indices have been extensively studied, and detail regarding the mathematical aspects of the two indices may be found in the review papers [2] and [1], respectively. By amalgamating the core idea of the ABC and SC indices, Ali et al. [4] defined a new topological index, called the *atom-bond sum-connectivity (ABS) index*, of a graph G, denoted by $ABS(G)$. It is formulated as

$$ABS(G) = \sum_{uv \in E(G)} \sqrt{1 - \frac{2}{d_G(u) + d_G(v)}}.$$

Ali, Gutman and Redžepović [3] investigated ABS, Randić, ABC and SC indices in terms of some physico-chemical properties, in the case of octane isomers. It is observed that the ABS index performs somewhat better than the other indices for some properties, such as boiling point, enthalpy of vaporization, and enthalpy of formation. Therefore, the ABS index has important physico-chemical applications. Moreover, the authors [4] determined the graphs attaining the extreme values of the ABS index over the classes of (molecular) trees and general graphs of a fixed order. Very recently, the authors [6] characterized the graphs having the maximum ABS index over the classes of graphs of a given order with a fixed parameter (such as, chromatic number, independence number, number of pendant vertices). In [3], the graphs with the maximum and second-maximum ABS index are determined over the class of connected unicyclic graphs with a fixed order. Compared to the maximum ABS index, characterizing the graphs with the minimum ABS index has been studied. In [3], the graphs with the minimum and second-minimum ABS index are determined among all connected unicyclic graphs. In [5] and [17], the authors provided independently a partial solution to the problem of characterizing graphs possessing the minimum ABS index among all trees of a fixed order and number of pendant vertices.

It is interesting to find the extremal graphs with the maximum or minimum index in some classes of graphs of a given order with a fixed parameter. For instance, the trees with the maximum ABC index among all trees of a given order with diameter or a perfect matching were determined in [14, 18], respectively. The extremal graph with the maximum ABC index among all connected unicyclic graphs of a fixed order with a perfect matching was characterized in [15]. The authors [8, 9] presented the extremal graph with the maximum ABC index in all graphs of a fixed order with a given matching number. Results on trees with given matching number having the maximum SC index are found in [20]. Extremal results concerning the minimum SC index and matching number were obtained in [10] for trees and connected unicyclic graphs, in [11] for connected bicyclic graphs, and in [16] for cacti.

Motivated by the known results, in this paper, we pay attention to trees with the maximum ABS index in the classes of trees of a given order with matching number or diameter, respectively.

2 Preliminaries

In the section, we give some useful lemmas and notations for the later use. First, we give a critical lemma on graph transformations leading to increase the value of the ABS index.

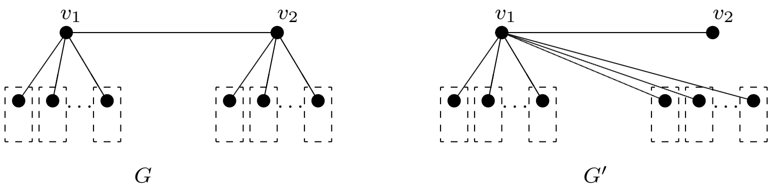

Figure 1. Graphs G and G' in Lemma 1.

In fact, the proof of Lemma 2.1 in [3] do not required the condition of degrees. Thus, Lemma 2.1 can be improved the following result.

Lemma 1. *Let v_1v_2 be an edge of a graph G such that $N_G(v_1) \cap N_G(v_2) = \emptyset$ and $d_G(v_1), d_G(v_2) \geq 2$. If $G' = G - \{v_2u : u \in N_G(v_2) \setminus \{v_1\}\} + \{v_1u : u \in N_G(v_2) \setminus \{v_1\}\}$ (see Fig. 1), then $ABS(G') > ABS(G)$.*

From Lemma 1, we immediately obtain the following result.

Corollary ([4]). *Among all trees of order $n \geq 4$, the star S_n uniquely attains the maximum value of the ABS index.*

For convenience, let us define two functions

$$f(x) = \sqrt{1 - \frac{2}{x}} - \sqrt{1 - \frac{2}{x+1}} \text{ and } h(x, y) = \sqrt{1 - \frac{2}{x+y}} - \sqrt{1 - \frac{2}{x+y-1}}.$$

Lemma 2. *The function $f(x) = \sqrt{1 - \frac{2}{x}} - \sqrt{1 - \frac{2}{x+1}}$ is increasing for $x \in [3, +\infty)$.*

Proof. By a simple calculation we have

$$f'(x) = \frac{1}{\sqrt{x^4 - 2x^3}} - \frac{1}{\sqrt{(x+1)^4 - 2(x+1)^3}}. \tag{1}$$

Let $g(x) = \sqrt{x^4 - 2x^3}$. Then we have

$$g'(x) = \frac{x^2(2x-3)}{\sqrt{x^4 - 2x^3}}.$$

It is clear that $g'(x) > 0$ for $x \in [3, +\infty)$. So, $g(x)$ is increasing for $x \in [3, +\infty)$. One can see from (1) that $f'(x) = \frac{1}{g(x)} - \frac{1}{g(x+1)} > 0$ for $x \in [3, +\infty)$. Thus $f(x)$ is increasing for $x \in [3, +\infty)$. ∎

Lemma 3. *Let $h(x, y) = \sqrt{1 - \frac{2}{x+y}} - \sqrt{1 - \frac{2}{x+y-1}}$, where $x \geq 3$ and $y \geq 1$. Then the function $h(x, y)$ is decreasing with respect to $x \in [3, +\infty)$ and $y \in [1, +\infty)$.*

Proof. It is easy to verify that $h(x, y) = -f(x + y - 1)$, where $f(x)$ is defined in Lemma 2. By a simple calculation we have

$$\frac{\partial h}{\partial x} = -f'(x + y - 1) \text{ and } \frac{\partial h}{\partial y} = -f'(x + y - 1).$$

It follows from Lemma 2 that $-f'(x + y - 1) < 0$ for $x + y - 1 \in [3, +\infty)$. Since $x \geq 3$ and $y \geq 1$, we have $x + y - 1 \geq 3$. Thus $\frac{\partial h}{\partial x}, \frac{\partial h}{\partial y} < 0$ for $x \geq 3$ and $y \geq 1$. The result holds. ∎

Lemma 4. *Let*

$$\phi(x,a)=\sqrt{1-\frac{2}{a-x+5}}+(a-x+2)\sqrt{1-\frac{2}{a-x+4}}+\sqrt{1-\frac{2}{x+2}}+(x-1)\sqrt{1-\frac{2}{x+1}}.$$

If $a \geq 2x-3$, then $\phi(x,a)$ is decreasing with respect to $x \in [2,+\infty)$.

Proof. Let $\varphi(t)=\sqrt{1-\frac{2}{t+1}}+(t-2)\sqrt{1-\frac{2}{t}}$. One can see

$$\phi(x,a)=\varphi(a-x+4)+\varphi(x+1).$$

It suffices to show that $\frac{\partial\phi}{\partial x}=-\frac{d\varphi}{dt}|_{t=a-x+4}+\frac{d\varphi}{dt}|_{t=x+1}<0$. Since $a \geq 2x-3$, we have $a-x+4 \geq x+1$. So, we need to prove that $\frac{d\varphi}{dt}$ is increasing for $t \in [3,+\infty)$, which is equivalent to $\frac{d^2\varphi}{dt^2}>0$ for $t \in [3,+\infty)$. Note that $\varphi(t)=(t-1)^{\frac{1}{2}}\cdot(t+1)^{-\frac{1}{2}}+(t-2)^{\frac{3}{2}}\cdot t^{-\frac{1}{2}}$. A simple calculation shows that

$$\begin{aligned}
\frac{d\varphi}{dt} &= \tfrac{1}{2}(t-1)^{-\frac{1}{2}}(t+1)^{-\frac{1}{2}}-\tfrac{1}{2}(t-1)^{\frac{1}{2}}(t+1)^{-\frac{3}{2}}+\tfrac{3}{2}(t-2)^{\frac{1}{2}}\cdot t^{-\frac{1}{2}} \\
&\quad -\tfrac{1}{2}(t-2)^{\frac{3}{2}}\cdot t^{-\frac{3}{2}} \\
&= \tfrac{1}{2}(t-1)^{-\frac{1}{2}}(t+1)^{-\frac{3}{2}}\cdot((t+1)-(t-1)) \\
&\quad +\tfrac{1}{2}(t-2)^{\frac{1}{2}}\cdot t^{-\frac{3}{2}}\cdot(3t-(t-2)) \\
&= (t-1)^{-\frac{1}{2}}(t+1)^{-\frac{3}{2}}+(t-2)^{\frac{1}{2}}\cdot t^{-\frac{3}{2}}\cdot(t+1)
\end{aligned}$$

and

$$\begin{aligned}
\frac{d^2\varphi}{dt^2} &= -\frac{1}{2}(t-1)^{-\frac{3}{2}}(t+1)^{-\frac{3}{2}}-\frac{3}{2}(t-1)^{-\frac{1}{2}}(t+1)^{-\frac{5}{2}} \\
&\quad +\frac{1}{2}(t-2)^{-\frac{1}{2}}\cdot t^{-\frac{3}{2}}\cdot(t+1)-\frac{3}{2}(t-2)^{\frac{1}{2}}\cdot t^{-\frac{5}{2}}\cdot(t+1)+(t-2)^{\frac{1}{2}}\cdot t^{-\frac{3}{2}} \\
&= -\frac{1}{2}(t-1)^{-\frac{3}{2}}(t+1)^{-\frac{5}{2}}\cdot[(t+1)+3(t-1)] \\
&\quad +\frac{1}{2}(t-2)^{-\frac{1}{2}}\cdot t^{-\frac{5}{2}}\cdot[t(t+1)-3(t-2)(t+1)+2(t-2)t] \\
&= -(t-1)^{-\frac{3}{2}}(t+1)^{-\frac{5}{2}}\cdot(2t-1)+3(t-2)^{-\frac{1}{2}}\cdot t^{-\frac{5}{2}}. \qquad (2)
\end{aligned}$$

For convenience, denote $\psi(t)=[3(t-2)^{-\frac{1}{2}}\cdot t^{-\frac{5}{2}}]^2-[(t-1)^{-\frac{3}{2}}(t+1)^{-\frac{5}{2}}\cdot(2t-1)]^2$. By simplification we have

$$\psi(t)=\frac{m(t)}{(t-1)^3(t+1)^5(t-2)t^5},$$

where $m(t) = 5t^8 + 30t^7 - 27t^6 - 52t^5 + 54t^3 + 18t^2 - 18t - 9$. Note that $m(t)$ is a polynomial function. Using Matlab, the largest real root of $m(t)$ is 0.9796. Since the coefficient of the first term of $m(t)$ is larger than 0, we have $m(t) > 0$ for $t \geq 3$, and so $\psi(t) > 0$ for $t \geq 3$. By (2) we have $\frac{d^2\varphi}{dt^2} > 0$ for $t \geq 3$.

It completes the proof. ■

3 Trees with matching number α'

In this section, let $\mathcal{T}_{n,\alpha'}$ be the family of all trees of order n with matching number α', where $n \geq 2\alpha' \geq 2$. Let $T_{n,\alpha'}$ be the tree obtained from the star $S_{n-\alpha'+1}$ by inserting a new vertex into its $\alpha' - 1$ pendant edges, respectively. Clearly, $T_{n,\alpha'} \in \mathcal{T}_{n,\alpha'}$. One can see $T_{n,\alpha'}$ and $T_{2\alpha',\alpha'}$ in Fig. 2. By a simple computation, we obtain

$$ABS(T_{n,\alpha'}) = \frac{\alpha'-1}{\sqrt{3}} + (\alpha'-1)\sqrt{1-\frac{2}{n-\alpha'+2}} + (n-2\alpha'+1)\sqrt{1-\frac{2}{n-\alpha'+1}}. \quad (3)$$

We will show that $T_{n,\alpha'}$ has the maximum ABS index among all trees in $\mathcal{T}_{n,\alpha'}$ with $n > 2\alpha' \geq 2$. We start with a useful lemma, due to Hou and Li [13].

$T_{n,\alpha'}$ $\qquad$ $T_{2\alpha',\alpha'}$

Figure 2. Graphs $T_{n,\alpha'}$ and $T_{2\alpha,\alpha'}$.

Lemma 5 ([13]). *If T is a tree of order $n > 2\alpha'$ with $\alpha'(T) = \alpha'$, then there is a maximum matching M and a pendant vertex u such that M does not saturate u.*

Lemma 6. *Assume that T^* has the maximum ABS index among trees in $\mathcal{T}_{n,\alpha'}$ with $n \geq 2\alpha' \geq 2$. If M is a maximum matching with $|M| = \alpha'$, then*
(1) e is a pendant edge of T^* for $e \in M$;
(2) u is saturated by M for $d_{T^*}(u) \geq 2$.

Proof. To show (1), let $e = uv \in M$. Suppose that e is not a pendant edge of T^*. So we have $d_{T^*}(u) \geq 2$ and $d_{T^*}(v) \geq 2$. Let $T' = T^* - \{vw : w \in N_{T^*}(v) \setminus \{u\}\} + \{uw : w \in N_{T^*}(v) \setminus \{u\}\}$.

Claim 1. $\alpha'(T') = \alpha'(T^*)$.

Since M is also a matching of T', $\alpha'(T') \geq |M| = \alpha'(T^*)$. It remains to show that $\alpha'(T') \leq \alpha'(T^*)$. By König's min-max theorem, it suffices to show that $\beta(T') \leq \beta(T^*)$, where $\beta(T')$ and $\beta(T^*)$ are the covering number of T' and T^*, respectively. Let S be a minimum covering of T^*. Observe that S' is a covering of T', where

$$S' = \begin{cases} S \setminus \{v\}, & u \in S, \\ (S \setminus \{v\}) \cup \{u\}, & \text{otherwise.} \end{cases}$$

Thus,

$$\alpha'(T^*) = \beta(T^*) = |S| \geq |S'| \geq \beta(T') = \alpha'(T').$$

This proves the claim.

However, by Lemma 1, we have $ABS(T') > ABS(T^*)$, contradicting the choice of T^*.

Next, we prove (2). If $T^* \cong S_n$, then the result holds. Assume that $T^* \ncong S_n$ and T^* has a non-pendant vertex u, which is not M-saturated. Since T^* is not a star, u has a neighbor v with $d_{T^*}(v) \geq 2$. By the maximality of M, v is M-saturated. Let $T'' = T^* - \{vw : w \in N_{T^*}(v) \setminus \{u\}\} + \{uw : w \in N_{T^*}(v) \setminus \{u\}\}$. By Claim 1, we have $\alpha'(T'') = \alpha'$. Again, by Lemma 1, $ABS(T'') > ABS(T^*)$, contradicting the maximality of T^*. ■

Recall that $S \subseteq V(G)$ is said to be an *independent set* of a graph G if no pair of vertices are adjacent in G. The independence number of G, denoted by $\alpha(G)$, is the maximum cardinality of an independent set of G. The well-known Gallai identity says that

$$\alpha(G) + \beta(G) = n$$

for any graph G.

Theorem 1. *If T is a tree in $\mathcal{T}_{n,\alpha'}$ with $n > 2\alpha'$, then*

$$ABS(T) \leq \frac{\alpha'-1}{\sqrt{3}} + (\alpha'-1)\sqrt{1-\frac{2}{n-\alpha'+2}} + (n-2\alpha'+1)\sqrt{1-\frac{2}{n-\alpha'+1}},$$

with equality if and only if $T \cong T_{n,\alpha'}$.

Proof. Assume that T has the maximum ABS index among all trees in $\mathcal{T}_{n,\alpha'}$ with $n > 2\alpha'$. If $n = 3$, then $T \cong P_3 \cong T_{3,1}$. Thus, the result trivially holds. Next, let $n \geq 4$ and assume that the result holds for all trees of order at most $n-1$ and at least $2\alpha'+1$. We proceed with the induction on n.

Let M be a matching of T with $|M| = \alpha'$. By Lemma 5, there is a pendant vertex u such that $T-u$ also contains the matching M. Let v be the unique neighbor of u. Set $x = d_T(v)$ and $N_T(v) \setminus \{u\} = \{v_1, v_2, \ldots, v_{x-1}\}$. Now, let $T' = T - u$. Clearly, T' is a tree of order $n-1$ with matching number α'.

By Gallai identity and König's min-max theorem, $x = d_T(v) \leq \alpha(T) = n - \beta(T) = n - \alpha'(T) = n - \alpha'$. Let t be the number of pendent vertices of T' belonging in $N_{T'}(v)$. Without loss of generality we assume that $v_1, \ldots, v_t$ are the pendant vertices in $N_{T'}(v)$. By Lemma 6, the number of pendant vertices of T is $n - \alpha'$. Thus,

$$t + 1 \leq n - \alpha' - (\alpha' - 1) = n - 2\alpha' + 1,$$

which is equivalent to $t \leq n - 2\alpha'$. By induction hypothesis,

$$ABS(T') \leq \frac{\alpha'-1}{\sqrt{3}} + (\alpha'-1)\sqrt{1-\frac{2}{n-\alpha'+1}} + (n-2\alpha')\sqrt{1-\frac{2}{n-\alpha'}}$$

Since $d_T(v_i) = d_{T'}(v_i) \geq 2$ for $i \in \{t+1, \ldots, x-1\}$, by Lemma 3,

$$\begin{aligned} &\sum_{i=t+1}^{x-1}\left(\sqrt{1-\frac{2}{x+d_T(v_i)}} - \sqrt{1-\frac{2}{x-1+d_T(v_i)}}\right) \\ \leq\ &\sum_{i=t+1}^{x-1}\left(\sqrt{1-\frac{2}{x+2}} - \sqrt{1-\frac{2}{x+1}}\right). \end{aligned} \tag{4}$$

In addition, note that $x \leq n-\alpha'$ and $t \leq n-2\alpha'$, we have

$$\begin{aligned}
& ABS(T) \\
= \;& ABS(T') + \sqrt{1-\frac{2}{d_T(v)+d_T(u)}} \\
& + \sum_{i=1}^{x-1}\left(\sqrt{1-\frac{2}{d_T(v)+d_T(v_i)}} - \sqrt{1-\frac{2}{d_{T'}(v)+d_{T'}(v_i)}}\right) \\
= \;& ABS(T') + \sqrt{1-\frac{2}{x+1}} + \sum_{i=1}^{t}\left(\sqrt{1-\frac{2}{x+1}} - \sqrt{1-\frac{2}{x}}\right) \\
& + \sum_{i=t+1}^{x-1}\left(\sqrt{1-\frac{2}{x+d_T(v_i)}} - \sqrt{1-\frac{2}{x-1+d_T(v_i)}}\right) \\
\leq \;& ABS(T') + \sqrt{1-\frac{2}{x+1}} + \sum_{i=1}^{t}\left(\sqrt{1-\frac{2}{x+1}} - \sqrt{1-\frac{2}{x}}\right) \\
& + \sum_{i=t+1}^{x-1}\left(\sqrt{1-\frac{2}{x+2}} - \sqrt{1-\frac{2}{x+1}}\right) \qquad \text{(due to (4))} \\
= \;& ABS(T') + \sqrt{1-\frac{2}{x+1}} + t \cdot h(x,1) + (x-t-1)\cdot h(x,2) \\
\leq \;& ABS(T') + \sqrt{1-\frac{2}{n-\alpha'+1}} + t \cdot h(n-\alpha',1) \\
& +(n-\alpha'-t-1)\cdot h(n-\alpha',2) \qquad \text{(due to Lemma 3)} \\
\leq \;& ABS(T') + \sqrt{1-\frac{2}{n-\alpha'+1}} + (n-\alpha'-1)\cdot h(n-\alpha',2) \\
& +t\cdot[h(n-\alpha',1)-h(n-\alpha',2)] \\
\leq \;& ABS(T') + \sqrt{1-\frac{2}{n-\alpha'+1}} + (n-\alpha'-1)\cdot h(n-\alpha',2) \\
& +(n-2\alpha')\cdot(h(n-\alpha',1)-h(n-\alpha',2)) \\
\leq \;& \frac{\alpha'-1}{\sqrt{3}} + (\alpha'-1)\sqrt{1-\frac{2}{n-\alpha'+1}} + (n-2\alpha')\sqrt{1-\frac{2}{n-\alpha'}} + \sqrt{1-\frac{2}{n-\alpha'+1}} \\
& +(n-\alpha'-1)\cdot h(n-\alpha',2)+(n-2\alpha')\cdot(h(n-\alpha',1)-h(n-\alpha',2)) \\
= \;& \frac{\alpha'-1}{\sqrt{3}} + (\alpha'-1)\sqrt{1-\frac{2}{n-\alpha'+2}} + (n-2\alpha'+1)\sqrt{1-\frac{2}{n-\alpha'+1}}.
\end{aligned}$$

It follows from (3) that if $T = T_{n,\alpha'}$ then the equality holds. On the other hand, if all equalities hold in the above expression, then $x = d_T(u) = n-\alpha'$, $t = n - 2\alpha'$ and $d_{T'}(v_i) = 2$ for $n - 2\alpha' + 1 \leq i \leq n - \alpha' - 1$, implying $T \cong T_{n,\alpha'}$. ■

By the inductive hypothesis and a similar way used in the proof of Theorem 1, we can show the following result, and here we omit the proof.

Theorem 2. *If T is a tree of order n with a perfect matching, then*

$$ABS(T) \leq \frac{\alpha' - 1}{\sqrt{3}} + (\alpha' - 1)\sqrt{1 - \frac{2}{\alpha' + 2}} + \sqrt{1 - \frac{2}{\alpha' + 1}},$$

with equality if and only if $T \cong T_{2\alpha',\alpha'}$, where $\alpha' = \alpha'(T)$.

4 Trees with diameter d

In this section, Let $\mathbb{T}_{n,d}$ be the family of trees of order n with diameter d, where $n \geq d + 1 \geq 3$. Let $T^1_{n,d}$ be the tree obtained from the path $P = u_0u_1 \cdots u_d$ by attaching $n - d - 1$ pendant edges to the vertex u_1, as shown in Fig. 3. Clearly, $T^1_{n,d} \in \mathbb{T}_{n,d}$. By a simple calculation, we have

$$ABS(T^1_{n,d}) = \frac{1}{\sqrt{3}} + \frac{d-3}{\sqrt{2}} + \sqrt{1 - \frac{2}{n-d+3}} + (n-d)\sqrt{1 - \frac{2}{n-d+2}}. \quad (5)$$

We will prove that $T^1_{n,d}$ has the maximum ABS index among all trees in $\mathbb{T}_{n,d}$.

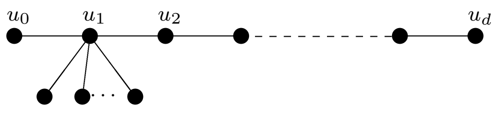

Figure 3. Graph $T^1_{n,d}$.

Lemma 7. *If T^* has the maximum ABS index among all trees in $\mathbb{T}_{n,d}$ with $n \geq d + 1 \geq 3$, then T^* is a caterpillar.*

Proof. Suppose to the contrary that T^* is not a caterpillar. Let $P = u_0u_1 \cdots u_d$ be a diametrical path of T^*. Clearly, u_0 and u_d are two leaves. Since T^* is not a caterpillar, there exists some vertex u_i $(1 \leq i \leq d - 1)$

such that a neighbor $v \notin \{u_{i-1}, u_{i+1}\}$ of u_i with $d_{T^*}(v) \geq 2$. Thus, the edge vu_i satisfies $d_{T^*}(v), d_{T^*}(u_i) \geq 2$. Let $T = T^* - \{vw : w \in N_{T^*}(v) \setminus \{u_i\}\} + \{u_i w : w \in N_{T^*}(v) \setminus \{u_i\}\}$. Clearly, $T \in \mathbb{T}_{n,d}$. By Lemma 1, we have $ABS(T) > ABS(T^*)$, contradicting the maximality of T^*. ■

Theorem 3. *If T is a tree in $\mathbb{T}_{n,d}$ with $n \geq d+1 \geq 3$, then*

$$ABS(T) \leq \frac{1}{\sqrt{3}} + \frac{d-3}{\sqrt{2}} + \sqrt{1 - \frac{2}{n-d+3}} + (n-d)\sqrt{1 - \frac{2}{n-d+2}},$$

with equality if and only if $T \cong T^1_{n,d}$.

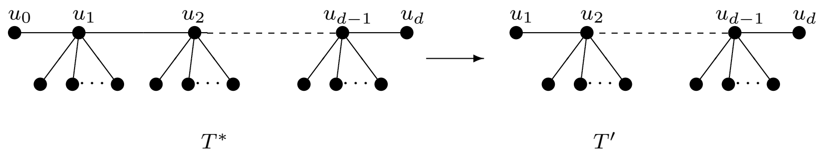

Figure 4. Graphs T^* and T' in Theorem 3.

Proof. Assume that T^* has the maximum ABS index among all trees in $\mathbb{T}_{n,d}$ with $n \geq d+1 \geq 3$. It is clear that if $d = 2$ then $T^* \cong S_n \cong T^1_{n,2}$, and if $d = n-1$ then $T^* \cong P_n \cong T^1_{n,n-1}$. Thus, the result trivially holds.

Next, let $3 \leq d \leq n-2$. Assume that the result holds for every tree of order n' with diameter d' satisfying $n' + d' < n + d$. It follows from Lemma 7 that T^* is a caterpillar. Let $P = u_0 u_1 \cdots u_{d-1} u_d$ be a diametrical path of T^*. Clearly, u_0 and u_d are two leaves, and $n(T^* - P) = n - d - 1$. One can see that one of u_1 and u_{d-1} hangs at most $\frac{n-d-1}{2} + 1 = \frac{n-d+1}{2}$ leaves. Without loss of generality assume that u_1 hangs at most $\frac{n-d+1}{2}$ leaves. Denote $x = d_{T^*}(u_1) \geq 2$, that is $2 \leq x \leq \frac{n-d+1}{2} + 1 = \frac{n-d+3}{2}$. Let $T' = T^* - N_{T^*}(u_1) \setminus \{u_2\}$ (see Fig.4). So, T' is a tree of order $n - x + 1$ with diameter $d-1$. By the induction hypothesis, we have

$$\begin{aligned} ABS(T') \quad \leq \quad & \frac{1}{\sqrt{3}} + \frac{d-4}{\sqrt{2}} + \sqrt{1 - \frac{2}{n-x-d+5}} \\ & + (n-x-d+2)\sqrt{1 - \frac{2}{n-x-d+4}}. \end{aligned}$$

For convenience, denote by $y = d_{T^*}(u_2) \geq 2$. Thus,

$$\begin{aligned}
ABS(T^*) &= ABS(T') - \sqrt{1-\frac{2}{y+1}} + \sqrt{1-\frac{2}{x+y}} + (x-1)\sqrt{1-\frac{2}{x+1}} \\
&\leq \frac{1}{\sqrt{3}} + \frac{d-4}{\sqrt{2}} + \sqrt{1-\frac{2}{n-x-d+5}} + (n-x-d+2)\sqrt{1-\frac{2}{n-x-d+4}} \\
&\quad -\sqrt{1-\frac{2}{y+1}} + \sqrt{1-\frac{2}{x+y}} + (x-1)\sqrt{1-\frac{2}{x+1}} \\
&:= \Phi(x,y).
\end{aligned} \tag{6}$$

By a simple calculation, we have

$$\frac{\partial \Phi(x,y)}{\partial y} = -\frac{1}{\sqrt{(y+1)^4 - 2(y+1)^3}} + \frac{1}{\sqrt{(x+y)^4 - 2(x+y)^3}} < 0.$$

Thus $\Phi(x,y)$ is decreasing with respect to $y \in [2, +\infty)$. From (6) we have

$$\begin{aligned}
ABS(T^*) \leq\ & \Phi(x,2) \\
=\ & \frac{d-4}{\sqrt{2}} + \sqrt{1-\frac{2}{n-x-d+5}} + (n-x-d+2)\sqrt{1-\frac{2}{n-x-d+4}} \\
& + \sqrt{1-\frac{2}{x+2}} + (x-1)\sqrt{1-\frac{2}{x+1}} \\
=\ & \frac{d-4}{\sqrt{2}} + \phi(x, n-d),
\end{aligned}$$

where $\phi(x, n-d)$ is defined in Lemma 4. Since $x \leq \frac{n-d+3}{2}$ (i.e., $n-d \geq 2x-3$), by Lemma 4, $\Phi(x,2)$ is decreasing for $x \in [2, +\infty)$. Thus,

$$\begin{aligned}
ABS(T^*) &\leq \Phi(2,2) \\
&= \frac{d-4}{\sqrt{2}} + \sqrt{1-\frac{2}{n-2-d+5}} + (n-2-d+2)\sqrt{1-\frac{2}{n-2-d+4}} \\
&\quad + \sqrt{1-\frac{2}{2+2}} + \sqrt{1-\frac{2}{2+1}} \\
&= \frac{1}{\sqrt{3}} + \frac{d-3}{\sqrt{2}} + \sqrt{1-\frac{2}{n-d+3}} + (n-d)\sqrt{1-\frac{2}{n-d+2}}.
\end{aligned}$$

If all equalities hold in the above expression then $x = y = 2$ and $T' \cong$

$T^1_{n-x+1,d-1}$, and so $T^* \cong T^1_{n,d}$. On the other hand, if $T^* \cong T^1_{n,d}$, from (5) then the equality holds. ■

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