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Extremal trees with fixed degree sequence for atom-bond connectivity index

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Abstract. The atom-bond connectivity (ABC) index of a graph G is the sum of $\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$ over all edges uv of G, where $d(u)$ is the degree of vertex u in G. We characterize the extremal trees with fixed degree sequence that maximize and minimize the ABC index, respectively. We also provide algorithms to construct such trees.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For any vertex $v \in V(G)$, denote by $d_G(v)$ or $d(v)$ the degree of v in G.

The atom-bond connectivity (ABC) index of G is defined as [1]

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

The ABC index displays an excellent correlation with the heat of formation of alkanes [1], and from it a basically topological approach was developed to explain the differences in the energy of linear and branched alkanes both qualitatively and quantitatively [2]. Various properties of the ABC index have been established, see [3–8].

The (general) Randić index of a graph G is defined as [9]

$$R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha,$$

where α is a nonzero real number. Delorme et al. [10] described an algorithm that determines a tree of fixed degree sequence that maximizes the (general) Randić index for $\alpha = 1$ (also known as the second Zagreb index [11]). Then Wang [12] characterized the extremal trees with fixed degree sequence that minimize the (general) Randić index for $\alpha > 0$, and maximize the (general) Randić index for $\alpha < 0$.

In this note, we use the techniques from [10, 12] to characterize the extremal trees with fixed degree sequence to maximize and minimize the ABC index.

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2. Preliminaries

For a tree T, the degree sequence of T is the sequence of degrees of the non-pendent vertices arranged in a non-increasing order.

First we give two lemmas.

Let $f(x,y) = \sqrt{\frac{x+y-2}{xy}}$ for $x, y \geq 1$ with $x + y > 2$.

Lemma 2.1. ([5]) *If $y \geq 2$ is fixed, then $f(x, y)$ is decreasing in x.*

For $s > r \geq 1$, let $g_{r,s}(x) = f(x,r) - f(x,s)$.

Lemma 2.2. *The fuction $g_{r,s}(x)$ is increasing in x.*

Proof. Obviously, $g_{r,s}(x) = \sqrt{\frac{1}{x} + \frac{1}{r} - \frac{2}{rx}} - \sqrt{\frac{1}{x} + \frac{1}{s} - \frac{2}{sx}}$. Then

$$\begin{aligned} g'_{r,s}(x) &= \frac{1}{2}\sqrt{\frac{rx}{r+x-2}}\left(-\frac{1}{x^2} + \frac{2}{rx^2}\right) - \frac{1}{2}\sqrt{\frac{sx}{s+x-2}}\left(-\frac{1}{x^2} + \frac{2}{sx^2}\right) \\ &= \frac{\sqrt{x}}{x^2\sqrt{r+x-2}}\left(\frac{1}{\sqrt{r}} - \frac{\sqrt{r}}{2}\right) - \frac{\sqrt{x}}{x^2\sqrt{s+x-2}}\left(\frac{1}{\sqrt{s}} - \frac{\sqrt{s}}{2}\right). \\ &= \frac{\sqrt{x}}{2x^2}\left(\frac{2-r}{\sqrt{r(r+x-2)}} - \frac{2-s}{\sqrt{s(s+x-2)}}\right). \end{aligned}$$

Let $h(t) = \frac{2-t}{\sqrt{t(t+x-2)}}$ for $t \geq 1$ with $t + x > 2$. It is easily seen that $h'(t) = -\frac{xt+2(t+x-2)}{2(t(t+x-2))^{\frac{3}{2}}} < 0$, implying that $h(t)$ is decreasing in t. Recall that $r < s$. Then $g'_{r,s}(x) = \frac{\sqrt{x}}{2x^2}(h(r) - h(s)) > 0$, and thus result follows. □

For a tree T and $i = 0, 1, \ldots$, let $L_i = L_i(T)$ be the set of vertices in T, the minimum distance from which to the set of pendent vertices of T is i. Clearly, L_0 is exactly the set of pendent vertices in T.

For a graph G with $F \subseteq E(G)$, denote by $G - F$ the subgraph of G obtained by deleting the edges of F. Similarly, $G + W$ denotes the graph obtained from G by adding edges in W, where W is an subset of edge set of the complement of G.

3. Upper bound for the ABC index of trees with fixed degree sequence

In this section, we characterize the extremal trees with maximum ABC index among the trees with fixed degree sequence, and provide an algorithm to construct such trees.

Lemma 3.1. *Let T be a tree with maximum ABC index among the trees with fixed degree sequence. Let $P = v_0v_1v_2\ldots v_t$ be a path in T, where $d(v_0) = d(v_t) = 1$. For $1 \leq i \leq \frac{t}{2}$, we may always assume*

(i) if i is odd, then $d(v_i) \geq d(v_{t-i}) \geq d(v_j)$ for $i + 1 \leq j \leq t - i - 1$;

(ii) if i is even, then $d(v_i) \leq d(v_{t-i}) \leq d(v_j)$ for $i + 1 \leq j \leq t - i - 1$.

Proof. We argue by induction on i. Suppose that $d(v_1) < d(v_j)$ for some $2 \leq j \leq t - 2$. Let $T' = T - \{v_0v_1, v_jv_{j+1}\} + \{v_0v_j, v_1v_{j+1}\}$. Obviously, T' has the same degree sequence as T. Note that $d(v_0) = 1$. Since $j + 1 \leq t - 1$, we have $d(v_{j+1}) \geq 2 > 1$. Since $d(v_j) > d(v_1) \geq 1$, we know by Lemma 2.2 that the function $g_{d(v_1),d(v_j)}(x)$ is increasing in x, and then

$$\begin{aligned} ABC(T) - ABC(T') &= f(d(v_0), d(v_1)) + f(d(v_j), d(v_{j+1})) - f(d(v_0), d(v_j)) - f(d(v_1), d(v_{j+1})) \\ &= \big(f(d(v_0), d(v_1)) - f(d(v_0), d(v_j))\big) - \big(f(d(v_1), d(v_{j+1})) - f(d(v_j), d(v_{j+1}))\big) \\ &= g_{d(v_1),d(v_j)}(d(v_0)) - g_{d(v_1),d(v_j)}(d(v_{j+1})) \\ &= g_{d(v_1),d(v_j)}(1) - g_{d(v_1),d(v_j)}(d(v_{j+1})) < 0, \end{aligned}$$

which is a contradiction. Thus $d(v_1) \geq d(v_j)$ for $2 \leq j \leq t-2$. Similarly, we have $d(v_{t-1}) \geq d(v_j)$ for $2 \leq j \leq t-2$. Thus we may assume that $d(v_1) \geq d(v_{t-1}) \geq d(v_j)$ for $2 \leq j \leq t-2$. The result for $i = 1$ follows.

Suppose that the result is true for $i = k \geq 1$. We consider the case $i = k+1$. Suppose that k is odd. Then $k+1$ is even, and by the induction hypothesis, we have $d(v_k) \geq d(v_{t-k}) \geq d(v_j)$ for $k+1 \leq j \leq t-k-1$. Suppose that $d(v_{k+1}) > d(v_j)$ for some j with $k+2 \leq j \leq t-k-2$. Let $T'' = T - \{v_k v_{k+1}, v_j v_{j+1}\} + \{v_k v_j, v_{k+1} v_{j+1}\}$. Obviously, T'' has the same degree sequence as T. Note that the path P in T is changed into the path $Q = v_0 v_1 \ldots v_k v_j v_{j-1} \ldots v_{k+2} v_{k+1} v_{j+1} v_{j+2} \ldots v_t$ in T'', and the degree of the $(k+1)$-th vertex (v_j) of Q is less than the degree of the j-th vertex (v_{k+1}) of Q in T''. Since $j+1 \leq t-k-1$, we have $d(v_k) \geq d(v_{j+1})$. Similarly as above, we have

$$\begin{aligned} ABC(T) - ABC(T'') &= f(d(v_k), d(v_{k+1})) + f(d(v_j), d(v_{j+1})) - f(d(v_k), d(v_j)) - f(d(v_{k+1}), d(v_{j+1})) \\ &= \Big(f(d(v_j), d(v_{j+1})) - f(d(v_{k+1}), d(v_{j+1}))\Big) - \Big(f(d(v_k), d(v_j)) - f(d(v_k), d(v_{k+1}))\Big) \\ &= g_{d(v_j), d(v_{k+1})}(d(v_{j+1})) - g_{d(v_j), d(v_{k+1})}(d(v_k)) \leq 0. \end{aligned}$$

Thus we may assume that $d(v_{k+1}) \leq d(v_j)$ for $k+2 \leq j \leq t-k-2$. Similarly, we may also have $d(v_{t-k-1}) \leq d(v_j)$ for $k+2 \leq j \leq t-k-2$. If $d(v_{k+1}) > d(v_{t-k-1})$, then as above, we have $ABC(T) \leq ABC(T - \{v_k v_{k+1}, v_{t-k-1} v_{t-k}\} + \{v_k v_{t-k-1}, v_{k+1} v_{t-k}\})$. Thus we may assume that $d(v_{k+1}) \leq d(v_{t-k-1}) \leq d(v_j)$ for $k+2 \leq j \leq t-k-2$. The result follows for $i = k+1$ with odd k. Similarly, the result follows for $i = k+1$ with even k. □

From Lemma 3.1, the following corollary follows easily.

Corollary 3.2. *Let T be a tree with maximum ABC index among the trees with fixed degree sequence. For $v_i \in L_i$ and $v_j \in L_j$ with $j > i \geq 1$, if i is odd, then $d(v_i) \geq d(v_j)$, and if i is even, then $d(v_i) \leq d(v_j)$.*

Given the degree sequence $D = \{d_1, d_2, \ldots, d_m\}$, an extremal tree T that achieves the maximum ABC index among the trees with degree sequence D can be constructed as follows:

(i) If $d_m \geq m-1$, then by Corollary 3.2, the vertices with degrees respectively $d_1, d_2, \ldots, d_{m-1}$ are all in L_1, and thus we construct an extremal tree T by rooting at vertex u with d_m children with degrees $d_1, d_2, \ldots, d_{m-1}$ and $\underbrace{1, \ldots, 1}_{d_m - m + 1 \text{ times}}$.

(ii) Suppose that $d_m \leq m-2$.

(a) For the extremal tree T, by Corollary 3.2, the vertices in L_1 take some largest degrees and they are adjacent to the vertices in L_2 with some smallest degrees. We construct some subtrees that contain vertices in L_0, L_1 and L_2 first. We produce subtree T_1: rooted at vertex u_1 with $d_m - 1$ children with degrees $d_1, d_2, \ldots, d_{d_m - 1}$, where $u_1 \in L_2$, $d_T(u_1) = d_m$, and the children of u_1 are all in L_1. Removing T_1 except the root u_1 from T results in a new tree S_1 with degree sequence $D_1 = \{d_{d_m}, d_{d_m+1}, \ldots, d_{m-1}\}$. By Lemma 3.1 and Corollary 3.2, S_1 is a tree with maximum ABC index among the trees with the degree sequence D_1. Then do the same to S_1 to get T_2 and S_2, and then T_3 and S_3, and so on, until S_k satisfies the condition of (i).

(b) For $i = k, k-1, \ldots, 1$, the remaining is to identify u_i with which pendent vertex of S_i. Let v_i be the pendent vertex in S_i with which u_i is identified, and let w_i be the unique neighbor of v_i in S_i. Since T is a tree of degree sequence D with maximum ABC index, we need to maximize

$$ABC(T) = f(d_{T_i}(u_i) + 1, d_{S_i}(w_i)) + F,$$

where F is a constant independent of the pendent vertex of S_i that we identify u_i with. Note that $d_{T_i}(u_i) + 1 \geq 2$. By Lemma 2.1, we need to minimize $d_{S_i}(w_i)$.

Hence, we construct T as: identifying u_i with a pendent vertex v_i in S_i, where w_i is the unique neighbor of v_i in S_i, such that $w_i \in L_1(S_i)$ and $d_{S_i}(w_i) = \min\{d_{S_i}(x) : x \in L_1(S_i)\}$.

For an example, consider the degree sequence $\{4, 4, 3, 3, 3, 2, 2\}$. First, by (ii) a, we have the subtree T_1 and new degree sequence $D_1 = \{4, 3, 3, 3, 2\}$, and similarly, the tree T_2 and still new degree sequence $D_2 = \{3, 3, 3\}$. It is easily seen that D_2 satisfies the condition of (i), and thus we have S_2. There are three vertices in $L_1(S_2)$ with degree three, two of which are symmetric in S_2, and then by (ii) b, we have two types of S_1 by identifying u_2 of T_2 and a pendent vertex of S_2. Similarly, by identifying u_1 of T_1 and a pendent vertex of S_1, we have three extremal trees (of fixed degree sequence $\{4, 4, 3, 3, 3, 2, 2\}$) with maximum ABC index, see Fig. 1.

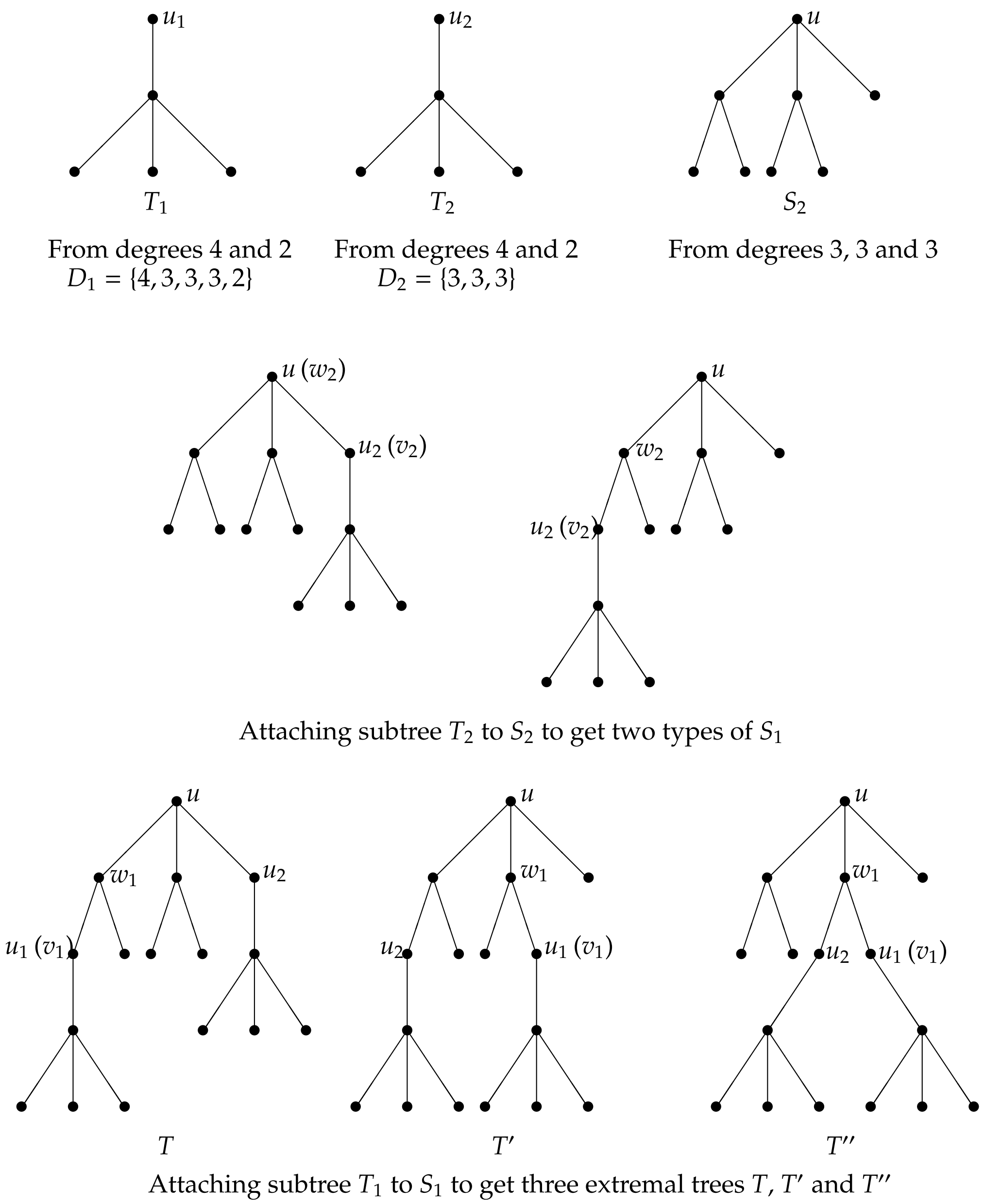

Fig. 1. The procedure to construct extremal trees of degree sequence $\{4, 4, 3, 3, 3, 2, 2\}$ with maximum ABC index.

Compared with the result in [12], an extremal tree T that achieves the maximum ABC index is just the tree that achieves the maximum (general) Randić index for $\alpha < 0$ among the trees with fixed degree sequence.

4. Lower bound for the ABC index of trees with fixed degree sequence

In this section, we characterize the extremal trees with minimum ABC index among the trees with fixed degree sequence, and provide an algorithm to construct such trees.

Lemma 4.1. *Let T be a tree with minimum ABC index among the trees with fixed degree sequence. Let $P = v_1v_2 \dots v_t$ be a path in T, where $t \geq 4$ and $d(v_1) < d(v_t)$. Then $d(v_2) \leq d(v_{t-1})$.*

Proof. Suppose that $d(v_2) > d(v_{t-1})$. Let $T' = T - \{v_1v_2, v_{t-1}v_t\} + \{v_1v_{t-1}, v_2v_t\}$. Obviously, T' has the same degree sequence as T. Since $d(v_1) < d(v_t)$, we know by Lemma 2.2 that the function $g_{d(v_1),d(v_t)}(x)$ is increasing in x, and then

$$\begin{aligned} ABC(T) - ABC(T') &= f(d(v_1), d(v_2)) + f(d(v_{t-1}), d(v_t)) - f(d(v_1), d(v_{t-1})) - f(d(v_2), d(v_t)) \\ &= (f(d(v_1), d(v_2)) - f(d(v_2), d(v_t))) - (f(d(v_1), d(v_{t-1})) - f(d(v_{t-1}), d(v_t))) \\ &= g_{d(v_1),d(v_t)}(d(v_2)) - g_{d(v_1),d(v_t)}(d(v_{t-1})) > 0, \end{aligned}$$

which is a contradiction. □

By Lemma 4.1, we have the following corollaries, as in [10].

Corollary 4.2. *Let T be a tree with minimum ABC index among the trees with fixed degree sequence. Then there is no path $P = v_1v_2 \dots v_t$ in T with $t \geq 3$ such that $d(v_1), d(v_t) > d(v_i)$ for some $2 \leq i \leq t-1$.*

Corollary 4.3. *Let T be a tree with minimum ABC index among the trees with fixed degree sequence. For every positive integer d, the vertices with degrees at least d induce a subtree of T.*

Corollary 4.4. *Let T be a tree with minimum ABC index among the trees with fixed degree sequence. Then there are no two non-adjacent edges v_1v_2 and v_3v_4 such that $d(v_1) < d(v_3) \leq d(v_4) < d(v_2)$.*

By Corollary 4.3, the degrees of vertices in L_i are no more than the degrees of vertices in L_{i+1} for all $i = 0, 1, 2, \dots$. Thus the vertices of larger degrees have farther distances from L_0 than the vertices of smaller degrees.

Given the degree sequence $D = \{d_1, d_2, \dots, d_m\}$, let T be a tree with minimum ABC index among the trees with fixed degree sequence. If $m = 1$, then $d_1 = |V(T)| - 1$, and thus T is the star. Suppose that $m \geq 2$. Delorme et al. [10] discovered that the properties of extremal trees with maximum (general) Randić index for $\alpha = 1$ are the same as the features of Kruskal's classical algorithm for the minimum spanning tree problem. Wang [12] generalized it to the greedy algorithm.

Now an extremal tree T who achieves the minimum ABC index among the trees with fixed degree sequence $D = \{d_1, d_2, \dots, d_m\}$ can be constructed as:

(i) Label a vertex with the largest degree d_1 as v, which is the root;

(ii) Label the neighbors of v as $v_1, v_2, \dots, v_{d_1}$, such that $d(v_1) = d_2 \geq d(v_2) = d_3 \geq \dots \geq d(v_{d_1}) = d_{d_1+1}$;

(iii) Label the neighbors of v_1 except v as $v_{1,1}, v_{1,2}, \dots, v_{1,d_2-1}$ such that $d(v_{1,1}) = d_{d_1+2} \geq d(v_{1,2}) = d_{d_1+3} \geq \dots \geq d(v_{1,d_2-1}) = d_{d_1+d_2}$, and do the same for the vertices $v_2, v_3, \dots$;

(iv) Repeat (iii) for all the newly labeled vertices, and always start with the neighbors of the labeled vertex with the largest degree whose neighbors are not labeled yet.

Now we give an example to construct extremal trees of degree sequence $\{4, 4, 4, 3, 3, 2, 2\}$ with the minimum ABC index, see Fig. 2.

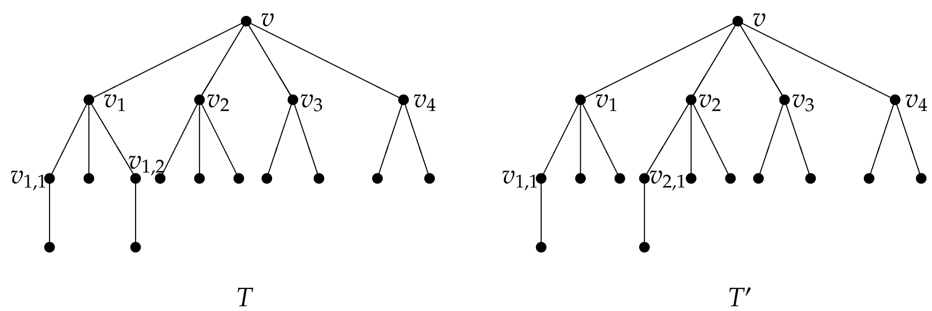

Fig. 2. Two extremal trees T and T' of degree sequence $\{4, 4, 4, 3, 3, 2, 2\}$ with minimum ABC index.

Compared with the result in [12], an extremal tree T that achieves the minimum ABC index is just the tree that achieves the minimum (general) Randić index for $\alpha < 0$ among the trees with fixed degree sequence.

5. Remark

Obviously, the ABC index of a graph G may be generalized to the general ABC index, defined as

$$ABC_\alpha(G) = \sum_{uv \in E(G)} \left(\frac{d(u) + d(v) - 2}{d(u)d(v)} \right)^\alpha$$

for real $\alpha \neq 0$, where G has no isolated K_2 (complete graph with two vertices) if $\alpha < 0$. Then $ABC_{\frac{1}{2}}(G) = ABC(G)$, and $ABC_{-3}(G)$ is the augmented Zagreb index of G proposed in [13].

Let $f_\alpha(x, y) = \left(\frac{x+y-2}{xy}\right)^\alpha$ for (integers) $x, y \geq 1$ with $x + y > 2$. Then $\frac{\partial f_\alpha(x,y)}{\partial x} = \frac{\alpha(2-y)(x+y-2)^{\alpha-1}}{x^{\alpha+1} y^\alpha}$. If $y \geq 2$ is fixed, then $f_\alpha(x, y)$ is decreasing in x for $\alpha > 0$ and increasing in x for $\alpha < 0$.

For $s > r \geq 1$, let $g_{\alpha;r,s}(x) = f_\alpha(x, r) - f_\alpha(x, s)$. Then $g'_{\alpha;r,s}(x) = \frac{\alpha}{x^{\alpha+1}} (h_\alpha(r) - h_\alpha(s))$, where $h_\alpha(t) = \frac{(2-t)(t+x-2)^{\alpha-1}}{t^\alpha}$ for (integer) $t \geq 1$ with $t + x > 2$. It is easily seen that $h'_\alpha(t) = \frac{(t+x-2)^{\alpha-2}}{t^{\alpha+1}} ((\alpha - 1)xt - 2\alpha(t + x - 2))$. Obviously, $h'_\alpha(t) < 0$ if $0 < \alpha \leq 1$. Suppose that $\alpha < 0$. If $x \geq 2$, then $h_\alpha(1) = (x - 1)^{\alpha-1} > 0 = h_\alpha(2)$, $h'_\alpha(t) < 0$ if $t \geq 2$, and thus $h_\alpha(t) > h_\alpha(t + 1)$ for (integer) $t \geq 1$. If $x = 1$, then $g_{\alpha;r,s}(1) = \left(1 - \frac{1}{r}\right)^\alpha - \left(1 - \frac{1}{s}\right)^\alpha > 0 = g_{\alpha;r,s}(2)$. It follows that $g_{\alpha;r,s}(x) > g_{\alpha;r,s}(x + 1)$ for (integer) $x \geq 1$ if $0 < \alpha \leq 1$ or $\alpha < 0$.

With these preparations, we have by similar analysis as in Sections 3 and 4 that an extremal tree that achieves the maximum (minimum, respectively) general ABC index for $0 < \alpha \leq 1$ is just the extremal tree with $\alpha = \frac{1}{2}$, and an extremal tree that achieves the maximum (minimum, respectively) general ABC index for $\alpha < 0$ is just the tree that achieves the minimum (maximum, respectively) ABC index.

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