

RESEARCH ARTICLE

The minimal-ABC trees with B_1 -branches

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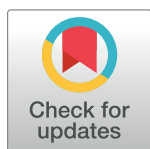
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Abstract

The atom-bond connectivity index (or, for short, ABC index) is a molecular structure descriptor bridging chemistry to graph theory. It is probably the most studied topological index among all numerical parameters of a graph that characterize its topology. For a given graph $G = (V, E)$, the ABC index of G is defined as $ABC(G) = \sum_{ij \in E} \sqrt{(d_i + d_j - 2)/(d_i d_j)}$, where d_i denotes the degree of the vertex i , and ij is the edge incident to the vertices i and j . A combination of physicochemical and the ABC index properties are commonly used to foresee the bioactivity of different chemical composites. Additionally, the applicability of the ABC index in chemical thermodynamics and other areas of chemistry, such as in dendrimer nanostars, benzenoid systems, fluoranthene congeners, and phenylenes is well studied in the literature. While finding of the graphs with the greatest ABC-value is a straightforward assignment, the characterization of the tree(s) with minimal ABC index is a problem largely open and has recently given rise to numerous studies and conjectures. A B_1 -branch of a graph is a pendent path of order 2. In this paper, we provide an important step forward to the full characterization of these minimal trees. Namely, we show that a minimal-ABC tree contains neither 4 nor 3 B_1 -branches. The case when the number of B_1 -branches is 2 is also considered.

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Introduction

The atom-bond connectivity index, widely known as ABC index, of a graph is a thoroughly studied vertex-degree-based graph invariant both in chemistry and mathematical communities. For a given simple graph $G = (V, E)$, let us denote by d_u the degree of vertex u , and uv the edge incident to the vertices u and v . The atom-bond connectivity index (or, simply, ABC index) is a vertex-degree-based graph topological index, which is a variation of the Randić graph-theoretic invariant [1], and is defined as

$$ABC(G) = \sum_{uv \in E} f(d_u, d_v),$$

where

$$f(d(u), d(v)) = \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

The relevance of the ABC index, in what we call today chemical graph theory, was first revealed two decades ago by Estrada, Torres, Rodríguez, and Gutman in [2]. They disclosed the importance of the ABC index as an analytical instrument for modeling thermodynamic properties of organic chemical compounds. Ten years later, Estrada [3] uncovered the significance of ABC index on the stability of branched alkanes, based on at that time a novel quantum-theory-like exposition. These studies were the trigger point for an uncountable number of papers on a new found area: chemical graph theory. Just to give two examples, in [4] it is proved that the ABC index of both benzenoid systems and fluoranthene congeners, consisting of two benzenoid fragments, depend exclusively on the number of vertices, hexagons and inlets. The author also characterized the extremal catacondensed benzenoid systems with the maximal and minimal ABC indices. The case of the phenylenes was considered by [5]. Another example of the importance of this topological descriptor can be seen on the calculation of the ABC index of an infinite class of nanostar dendrimers, artificially manufactured or synthesized molecule built up from branched units called monomers [6].

Many problems persist open, though. For example, it is known that the star of a given order has the maximal ABC index [7]. However for the trees with minimal ABC index, we are still far from a full characterization. For some further conjectures and partial results the reader is referred to [8–12]. More progress about minimal ABC trees can be found in [13–18].

A path $v_0 v_1 \cdots v_r$ in a graph G is said to be a pendent path of length r , where $d_{v_0} \geq 3$, $d_{v_1} = \cdots = d_{v_{r-1}} = 2$, and $d_{v_r} = 1$.

For the tree(s) with minimal ABC index, the length of its pendent paths is of crucial importance. In particular, the next lemma has become a key result in this area:

Lemma 1 [11, 19] *If T is a tree with minimal ABC index, then every pendent path in T is of length 2 or 3, and there is at most one pendent path of length 3 in T .*

In [20], Wang defined the greedy trees, for a given degree sequence, as follows:

Definition 1. *Suppose that the degrees of the non-leaf vertices are given, the greedy tree is achieved by the following ‘greedy algorithm’:*

1. Label the vertex with the largest degree as v (the root);
2. Label the neighbors of v as v_1, v_2, \dots , assign the largest degree available to them such that $d(v_1) \geq d(v_2) \geq \dots$;
3. Label the neighbors of v_1 (except v) as v_{11}, v_{12}, \dots , such that they take all the largest degrees available and that $d(v_{11}) \geq d(v_{12}) \geq \dots$, then do the same for v_2, v_3, \dots ;
4. Repeat (3) for all newly labeled vertices, always starting with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.

In particular, the vertex i is said to be the root of T , which is also the vertex lying on the first layer of T ; the vertices i_1, i_2, \dots are said to be the vertices lying on the second layer of T ; the vertices i_{11}, i_{12}, \dots are said to be the vertices lying on the third layer of T , and so on.

A major result attesting the importance of the greedy trees is the next proposition.

Proposition 2 ([21, 22]). *Given the degree sequence, the greedy tree minimizes the ABC index.*

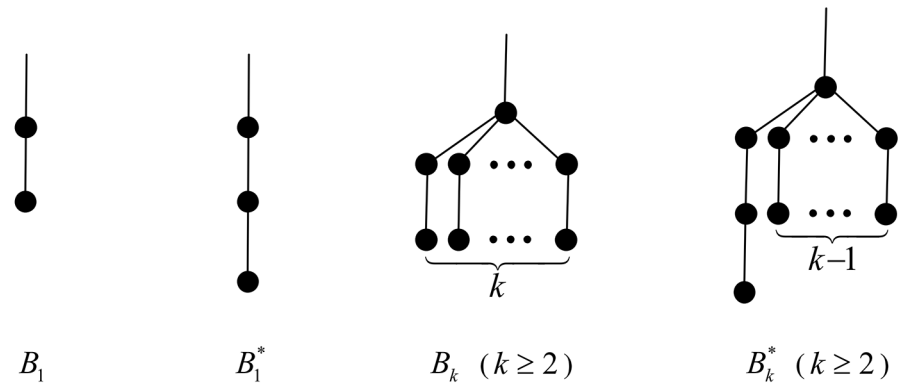


Fig 1. The B_k - and B_k^* -branches for $k \geq 1$.

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From the previous considerations, different types of branches will play a crucial role in our quest. Namely, the B_k -branches, with $k \geq 1$, and the B_k^* -branches, with $k \geq 1$, are illustrated in Fig 1.

In this regard, the most relevant results on minimal-ABC trees are listed next.

Proposition 3 ([23, Theorem 3.2]). *A minimal-ABC tree does not contain a B_k -branch, with $k > 4$.*

Proposition 4 ([24, Proposition 3.4]). *A minimal-ABC tree does not contain a B_3 -branch and a B_1^* -branch sharing a common parent vertex.*

Proposition 5 ([23, Lemma 3.3(a)]). *A minimal-ABC tree does not contain a B_4 -branch and a B_1 -branch sharing a common parent vertex.*

Proposition 6 ([25, Theorem 3.4]). *A minimal-ABC tree of order $n > 18$ with a pendent path of length 3 may contain a B_2 -branch if and only if it is of order 161 or 168. Moreover, in this case, a minimal-ABC tree is comprised of a single central vertex, B_3 -branches and one B_2 , including a pendent path of length 3 that may belong to a B_3^* -branch or B_2^* -branch.*

As a consequence of Proposition 6, we get the following proposition immediately.

Proposition 7. *A minimal-ABC tree cannot contain a B_2 -branch and a B_1^* -branch simultaneously.*

Recently, the authors were able to show in [26] that a minimal-ABC tree cannot contain simultaneously a B_4 -branch and B_1 - or B_2 -branches.

Recall that a k -terminal vertex of a rooted tree is a vertex of degree $k + 1 \geq 3$, which is a parent of only $B_{\geq 1}$ -branches, such that at least one branch among them is a B_1 -branch (or B_1^* -branch). The (sub)tree, induced by a k -terminal vertex and all its (direct and indirect) children (descendant) vertices, is called a k -terminal branch or T_k -branch.

Proposition 8 ([27, Proposition 2.13]). *A minimal-ABC tree contains at most one T_k -branch, with $k \geq 2$.*

Proposition 9 ([27, Theorem 3.5]). *A minimal-ABC tree contains at most four B_1 -branches.*

Although all the progress that has been lately made, the minimal-ABC trees seem still far from a full characterization. This paper contributes for this task. Specifically, we show that such trees contain neither 4 nor 3 B_1 -branches. The case when we have 2 B_1 -branches is also considered in the last section.

Preliminaries and methods

Lemmas

First we recall some technical lemmas.

Lemma 10 ([23, Proposition A.3]). *Let*

$$g(x, y) = f(x + \Delta x, y - \Delta y) - f(x, y)$$

with real numbers $x, y \geq 2, \Delta x \geq 0, 0 \leq \Delta y < y$. Then $g(x, y)$ increases in x and decreases in y .

Due to the symmetry of the function $g(x, y)$, we can also get an equivalent version of Lemma 10.

Lemma 11. *Let*

$$g(x, y) = f(x - \Delta x, y + \Delta y) - f(x, y)$$

with real numbers $x, y \geq 2, 0 \leq \Delta x < x, \Delta y \geq 0$. Then $g(x, y)$ decreases in x and increases in y .

In a similar fashion we have:

Lemma 12. *Let $h(x, y) = (y - 4)f(x + y - 5, 4) - f(x, y)$, where $x \geq y$ and $y = 6, 7, 8, 9, 10, 11$. Then for every fixed y , the function $h(x, y)$ decreases in $x \geq y$.*

proof. We only prove the case when $y = 6$. The other cases are similar.

Suppose that $y = 6$. Then $h(x, 6) = 2f(x + 1, 4) - f(x, 6)$.

First we have

$$\sqrt{6}x^2(x + 1)^{\frac{3}{2}}\sqrt{(x + 3)(x + 4)}h'(x, 6) = 2(x + 1)^{\frac{3}{2}}\sqrt{x(x + 3)} - \sqrt{6}x^2\sqrt{x + 4}.$$

Next, it is readily verified that

$$2(x + 1)^{\frac{3}{2}}\sqrt{x(x + 3)} - \sqrt{6}x^2\sqrt{x + 4} < 0$$

for $x \geq 6$.

Now it follows that $h'(x, 6) < 0$, i.e., $h(x, 6)$ decreases in $x \geq 6$.

Similar to the proof of Lemma 12, we can also get the following lemma.

Lemma 13. *Let $\ell(x, y) = (y - 3)f(x + y - 4, 3) - f(x, y)$, where $y = 5, 7, 8, 9$.*

1. *When $y = 5$, the function $\ell(x, 5)$ increases in $x > 0$.*
2. *When $y = 7$, the function $\ell(x, 7)$ decreases in $x \geq 19$.*
3. *When $y = 8$, the function $\ell(x, 8)$ decreases in $x \geq 17$.*
4. *When $y = 9$, the function $\ell(x, 9)$ decreases in $x \geq 16$.*

The root of B_1 -branches

A Kragujevac tree is a tree comprising of a single central vertex, B_k -branches, with $k \geq 1$, and at most one B_k^* -branch.

Lemma 14 ([28, Theorem 11]). *If T is a Kragujevac tree with minimal ABC index, and the degree of the central vertex of T is at least 19, then T contains no B_1 -branch.*

Taking into account Lemma 14, we can establish the main result in this section.

Proposition 15. *If T is a minimal-ABC tree on more than 122 vertices containing B_1 -branches, then the B_1 -branches cannot be attached to the root vertex of T .*

proof. Observe that the B_1 -branches of T are attached to the same vertex, say u , otherwise, there are at least two T_k -branches, which is a contradiction to Proposition 8. Suppose to the contrary that u is the root vertex of T .

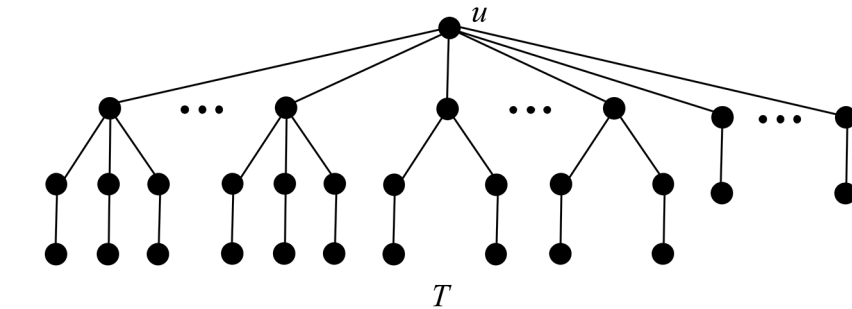


Fig 2. The tree T in the proof of Proposition 15.

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First, by Proposition 3, u contains no B_k -branch with $k > 4$. Next by Proposition 5, u contains no B_4 -branch, and by Propositions 4 and 7, u contains no B_1^* -branch, no matter u has B_3 -branches or B_2 -branches. Now we may deduce that the branches attached to u must be B_3 -, B_2 - or B_1 -branches, i.e., T is of the structure as depicted in Fig 2.

Notice that T is actually a Kragujevac tree. Denote by d_u the degree of u in T .

If $d_u \geq 19$, then from Lemma 14, T contains no B_1 -branch, which is a contradiction to the assumption for the existence of B_1 -branches in T .

If $d_u \leq 18$, then recall that every branch attached to u in T is a B_k -branch with $k = 1, 2, 3$, and thus the order of T is at most

$$1 + 7(d_u - 1) + 2 = 7d_u - 4 \leq 122,$$

which is a contradiction to the assumption for the order of T .

Now the result follows.

Since all the minimal-ABC trees of order up to 300 are completely determined in [29], we may assume that the trees considered in our main results have more than 300 vertices.

Switching transformation

Before we proceed with the main results of this paper, we present the so-called *switching transformation* explicitly stated by Lin, Gao, Chen, and Lin [30].

Lemma 16 (Switching transformation). *Let $G = (V, E)$ be a connected graph with $uv, xy \in E(G)$ and $uy, xv \notin E(G)$. Let $G_1 = G - uv - xy + uy + xv$. If $d(u) \geq d(x)$ and $d(v) \leq d(y)$, then $ABC(G_1) \leq ABC(G)$, with the equality if and only if $d(u) = d(x)$ or $d(v) = d(y)$.*

The switching transformation was used in the proofs of some characterizations of the minimal-ABC trees, and the following observation that will be applied in the further analysis.

Observation 1. *Let G be a minimal-ABC tree with the root vertex v_0 and let v_0, v_1, \dots, v_n be the sequence of vertices obtain by the breadth-first search of G . If $d(v_i), d(v_j) \geq 3$ and $i < j$, then by Lemma 16, we may assume that $d(v_i) \geq d(v_j)$.*

From Observation 1, we may assume that the trees considered are all greedy trees.

Results

The existence of four B_1 -branches

In this section we will prove our first main result: Any minimal-ABC tree cannot contain four B_1 -branches.

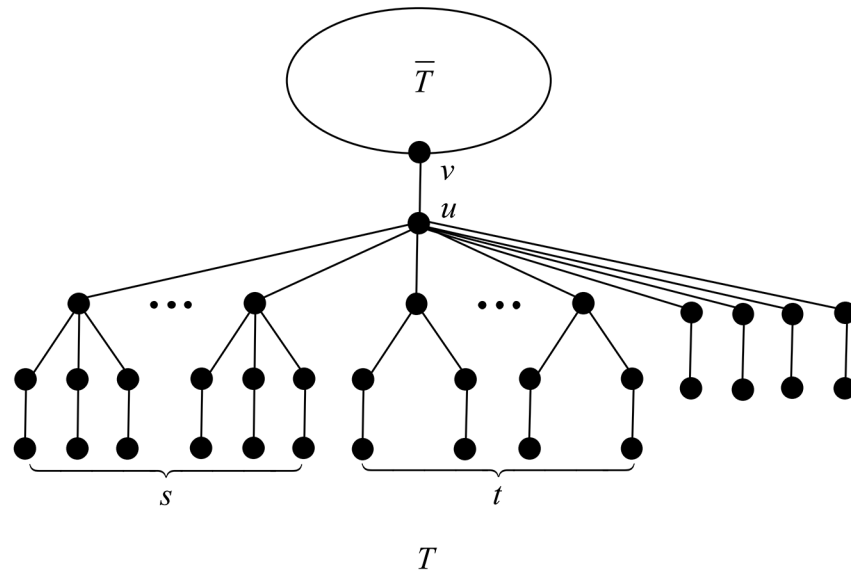


Fig 3. The tree T in Proposition 17 and Theorem 18.

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The following result is recent and establishes a forbidden configuration for minimal-ABC trees.

Proposition 17 ([27, Proposition 3.2]). *When $s + t > 6$, the configuration T depicted in Fig 3 cannot occur in a minimal-ABC tree.*

We are ready now to state the main result of this section.

Theorem 18. *A minimal-ABC tree cannot contain four B_1 -branches.*

proof. Suppose to the contrary that T is a minimal-ABC tree containing exactly four B_1 -branches. Observe that the four B_1 -branches are attached to the same vertex, say u , otherwise, there are at least two T_k -branches, which is a contradiction to Proposition 8. Moreover, by Proposition 15, u is not the root vertex of T . Let us denote by v the parent of u .

First, by Proposition 3, u contains no B_k -branch with $k > 4$. Next by Proposition 5, u contains no B_4 -branch, and by Propositions 4 and 7, u contains no B_1^* -branch, no matter u has B_3 -branches or B_2 -branches. Now we may deduce that the branches attached to u must be B_3 -, B_2 - or B_1 -branches, i.e., T is of the structure depicted in Fig 3.

Denote by s the number of B_3 -branches attached to u , and t the number of B_2 -branches attached to u . Clearly, $s + t \geq 1$, and $s + t \leq 6$ from Proposition 17.

Let d_x be the degree of vertex x in T .

Observe that $d_v \geq d_u = s + t + 5$ from Proposition 2.

Case 1. $t = 0$.

In this case, we apply the transformation \mathcal{T}_1 depicted in Fig 4.

After applying \mathcal{T}_1 , the degree of vertex v increases by s , while the degree of vertex u decreases by s . The rest of the vertices do not change their degrees. The change of the ABC

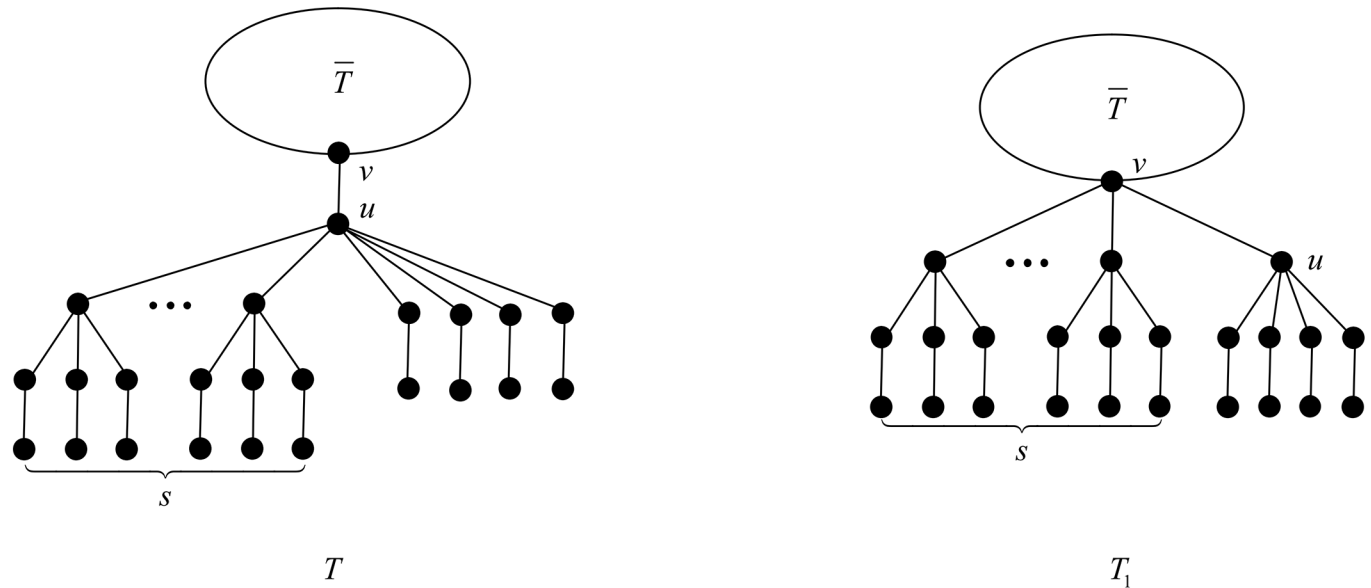


Fig 4. The transformation T_1 in Case 1 of Theorem 18.

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index after applying T_1 is

$$\begin{aligned}
 ABC(T_1) - ABC(T) &= \sum_{xv \in E(\bar{T})} (f(d_v + s, d_x) - f(d_v, d_x)) \\
 &\quad + f(d_v + s, 5) - f(d_v, s + 5) + s(f(d_v + s, 4) - f(s + 5, 4)).
 \end{aligned}$$

Clearly, $f(d_v + s, d_x) - f(d_v, d_x) < 0$ for $xv \in E(\bar{T})$, and thus

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< f(d_v + s, 5) - f(d_v, s + 5) + s[f(d_v + s, 4) - f(s + 5, 4)] \\
 &= (s + 1)f(d_v + s, 4) - f(d_v, s + 5) \\
 &\quad + f(d_v + s, 5) - f(d_v, s + 4) - s \cdot f(s + 5, 4).
 \end{aligned}$$

Recall that $d_v \geq s + 5$ from Proposition 2. On one hand, by Lemma 12, $(s + 1)f(d_v + s, 4) - f(d_v, s + 5)$ decreases in $d_v \geq s + 5$. On the other hand, by Lemma 11, $f(d_v + s, 5) - f(d_v, s + 4)$ also decreases in $d_v \geq s + 5$. So we get that

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< (s + 1)f((s + 5) + s, 4) - f(s + 5, s + 5) \\
 &\quad + f((s + 5) + s, 5) - f((s + 5) + s, 4) - s \cdot f(s + 5, 4) \\
 &= (s + 1)f(2s + 5, 4) - f(s + 5, s + 5) \\
 &\quad + f(2s + 5, 5) - f(2s + 5, 4) - s \cdot f(s + 5, 4).
 \end{aligned} \tag{1}$$

By virtue of Mathematica, the right-hand side of (1) is negative, equivalently $ABC(T_1) < ABC(T)$, follows from direct calculation, for $1 \leq s \leq 6$.

Case 2. $t \geq 1$.

In this case, we apply the transformation T_2 depicted in Fig 5.

After applying T_2 , the degree of vertex v increases by $s + t$, while the degree of vertex u decreases to 4, and a child of u in T belonging to a B_2 -branch increases its degree from 3 to 4.

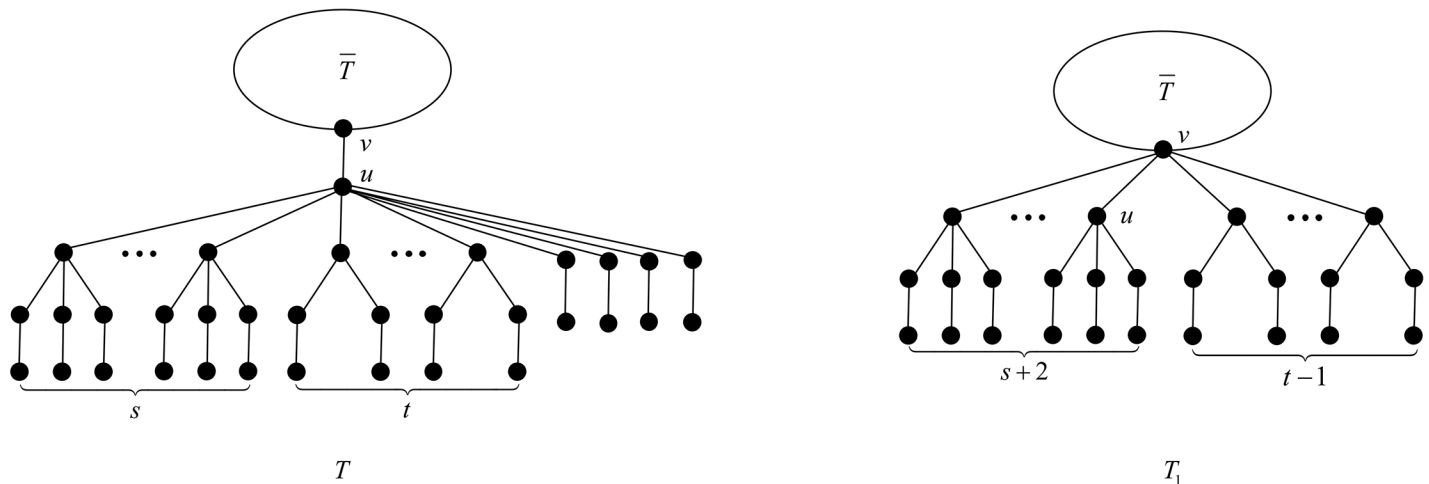


Fig 5. The transformation \mathcal{T}_2 in Case 2 of Theorem 18.

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The rest of the vertices do not change their degrees. The change of the ABC index after applying \mathcal{T}_2 is

$$\begin{aligned}
 ABC(T_1) - ABC(T) &= \sum_{xv \in E(\bar{T})} (f(d_v + s + t, d_x) - f(d_v, d_x)) \\
 &+ s(f(d_v + s + t, 4) - f(s + t + 5, 4)) \\
 &+ (t - 1)(f(d_v + s + t, 3) - f(s + t + 5, 3)) \\
 &+ 2f(d_v + s + t, 4) - f(s + t + 5, 3) \\
 &- f(d_v, s + t + 5).
 \end{aligned} \tag{2}$$

Clearly, $f(d_v + s + t, d_x) - f(d_v, d_x) < 0$ for $xv \in E(\bar{T})$, and thus

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< s(f(d_v + s + t, 4) - f(s + t + 5, 4)) \\
 &+ (t - 1)(f(d_v + s + t, 3) - f(s + t + 5, 3)) \\
 &+ 2f(d_v + s + t, 4) - f(s + t + 5, 3) - f(d_v, s + t + 5).
 \end{aligned}$$

Let $r = s + t$ be a fixed number. Recall that $1 \leq r \leq 6$.

Now we have

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< (r - t)(f(d_v + r, 4) - f(r + 5, 4)) \\
 &+ (t - 1)(f(d_v + r, 3) - f(r + 5, 3)) \\
 &+ 2f(d_v + r, 4) - f(r + 5, 3) - f(d_v, r + 5).
 \end{aligned} \tag{3}$$

For the right-hand side of (3), notice that the coefficient of t is

$$(f(d_v + r, 3) - f(r + 5, 3)) - (f(d_v + r, 4) - f(r + 5, 4)).$$

Since $d_v > 5$, from Lemma 10, $f(d_v + r, y) - f(r + 5, y)$ decreases in $y \geq 2$, thus we may deduce that

$$(f(d_v + r, 3) - f(r + 5, 3)) - (f(d_v + r, 4) - f(r + 5, 4)) > 0.$$

Together with $t \leq r$, we have

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< (r - r)(f(d_v + r, 4) - f(r + 5, 4)) \\
 &\quad + (r - 1)(f(d_v + r, 3) - f(r + 5, 3)) \\
 &\quad + 2f(d_v + r, 4) - f(r + 5, 3) - f(d_v, r + 5) \\
 &= (r - 1)f(d_v + r, 3) + 2f(d_v + r, 4) \\
 &\quad - f(d_v, r + 5) - r \cdot f(r + 5, 3).
 \end{aligned} \tag{4}$$

Recall that $d_v \geq r + 5$ from Proposition 2.

Subcase 2.1. $r = 1$.

If $r = 1$, then by (4), we have

$$ABC(T_1) - ABC(T) < 2f(d_v + 1, 4) - f(d_v, 6) - f(6, 3).$$

Moreover, by Lemma 12, we know that $2f(d_v + 1, 4) - f(d_v, 6)$ decreases in $d_v \geq 6$, thus

$$ABC(T_1) - ABC(T) < 2f(6 + 1, 4) - f(6, 6) - f(6, 3) < 0,$$

i.e., $ABC(T_1) < ABC(T)$.

Subcase 2.2. $r = 2$.

If $r = 2$, then by (4), we have

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< f(d_v + 2, 3) + 2f(d_v + 2, 4) - f(d_v, 7) - 2f(7, 3) \\
 &= 3f(d_v + 2, 4) - f(d_v, 7) \\
 &\quad + f(d_v + 2, 3) - f(d_v + 2, 4) - 2f(7, 3).
 \end{aligned}$$

Moreover, by Lemma 12, we know that $3f(d_v + 2, 4) - f(d_v, 7)$ decreases in $d_v \geq 7$, and by Lemma 10, $f(d_v + 2, 3) - f(d_v + 2, 4)$ increases in d_v , thus

$$f(d_v + 2, 3) - f(d_v + 2, 4) \leq \lim_{d_v \rightarrow +\infty} (f(d_v + 2, 3) - f(d_v + 2, 4)) = \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{4}}.$$

So for $d_v \geq 11$, we get that

$$ABC(T_1) - ABC(T) < 3f(11 + 2, 4) - f(11, 7) + \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{4}} - 2f(7, 3) < 0,$$

i.e., $ABC(T_1) < ABC(T)$. For the remaining cases that $7 \leq d_v \leq 10$, by virtue of Mathematica, the right-hand side of (4) is negative, equivalently $ABC(T_1) < ABC(T)$, follows from direct calculation easily.

Subcase 2.3. $r = 3$.

If $r = 3$, then by (4), we have

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< 2f(d_v + 3, 3) + 2f(d_v + 3, 4) - f(d_v, 8) - 3f(8, 3) \\
 &= 4f(d_v + 3, 4) - f(d_v, 8) \\
 &\quad + 2(f(d_v + 3, 3) - f(d_v + 3, 4)) - 3f(8, 3).
 \end{aligned}$$

Moreover, by Lemma 12, we know that $4f(d_v + 3, 4) - f(d_v, 8)$ decreases in $d_v \geq 8$, and by

Lemma 10, $f(d_v + 3, 3) - f(d_v + 3, 4)$ increases in d_v , thus

$$f(d_v + 3, 3) - f(d_v + 3, 4) \leq \lim_{d_v \rightarrow +\infty} (f(d_v + 3, 3) - f(d_v + 3, 4)) = \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{4}}.$$

So for $d_v \geq 20$, we get that

$$ABC(T_1) - ABC(T) < 4f(20 + 3, 4) - f(20, 8) + 2\left(\sqrt{\frac{1}{3}} - \sqrt{\frac{1}{4}}\right) - 3f(8, 3) < 0,$$

i.e., $ABC(T_1) < ABC(T)$. For the remaining cases that $8 \leq d_v \leq 19$, by virtue of Mathematica, the right-hand side of (4) is negative, equivalently $ABC(T_1) < ABC(T)$, follows from direct calculation easily.

Subcase 2.4. $r = 4$.

If $r = 4$, then by (4), we have

$$\begin{aligned} ABC(T_1) - ABC(T) &< 3f(d_v + 4, 3) + 2f(d_v + 4, 4) - f(d_v, 9) - 4f(9, 3) \\ &= 5f(d_v + 4, 4) - f(d_v, 9) \\ &\quad + 3(f(d_v + 4, 3) - f(d_v + 4, 4)) - 4f(9, 3). \end{aligned}$$

Moreover, by Lemma 12, we know that $5f(d_v + 4, 4) - f(d_v, 9)$ decreases in $d_v \geq 9$, and by Lemma 10, $f(d_v + 4, 3) - f(d_v + 4, 4)$ increases in d_v , thus

$$f(d_v + 4, 3) - f(d_v + 4, 4) \leq \lim_{d_v \rightarrow +\infty} (f(d_v + 4, 3) - f(d_v + 4, 4)) = \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{4}}.$$

So for $d_v \geq 31$, we get that

$$ABC(T_1) - ABC(T) < 5f(31 + 4, 4) - f(31, 9) + 3\left(\sqrt{\frac{1}{3}} - \sqrt{\frac{1}{4}}\right) - 4f(9, 3) < 0,$$

i.e., $ABC(T_1) < ABC(T)$. For the remaining cases that $9 \leq d_v \leq 30$, by virtue of Mathematica, the right-hand side of (4) is negative, equivalently $ABC(T_1) < ABC(T)$, follows from direct calculation easily.

Subcase 2.5. $r = 5$.

If $r = 5$, then by (4), we have

$$\begin{aligned} ABC(T_1) - ABC(T) &< 4f(d_v + 5, 3) + 2f(d_v + 5, 4) - f(d_v, 10) - 5f(10, 3) \\ &= 6f(d_v + 5, 4) - f(d_v, 10) \\ &\quad + 4(f(d_v + 5, 3) - f(d_v + 5, 4)) - 5f(10, 3). \end{aligned}$$

Moreover, by Lemma 12, we know that $6f(d_v + 5, 4) - f(d_v, 10)$ decreases in $d_v \geq 10$, and by Lemma 10, $f(d_v + 5, 3) - f(d_v + 5, 4)$ increases in d_v , thus

$$f(d_v + 5, 3) - f(d_v + 5, 4) \leq \lim_{d_v \rightarrow +\infty} (f(d_v + 5, 3) - f(d_v + 5, 4)) = \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{4}}.$$

So for $d_v \geq 42$, we get that

$$ABC(T_1) - ABC(T) < 6f(42 + 5, 4) - f(42, 10) + 4\left(\sqrt{\frac{1}{3}} - \sqrt{\frac{1}{4}}\right) - 5f(10, 3) < 0,$$

i.e., $ABC(T_1) < ABC(T)$. For the remaining cases that $10 \leq d_v \leq 41$, by virtue of Mathematica, the right-hand side of (4) is negative, equivalently $ABC(T_1) < ABC(T)$, follows from direct calculation easily.

Subcase 2.6. $r = 6$.

If $r = 6$, then by (4), we have

$$\begin{aligned} ABC(T_1) - ABC(T) &< 5f(d_v + 6, 3) + 2f(d_v + 6, 4) - f(d_v, 11) - 6f(11, 3) \\ &= 7f(d_v + 6, 4) - f(d_v, 11) + 5(f(d_v + 6, 3) - f(d_v + 6, 4)) \\ &\quad - 6f(11, 3). \end{aligned}$$

Moreover, by Lemma 12, we know that $7f(d_v + 6, 4) - f(d_v, 11)$ decreases in $d_v \geq 11$, and by Lemma 10, $f(d_v + 6, 3) - f(d_v + 6, 4)$ increases in d_v , thus

$$f(d_v + 6, 3) - f(d_v + 6, 4) \leq \lim_{d_v \rightarrow +\infty} (f(d_v + 6, 3) - f(d_v + 6, 4)) = \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{4}}.$$

So for $d_v \geq 56$, we get that

$$ABC(T_1) - ABC(T) < 7f(56 + 6, 4) - f(56, 11) + 5\left(\sqrt{\frac{1}{3}} - \sqrt{\frac{1}{4}}\right) - 6f(11, 3) < 0,$$

i.e., $ABC(T_1) < ABC(T)$. For the cases that $18 \leq d_v \leq 55$, by virtue of Mathematica, the right-hand side of (4) is negative, equivalently $ABC(T_1) < ABC(T)$, follows from direct calculation easily.

As to the remaining cases that $11 \leq d_v \leq 17$, let us be a bit more precisely in (2) about the term

$$\sum_{xv \in E(\bar{T})} (f(d_v + s + t, d_x) - f(d_v, d_x)) = \sum_{xv \in E(\bar{T})} (f(d_v + 6, d_x) - f(d_v, d_x)).$$

Notice that the degree of every neighbor of v in \bar{T} is at least 3 from Proposition 2. Furthermore, by Lemma 10, $f(d_v + 6, d_x) - f(d_v, d_x)$ decreases in $d_x \geq 3$, we may deduce that

$$\sum_{xv \in E(\bar{T})} (f(d_v + 6, d_x) - f(d_v, d_x)) < f(d_v + 6, 3) - f(d_v, 3).$$

Now together with (4), it follows that

$$\begin{aligned} ABC(T_1) - ABC(T) &< f(d_v + 6, 3) - f(d_v, 3) \\ &\quad + 5f(d_v + 6, 3) + 2f(d_v + 6, 4) \\ &\quad - f(d_v, 11) - 6f(11, 3). \end{aligned} \tag{5}$$

By virtue of Mathematica, the right-hand side of (5) is negative, equivalently $ABC(T_1) < ABC(T)$, for $11 \leq d_v \leq 17$, follows from direct calculation easily.

Combining the above cases, the result follows easily.

The existence of three B_1 -branches

We proceed proving in this section that a minimal-ABC tree does not contain three B_1 -branches. Before that, we consider some preliminary results.

Proposition 19 ([27, Proposition 3.2]). *When $s + t > 8$, the configuration T depicted in Fig 6 cannot occur in a minimal-ABC tree.*

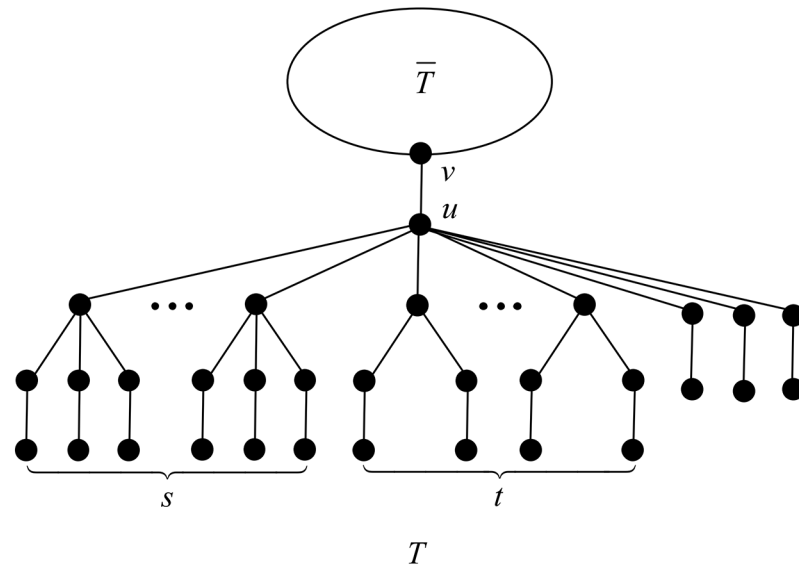


Fig 6. The tree T in Propositions 19, 20 and 21, and Theorem 22.

<https://doi.org/10.1371/journal.pone.0195153.g006>

Proposition 20 ([27, Proposition 3.4]). When $s = 0$ and $t > 3$, the configuration T depicted in Fig 6 cannot occur in a minimal-ABC tree.

Proposition 21. The configuration T depicted in Fig 6 cannot occur in a minimal-ABC tree, for the following cases:

- $t = 3$ and $s = 0, 4, 5$;
- $t = 4$ and $s = 2, 3, 4$;
- $t = 5$ and $s = 1, 2, 3$;
- $t = 6$ and $s = 1, 2$;
- $t = 7$ and $s = 1$.

proof. Let d_x be the degree of vertex x in T .

First we apply the transformation \mathcal{T}_1 illustrated in Fig 7.

After applying \mathcal{T}_1 , the degree of vertex u decreases by 3, while the degrees of three children of u in T belonging to a B_2 -branch increase from 3 to 4, and the rest of the vertices do not change their degrees. The change of the ABC index after applying \mathcal{T}_1 is

$$\begin{aligned} ABC(\mathcal{T}_1) - ABC(T) &= f(s + t + 1, d_v) - f(s + t + 4, d_v) \\ &\quad + (s + 3)f(s + t + 1, 4) + (t - 3)f(s + t + 1, 3) \\ &\quad - s \cdot f(s + t + 4, 4) - t \cdot f(s + t + 4, 3). \end{aligned}$$

From Lemma 11, $f(s + t + 1, d_v) - f(s + t + 4, d_v)$ increases in d_v , and thus

$$\begin{aligned} f(s + t + 1, d_v) - f(s + t + 4, d_v) &\leq \lim_{d_v \rightarrow +\infty} (f(s + t + 1, d_v) - f(s + t + 4, d_v)) \\ &= \sqrt{\frac{1}{s + t + 1}} - \sqrt{\frac{1}{s + t + 4}}. \end{aligned}$$

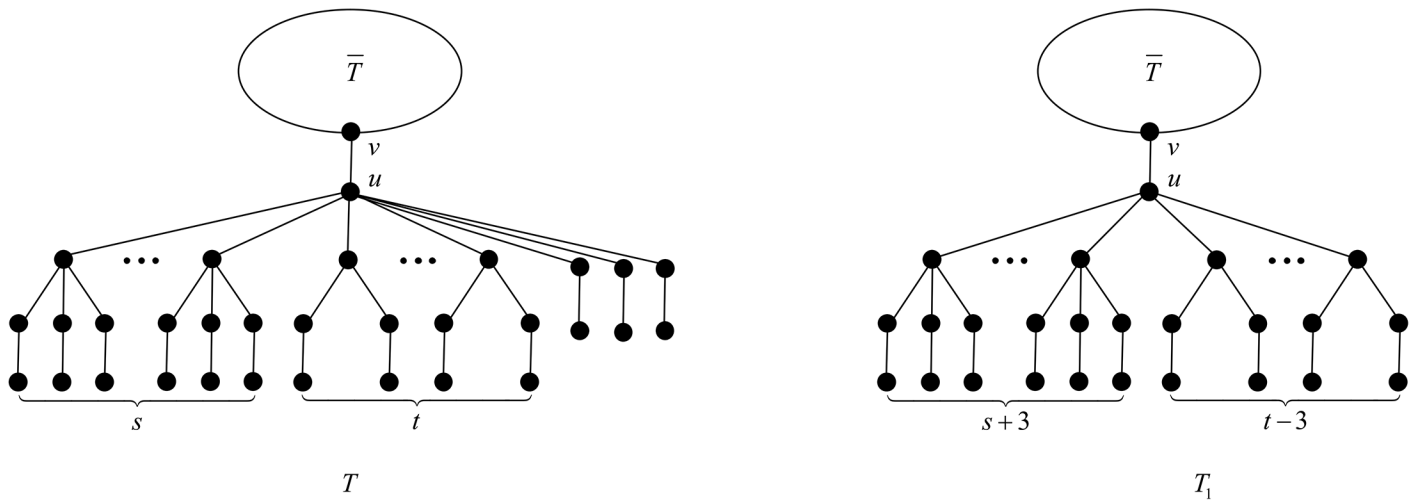


Fig 7. The transformation \mathcal{T}_1 in the proof of Proposition 21.

<https://doi.org/10.1371/journal.pone.0195153.g007>

Now it follows that

$$\begin{aligned}
 ABC(T_1) - ABC(T) \leq & \sqrt{\frac{1}{s+t+1}} - \sqrt{\frac{1}{s+t+4}} \\
 & + (s+3)f(s+t+1, 4) + (t-3)f(s+t+1, 3) \\
 & - s \cdot f(s+t+4, 4) - t \cdot f(s+t+4, 3).
 \end{aligned} \tag{6}$$

By virtue of Mathematica, the right-hand side of (6) is negative, equivalently $ABC(T_1) < ABC(T)$, follows from direct calculation easily, except the case $t = 3$ and $s = 0$. In such case, we apply the transformation \mathcal{T}_2 illustrated in Fig 8.

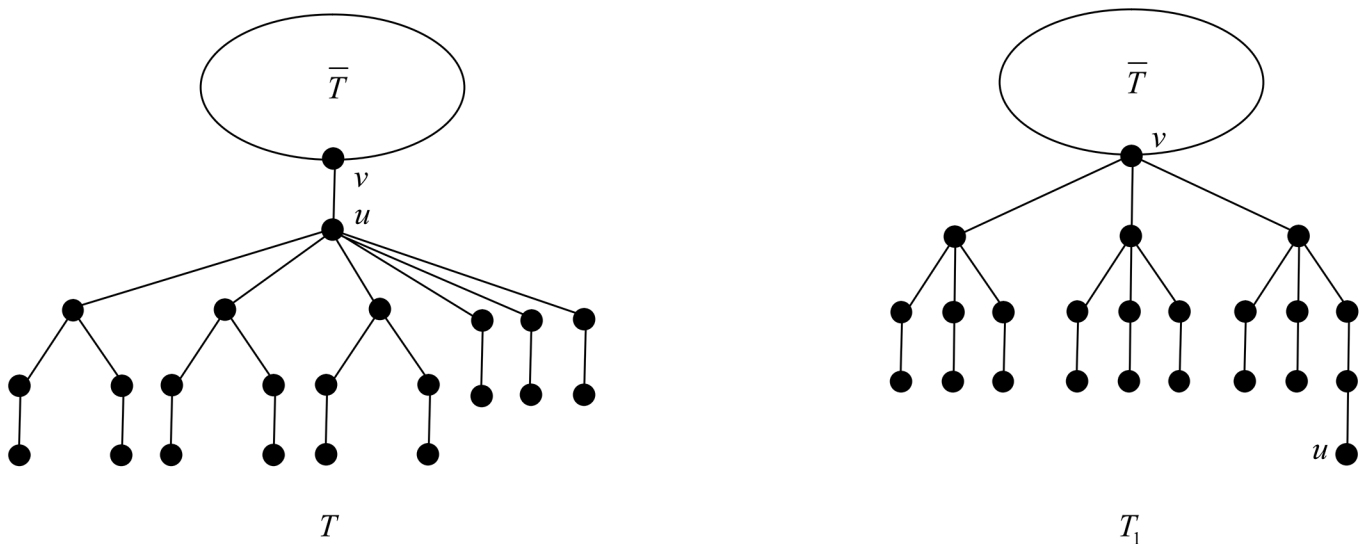


Fig 8. The transformation \mathcal{T}_2 in the proof of Proposition 21.

<https://doi.org/10.1371/journal.pone.0195153.g008>

After applying \mathcal{T}_2 , the degree of vertex v increases by 2, the degrees of three children of u in T belonging to a B_2 -branch increase from 3 to 4, a pendent vertex in T belonging to a B_2 -branch increases its degree from 1 to 2, the degree of u decreases from 7 to 1, and the rest of the vertices do not change their degrees. The change of the ABC index after applying \mathcal{T}_2 is

$$\begin{aligned}
 ABC(T_1) - ABC(T) &= \sum_{xv \in E(\bar{T})} (f(d_v + 2, d_x) - f(d_v, d_x)) \\
 &\quad + f(2, 1) - f(d_v, 7) + 3(f(d_v + 2, 4) - f(7, 3)).
 \end{aligned} \tag{7}$$

Clearly, $f(d_v + 2, d_x) - f(d_v, d_x) < 0$ for $xv \in E(\bar{T})$. So

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< f(2, 1) - f(d_v, 7) + 3(f(d_v + 2, 4) - f(7, 3)) \\
 &= 3f(d_v + 2, 4) - f(d_v, 7) + f(2, 1) - 3f(7, 3).
 \end{aligned}$$

Note that $d_v \geq d_u = 7$ from Proposition 2, and from Lemma 12, we know that $3f(d_v + 2, 4) - f(d_v, 7)$ decreases in $d_v \geq 7$. Therefore, for $d_v \geq 20$, we get that

$$ABC(T_1) - ABC(T) < 3f(20 + 2, 4) - f(20, 7) + f(2, 1) - 3f(7, 3) < 0.$$

For the remaining cases that $7 \leq d_v \leq 19$, let us be a bit more precisely in (7) for the term

$$\sum_{xv \in E(\bar{T})} (f(d_v + 2, d_x) - f(d_v, d_x)).$$

Note that every neighbor of v in \bar{T} has degree at least three from Proposition 2. By Lemma 10, $f(d_v + 2, d_x) - f(d_v, d_x)$ decreases in $d_x \geq 3$, and thus

$$\sum_{xv \in E(\bar{T})} (f(d_v + 2, d_x) - f(d_v, d_x)) \leq (d_v - 1)(f(d_v + 2, 3) - f(d_v, 3)).$$

Now together with (7), it follows that

$$\begin{aligned}
 ABC(T_1) - ABC(T) &\leq (d_v - 1)(f(d_v + 2, 3) - f(d_v, 3)) \\
 &\quad + f(2, 1) - f(d_v, 7) + 3(f(d_v + 2, 4) - f(7, 3)).
 \end{aligned} \tag{8}$$

By virtue of Mathematica, the right-hand side of (8) is negative, equivalently $ABC(T_1) < ABC(T)$, for $7 \leq d_v \leq 19$, follows from direct calculation easily.

Then the result follows.

We are now prepared to establish the main result of this section.

Theorem 22. *A minimal-ABC tree cannot contain three B_1 -branches.*

proof. Similarly to Theorem 18, let us suppose to the contrary that T is a minimal-ABC tree containing exactly three B_1 -branches. Observe that the three B_1 -branches are attached to the same vertex, say u , otherwise, there are at least two T_k -branches, which is a contradiction to Proposition 8. Moreover, by Proposition 15, u is not the root vertex of T . Denote by v the parent of u .

First, by Proposition 3, u contains no B_k -branch with $k > 4$. Next by Proposition 5, u contains no B_4 -branch, and by Propositions 4 and 7, u contains no B_1^* -branch, no matter u has B_3 -branches or B_2 -branches. Now we may deduce that the branches attached to u must be B_3 -, B_2 - or B_1 -branches, i.e., T is of the structure depicted in Fig 6.

Let us denote by s the number of B_3 -branches attached to u , and by t the number of B_2 -branches attached to u . Clearly, $s + t \geq 1$, and $s + t \leq 8$, from Proposition 19.

We apply the transformation \mathcal{T} depicted in Fig 9. And let d_x be the degree of vertex x in T .

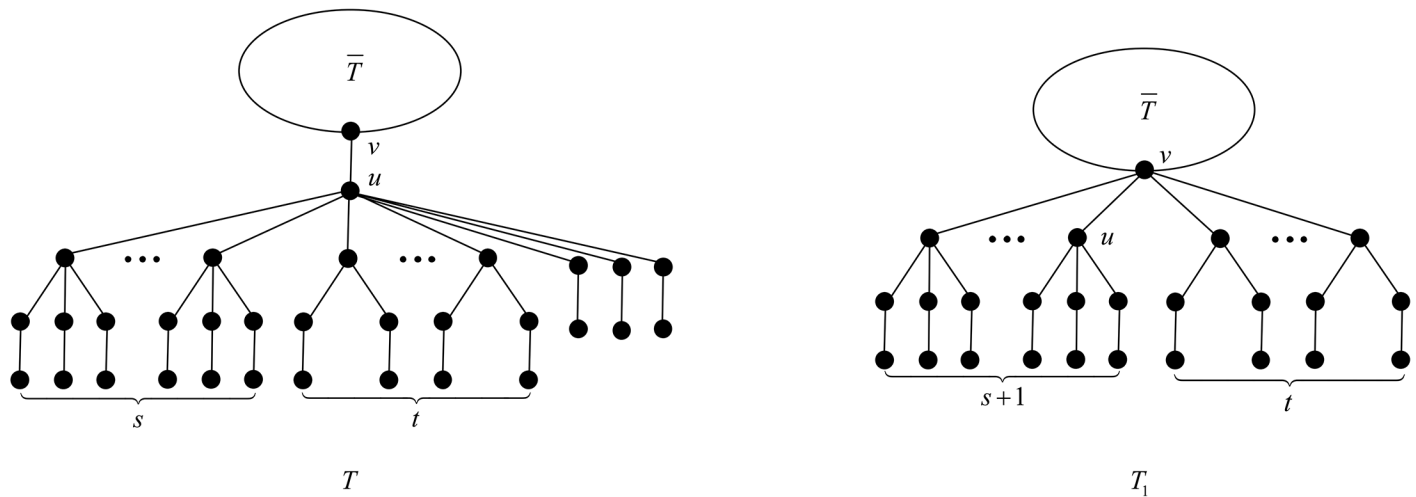


Fig 9. The transformation \mathcal{T} in the proof of Theorem 22.

<https://doi.org/10.1371/journal.pone.0195153.g009>

After applying \mathcal{T} , the degree of vertex v increases by $s + t$, while the degree of vertex u decreases by $s + t$, and the rest of the vertices do not change their degrees. The change of the ABC index after applying \mathcal{T} is

$$\begin{aligned}
 ABC(T_1) - ABC(T) &= \sum_{xv \in E(\bar{T})} (f(d_v + s + t, d_x) - f(d_v, d_x)) \\
 &+ s(f(d_v + s + t, 4) - f(s + t + 4, 4)) \\
 &+ t(f(d_v + s + t, 3) - f(s + t + 4, 3)) \\
 &+ f(d_v + s + t, 4) - f(d_v, s + t + 4).
 \end{aligned} \tag{9}$$

Clearly, $f(d_v + s + t, d_x) - f(d_v, d_x) < 0$ for $xv \in E(\bar{T})$, and thus

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< s(f(d_v + s + t, 4) - f(s + t + 4, 4)) \\
 &+ t(f(d_v + s + t, 3) - f(s + t + 4, 3)) \\
 &+ f(d_v + s + t, 4) - f(d_v, s + t + 4).
 \end{aligned}$$

On one hand, from Lemma 10, $f(d_v + s + t, 4) - f(d_v, s + t + 4)$ increases in d_v , thus

$$\begin{aligned}
 f(d_v + s + t, 4) - f(d_v, s + t + 4) &\leq \lim_{d_v \rightarrow +\infty} (f(d_v + s + t, 4) - f(d_v, s + t + 4)) \\
 &= \sqrt{\frac{1}{4}} - \sqrt{\frac{1}{s + t + 4}}.
 \end{aligned}$$

So it follows that

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< s(f(d_v + s + t, 4) - f(s + t + 4, 4)) \\
 &+ t(f(d_v + s + t, 3) - f(s + t + 4, 3)) \\
 &+ \sqrt{\frac{1}{4}} - \sqrt{\frac{1}{s + t + 4}}.
 \end{aligned} \tag{10}$$

On the other hand, note that $d_v \geq d_u = s + t + 4$ from Proposition 2, and both $f(d_v + s + t, 4)$ and $f(d_v + s + t, 3)$ decrease in $d_v \geq s + t + 4$, i.e., the right-hand side of (10) also decreases in $d_v \geq s + t + 4$.

Besides the upper bound about $ABC(T_1) - ABC(T)$ as (10), by considering a bit precisely in (9) for the term

$$\sum_{xv \in E(\bar{T})} (f(d_v + s + t, d_x) - f(d_v, d_x)),$$

we may get a somewhat stricter upper bound about $ABC(T_1) - ABC(T)$. Note that, from Lemma 10, $f(d_v + s + t, d_x) - f(d_v, d_x)$ decreases in d_x , and from Proposition 2, every neighbor of v in \bar{T} has degree at least three, thus

$$\sum_{xv \in E(\bar{T})} (f(d_v + s + t, d_x) - f(d_v, d_x)) \leq (d_v - 1)(f(d_v + s + t, 3) - f(d_v, 3)).$$

Now together with (9), it follows that

$$\begin{aligned} ABC(T_1) - ABC(T) \leq & (d_v - 1)(f(d_v + s + t, 3) - f(d_v, 3)) \\ & + s(f(d_v + s + t, 4) - f(s + t + 4, 4)) \\ & + t(f(d_v + s + t, 3) - f(s + t + 4, 3)) \\ & + f(d_v + s + t, 4) - f(d_v, s + t + 4). \end{aligned} \tag{11}$$

Case 1. $t = 0$.

In this case, note that $1 \leq s \leq 8$, and $d_v \geq s + 4$.

By direct calculation, we may deduce that the right-hand side of (10) is negative, equivalently $ABC(T_1) < ABC(T)$, holds for the following cases:

- $s = 1$ and $d_v \geq 12$;
- $s = 2$ and $d_v \geq 14$;
- $s = 3$ and $d_v \geq 16$;
- $s = 4$ and $d_v \geq 18$;
- $s = 5$ and $d_v \geq 21$;
- $s = 6$ and $d_v \geq 23$;
- $s = 7$ and $d_v \geq 26$;
- $s = 8$ and $d_v \geq 26$.

For the remaining cases as follows:

- $s = 1$ and $5 \leq d_v \leq 11$;
- $s = 2$ and $6 \leq d_v \leq 13$;
- $s = 3$ and $7 \leq d_v \leq 15$;
- $s = 4$ and $8 \leq d_v \leq 17$;
- $s = 5$ and $9 \leq d_v \leq 20$;
- $s = 6$ and $10 \leq d_v \leq 22$;
- $s = 7$ and $11 \leq d_v \leq 25$;

- $s = 8$ and $12 \leq d_v \leq 25$,

we would turn to use (11), and negative upper bounds, equivalently $ABC(T_1) < ABC(T)$, follow from direct calculation.

Case 2. $t = 1$.

In this case, note that $0 \leq s \leq 7$, and $d_v \geq s + 5$.

By direct calculation, we may deduce that the right-hand side of (10) is negative, equivalently $ABC(T_1) < ABC(T)$, holds for the following cases:

- $s = 0$ and $d_v \geq 124$;
- $s = 1$ and $d_v \geq 23$;
- $s = 2$ and $d_v \geq 22$;
- $s = 3$ and $d_v \geq 22$;
- $s = 4$ and $d_v \geq 25$;
- $s = 5$ and $d_v \geq 28$;
- $s = 6$ and $d_v \geq 30$;
- $s = 7$ and $d_v \geq 33$.

For the remaining cases as follows:

- $s = 0$ and $5 \leq d_v \leq 123$;
- $s = 1$ and $6 \leq d_v \leq 22$;
- $s = 2$ and $7 \leq d_v \leq 21$;
- $s = 3$ and $8 \leq d_v \leq 21$;
- $s = 4$ and $9 \leq d_v \leq 24$;
- $s = 5$ and $10 \leq d_v \leq 27$;
- $s = 6$ and $11 \leq d_v \leq 29$;
- $s = 7$ and $12 \leq d_v \leq 32$,

we would turn to use (11), and negative upper bounds, equivalently $ABC(T_1) < ABC(T)$, follow from direct calculation easily.

Case 3. $t = 2$.

In this case, note that $0 \leq s \leq 6$, and $d_v \geq s + 6$.

By direct calculation, we may deduce that the right-hand side of (10) is negative, equivalently $ABC(T_1) < ABC(T)$, holds for the following cases:

- $s = 0$ and $d_v \geq 751$;
- $s = 1$ and $d_v \geq 41$;
- $s = 2$ and $d_v \geq 34$;
- $s = 3$ and $d_v \geq 33$;
- $s = 4$ and $d_v \geq 35$;
- $s = 5$ and $d_v \geq 37$;
- $s = 6$ and $d_v \geq 39$.

For the remaining cases as follows:

- $s = 0$ and $6 \leq d_v \leq 750$;
- $s = 1$ and $7 \leq d_v \leq 40$;
- $s = 2$ and $8 \leq d_v \leq 33$;
- $s = 3$ and $9 \leq d_v \leq 32$;
- $s = 4$ and $10 \leq d_v \leq 34$;
- $s = 5$ and $11 \leq d_v \leq 36$;
- $s = 6$ and $12 \leq d_v \leq 38$,

we would turn to use (11), and negative upper bounds, equivalently $ABC(T_1) < ABC(T)$, follow from direct calculation easily.

Case 4. $t = 3$.

In this case, note that $0 \leq s \leq 5$, and $d_v \geq s + 7$.

On one hand, the contradiction for the cases $s = 0, 4, 5$ may be deduced from Proposition 21.

On the other hand, by direct calculation, we may deduce that the right-hand side of (10) is negative, equivalently $ABC(T_1) < ABC(T)$, holds for the following cases:

- $s = 1$ and $d_v \geq 74$;
- $s = 2$ and $d_v \geq 52$;
- $s = 3$ and $d_v \geq 48$.

For the remaining cases as follows:

- $s = 1$ and $8 \leq d_v \leq 73$;
- $s = 2$ and $9 \leq d_v \leq 51$;
- $s = 3$ and $10 \leq d_v \leq 47$,

we would turn to use (11), and negative upper bounds, equivalently $ABC(T_1) < ABC(T)$, follow from direct calculation easily.

Case 5. $t = 4$.

In this case, note that $0 \leq s \leq 4$, and $d_v \geq s + 8$.

The contradiction for the cases $s = 0$ and $s = 2, 3, 4$ may be, respectively, deduced from Propositions 20 and 21.

Besides that, by direct calculation, we may deduce that the right-hand side of (10) is negative, equivalently $ABC(T_1) < ABC(T)$, for $s = 1$ and $d_v \geq 145$. For the remaining cases $s = 1$ and $9 \leq d_v \leq 144$, we would turn to use (11), and a negative upper bound, equivalently $ABC(T_1) < ABC(T)$, follows from direct calculation easily.

Case 6. $t = 5$.

In this case, note that $s = 0, 1, 2, 3$. The contradiction for the cases $s = 0$ and $s = 1, 2, 3$ may be, respectively, deduced from Propositions 20 and 21.

Case 7. $t = 6$.

In this case, note that $s = 0, 1, 2$. The contradiction for the cases $s = 0$ and $s = 1, 2$ may be, respectively, deduced from Propositions 20 and 21.

Case 8. $t = 7$.

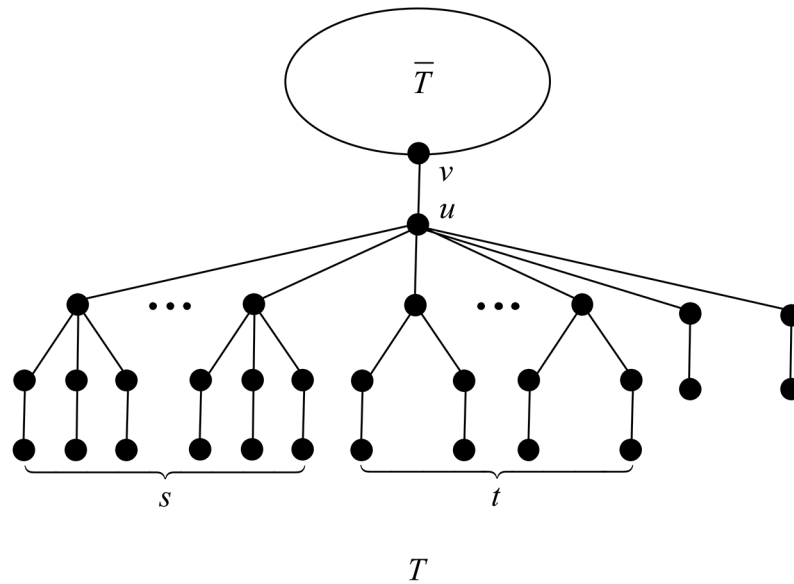


Fig 10. The tree T in Propositions 23, 24 and 25, and Theorem 26.

<https://doi.org/10.1371/journal.pone.0195153.g010>

In this case, note that $s = 0, 1$. The contradiction for the cases $s = 0$ and $s = 1$ may be, respectively, deduced from Propositions 20 and 21.

Case 9. $t = 8$.

In this case, note that $s = 0$. The contradiction may be deduced from Proposition 20 directly.

Combining the above cases, the result follows.

The existence of two B_1 -branches

This last section is devoted to the analysis of the existence of two B_1 -branches in a minimal-ABC tree. The first two propositions are known results establishing forbidden configurations in such cases.

Proposition 23 ([27, Proposition 3.2]). *When $s + t > 10$, the configuration T depicted in Fig 10 cannot occur in a minimal-ABC tree.*

Proposition 24 ([27, Proposition 3.4]). *When $s = 0$ and $t > 4$, the configuration T depicted in Fig 10 cannot occur in a minimal-ABC tree.*

We next list several cases more where the configuration depicted in Fig 10 is not possible in a minimal-ABC tree.

Proposition 25. *The configuration T depicted in Fig 10 cannot occur in a minimal-ABC tree, for the following cases:*

- $t = 2$ and $s = 0$;
- $t = 3$ and $s = 1, 2$;
- $t = 4$ and $s = 0, 1, 2, 3, 4, 5, 6$;
- $t = 5$ and $s = 1, 2, 3, 4, 5$;
- $t = 6$ and $s = 1, 2, 3, 4$;

- $t = 7$ and $s = 1, 2, 3$;
- $t = 8$ and $s = 1, 2$;
- $t = 9$ and $s = 1$.

proof. First we apply the transformation \mathcal{T}_1 illustrated in Fig 11. Let d_x be the degree of vertex x in T .

After applying \mathcal{T}_1 , the degree of vertex u decreases by 2, while the degrees of two children of u in T belonging to a B_2 -branch increase from 3 to 4. The rest of the vertices do not change their degrees. The change of the ABC index after applying \mathcal{T}_1 is

$$\begin{aligned} ABC(\mathcal{T}_1) - ABC(T) &= f(s+t+1, d_v) - f(s+t+3, d_v) \\ &\quad + (s+2)f(s+t+1, 4) + (t-2)f(s+t+1, 3) \\ &\quad - s \cdot f(s+t+3, 4) - t \cdot f(s+t+3, 3). \end{aligned}$$

From Lemma 11, $f(s+t+1, d_v) - f(s+t+3, d_v)$ increases in d_v , and thus

$$\begin{aligned} f(s+t+1, d_v) - f(s+t+3, d_v) &\leq \lim_{d_v \rightarrow +\infty} (f(s+t+1, d_v) - f(s+t+3, d_v)) \\ &= \sqrt{\frac{1}{s+t+1}} - \sqrt{\frac{1}{s+t+3}}. \end{aligned}$$

Now it follows that

$$\begin{aligned} ABC(\mathcal{T}_1) - ABC(T) &\leq \sqrt{\frac{1}{s+t+1}} - \sqrt{\frac{1}{s+t+3}} \\ &\quad + (s+2)f(s+t+1, 4) + (t-2)f(s+t+1, 3) \\ &\quad - s \cdot f(s+t+3, 4) - t \cdot f(s+t+3, 3). \end{aligned} \tag{12}$$

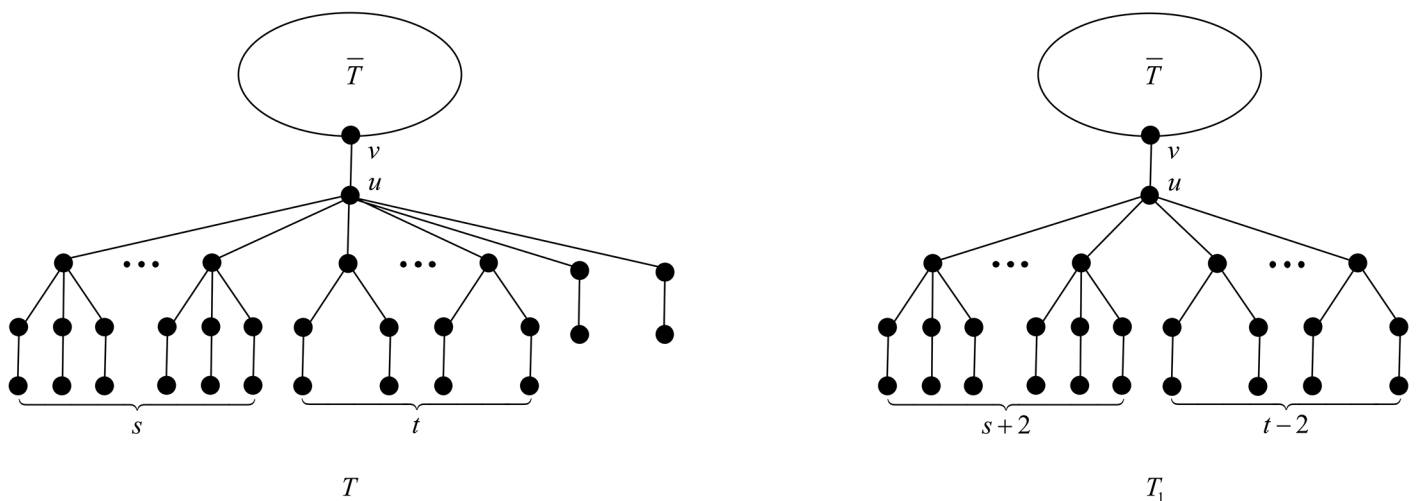


Fig 11. The transformation \mathcal{T}_1 in the proof of Proposition 25.

<https://doi.org/10.1371/journal.pone.0195153.g011>

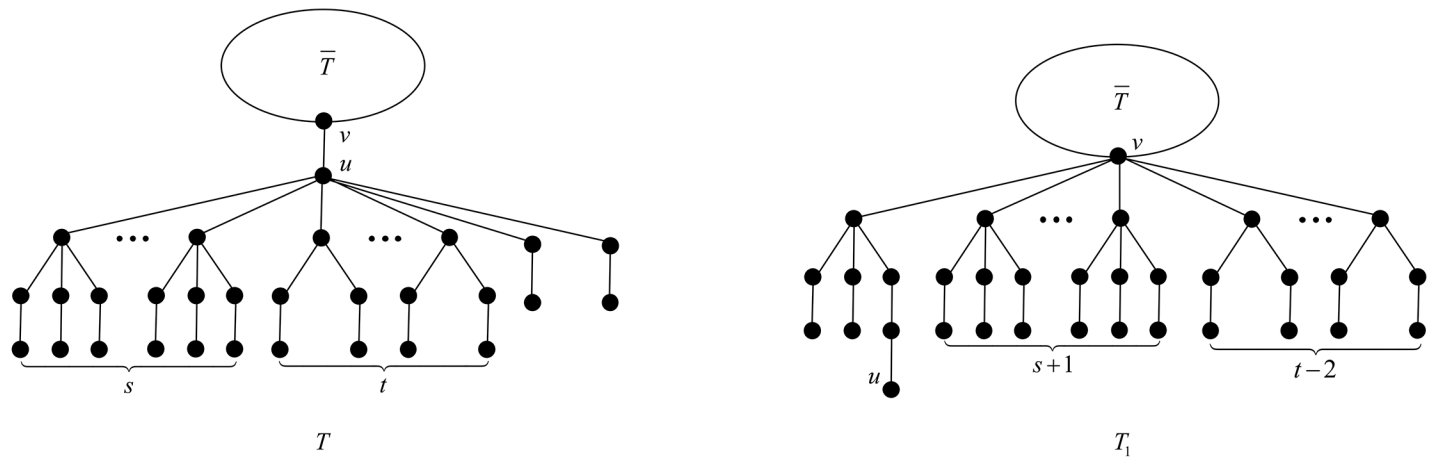


Fig 12. The transformation \mathcal{T}_2 in the proof of Proposition 25.

<https://doi.org/10.1371/journal.pone.0195153.g012>

The right-hand side of (12) is negative, equivalently $ABC(T_1) < ABC(T)$, holds for the following cases:

- $t = 4$ and $s = 3, 4, 5, 6$;
- $t = 5$ and $s = 2, 3, 4, 5$;
- $t = 6$ and $s = 1, 2, 3, 4$;
- $t = 7$ and $s = 1, 2, 3$;
- $t = 8$ and $s = 1, 2$;
- $t = 9$ and $s = 1$.

Next for the following cases:

- $t = 2$ and $s = 0$;
- $t = 3$ and $s = 1, 2$;
- $t = 4$ and $s = 1, 2$,

we apply the transformation \mathcal{T}_2 illustrated in Fig 12.

After applying \mathcal{T}_2 , the degree of vertex v increases by $s + t - 1$, the degrees of two children of u in T belonging to a B_2 -branch increase from 3 to 4, a pendent vertex in T belonging to a B_3 -branch increases its degree from 1 to 2, the degree of u decreases from $s + t + 3$ to 1, and the rest of the vertices do not change their degrees. The change of the ABC index after applying \mathcal{T}_2 is

$$\begin{aligned}
 ABC(T_1) - ABC(T) &= \sum_{xv \in E(\bar{T})} (f(d_v + s + t - 1, d_x) - f(d_v, d_x)) \\
 &+ s(f(d_v + s + t - 1, 4) - f(s + t + 3, 4)) \\
 &+ t(f(d_v + s + t - 1, 3) - f(s + t + 3, 3)) \\
 &+ 2(f(d_v + s + t - 1, 4) - f(d_v + s + t - 1, 3)) \\
 &+ f(1, 2) - f(d_v, s + t + 3).
 \end{aligned} \tag{13}$$

Clearly, $f(d_v + s + t - 1, d_x) - f(d_v, d_x) \leq 0$, for $xv \in E(\bar{T})$. So

$$\begin{aligned}
 ABC(T_1) - ABC(T) &\leq s(f(d_v + s + t - 1, 4) - f(s + t + 3, 4)) \\
 &\quad + t(f(d_v + s + t - 1, 3) - f(s + t + 3, 3)) \\
 &\quad + 2(f(d_v + s + t - 1, 4) - f(d_v + s + t - 1, 3)) \\
 &\quad + f(1, 2) - f(d_v, s + t + 3) \\
 &= (s + t)f(d_v + s + t - 1, 3) - f(d_v, s + t + 3) \\
 &\quad + (s + 2)(f(d_v + s + t - 1, 4) - f(d_v + s + t - 1, 3)) \\
 &\quad - s \cdot f(s + t + 3, 4) - t \cdot f(s + t + 3, 3) + f(1, 2).
 \end{aligned} \tag{14}$$

Note that $d_v \geq d_u = s + t + 3$ from Proposition 2, and from Lemma 13, we know that $(s + t)f(d_v + s + t - 1, 3) - f(d_v, s + t + 3)$ increases in $d_v \geq 5$ when $t = 2$ and $s = 0$, and decreases in

- $d_v \geq 19$ when $t = 3$ and $s = 1$;
- $d_v \geq 17$ when $t = 3$ and $s = 2$, or $t = 4$ and $s = 1$;
- $d_v \geq 16$ when $t = 4$ and $s = 2$.

On the other hand, from Lemma 11, $f(d_v + s + t - 1, 4) - f(d_v + s + t - 1, 3)$ also decreases in $d_v \geq s + t + 3$.

So if $t = 2$ and $s = 0$, and $d_v \geq 83$, then by (14),

$$\begin{aligned}
 ABC(T_1) - ABC(T) &\leq 2f(d_v + 1, 3) - f(d_v, 5) \\
 &\quad + 2(f(d_v + 1, 4) - f(d_v + 1, 3)) \\
 &\quad - 2f(5, 3) + f(1, 2) \\
 &\leq \lim_{d_v \rightarrow +\infty} (2f(d_v + 1, 3) - f(d_v, 5)) \\
 &\quad + 2(f(83 + 1, 4) - f(83 + 1, 3)) \\
 &\quad - 2f(5, 3) + f(1, 2) \\
 &< 0.
 \end{aligned}$$

Otherwise, the right-hand of (14) decreases in the following cases:

- $d_v \geq 19$ when $t = 3$ and $s = 1$;
- $d_v \geq 17$ when $t = 3$ and $s = 2$ or $t = 4$ and $s = 1$;
- $d_v \geq 16$ when $t = 4$ and $s = 2$.

Besides the upper bound about $ABC(T_1) - ABC(T)$ as (14), by considering in particular in (13) the term

$$\sum_{xv \in E(\bar{T})} (f(d_v + s + t - 1, d_x) - f(d_v, d_x)),$$

we may get a somewhat stricter upper bound about $ABC(T_1) - ABC(T)$. Note that, from Lemma 10, $f(d_v + s + t - 1, d_x) - f(d_v, d_x)$ decreases in d_x , and from Proposition 2, every neighbor of v in \bar{T} has degree at least three, thus

$$\sum_{xv \in E(\bar{T})} (f(d_v + s + t - 1, d_x) - f(d_v, d_x)) \leq (d_v - 1)(f(d_v + s + t - 1, 3) - f(d_v, 3)).$$

Now together with (13), it follows that

$$\begin{aligned}
 ABC(T_1) - ABC(T) \leq & (d_v - 1)(f(d_v + s + t - 1, 3) - f(d_v, 3)) \\
 & + s(f(d_v + s + t - 1, 4) - f(s + t + 3, 4)) \\
 & + t(f(d_v + s + t - 1, 3) - f(s + t + 3, 3)) \\
 & + 2(f(d_v + s + t - 1, 4) - f(d_v + s + t - 1, 3)) \\
 & + f(1, 2) - f(d_v, s + t + 3).
 \end{aligned} \tag{15}$$

By direct calculation, we may deduce that the right-hand side of (14) is negative, equivalently $ABC(T_1) < ABC(T)$, holds for the following cases:

- $t = 3, s = 1$, and $d_v \geq 64$;
- $t = 3, s = 2$, and $d_v \geq 44$;
- $t = 4, s = 1$, and $d_v \geq 4015$;
- $t = 4, s = 2$, and $d_v \geq 116$.

For the remaining cases as follows:

- $t = 2, s = 0$, and $5 \leq d_v \leq 82$;
- $t = 3, s = 1$, and $7 \leq d_v \leq 63$;
- $t = 3, s = 2$, and $8 \leq d_v \leq 43$;
- $t = 4, s = 1$, and $8 \leq d_v \leq 4014$;
- $t = 4, s = 2$, and $9 \leq d_v \leq 115$,

we would turn to use (15), and negative upper bounds, equivalently $ABC(T_1) < ABC(T)$, follow from direct calculation easily.

At this point, there are still two remaining cases: $t = 4, s = 0$, and $t = 5, s = 1$.

For the case $t = 4$ and $s = 0$, we apply the transformation \mathcal{T}_3 illustrated in Fig 13.

After applying \mathcal{T}_3 , the degree of vertex v increases by 2, the degrees of two children of u in T belonging to a B_2 -branch increase from 3 to 5, one child of u in T belonging to another B_2 -branch increases its degree from 3 to 4, the remaining child of u in T belonging to a B_2 -branch decreases its degree from 3 to 2, the degree of u decreases from 7 to 1, and the rest of the vertices do not change their degrees. The change of the ABC index after applying \mathcal{T}_3 is

$$\begin{aligned}
 ABC(T_1) - ABC(T) = & \sum_{xv \in E(\bar{T})} (f(d_v + 2, d_x) - f(d_v, d_x)) \\
 & + 2(f(d_v + 2, 5) - f(7, 3)) + f(d_v + 2, 4) - f(d_v, 7) \\
 & + 2(f(1, 2) - f(7, 3)).
 \end{aligned} \tag{16}$$

Clearly,

$$f(d_v + 2, d_x) - f(d_v, d_x) < 0,$$

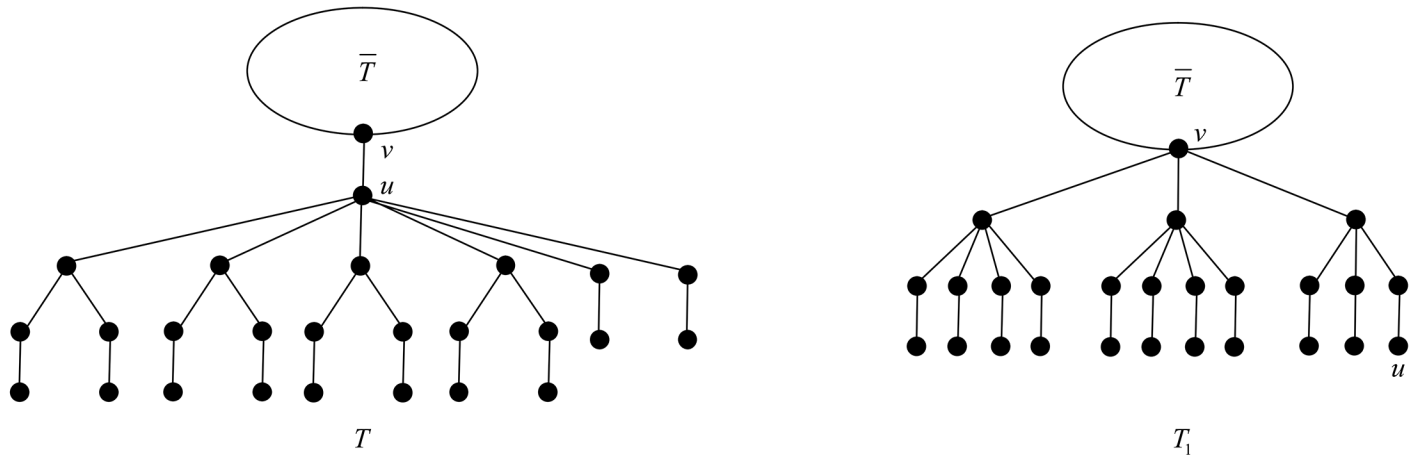


Fig 13. The transformation T_3 in the proof of Proposition 25.

<https://doi.org/10.1371/journal.pone.0195153.g013>

for $xv \in E(\bar{T})$. So

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< 2(f(d_v + 2, 5) - f(7, 3)) + f(d_v + 2, 4) - f(d_v, 7) \\
 &\quad + 2(f(1, 2) - f(7, 3)) \\
 &= 2(f(d_v + 2, 5) - f(d_v + 2, 4)) + 3f(d_v + 2, 4) - f(d_v, 7) \\
 &\quad - 4f(7, 3) + 2f(1, 2). \tag{17}
 \end{aligned}$$

Note that $d_v \geq d_u = 7$ from Proposition 2, and by Lemma 11, $f(d_v + 2, 5) - f(d_v + 2, 4)$ decreases in $d_v \geq 7$. On the other hand, by Lemma 12, $3f(d_v + 2, 4) - f(d_v, 7)$ decreases in $d_v \geq 7$. So the right-hand side of (17) also decreases in $d_v \geq 7$.

Besides the upper bound about $ABC(T_1) - ABC(T)$ as (17), by considering in (16) the term

$$\sum_{xv \in E(\bar{T})} (f(d_v + 2, d_x) - f(d_v, d_x)),$$

we may get a somewhat stricter upper bound about $ABC(T_1) - ABC(T)$. Note that, from Lemma 10, $f(d_v + 2, d_x) - f(d_v, d_x)$ decreases in d_x , and from Proposition 2, every neighbor of v in \bar{T} has degree at least three, thus

$$\sum_{xv \in E(\bar{T})} (f(d_v + 2, d_x) - f(d_v, d_x)) \leq (d_v - 1)(f(d_v + 2, 3) - f(d_v, 3)).$$

Now together with (16), it follows that

$$\begin{aligned}
 ABC(T_1) - ABC(T) &\leq (d_v - 1)(f(d_v + 2, 3) - f(d_v, 3)) \\
 &\quad + 2(f(d_v + 2, 5) - f(7, 3)) + f(d_v + 2, 4) - f(d_v, 7) \\
 &\quad + 2(f(1, 2) - f(7, 3)). \tag{18}
 \end{aligned}$$

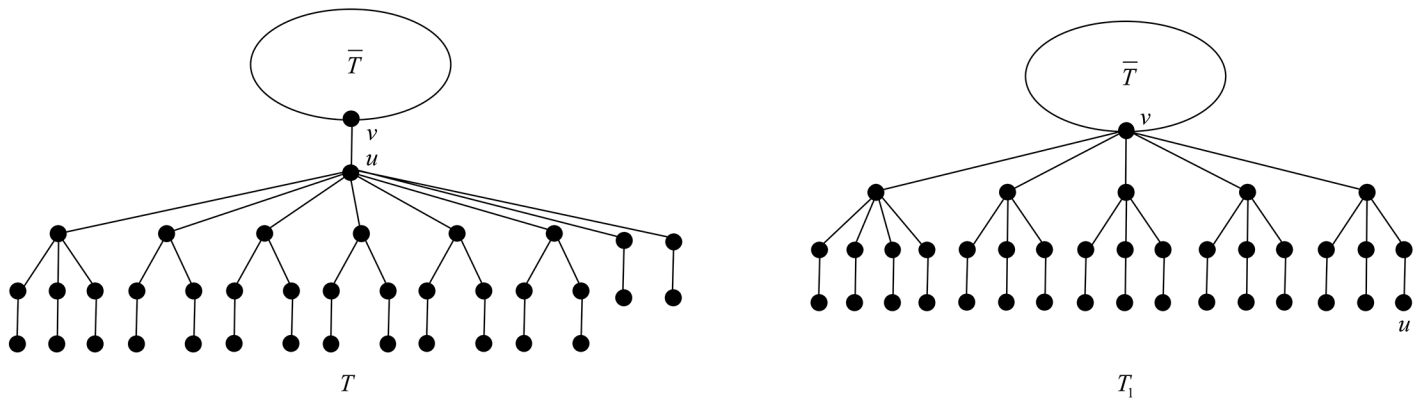


Fig 14. The transformation \mathcal{T}_4 in the proof of Proposition 25.

<https://doi.org/10.1371/journal.pone.0195153.g014>

For $d_v \geq 20$, by (17), we have

$$\begin{aligned} ABC(T_1) - ABC(T) &< 2(f(20 + 2, 5) - f(7, 3)) + f(20 + 2, 4) - f(20, 7) \\ &\quad + 2(f(1, 2) - f(7, 3)) \\ &< 0, \end{aligned}$$

i.e., $ABC(T_1) < ABC(T)$. For the remaining cases $7 \leq d_v \leq 19$, we would turn to use (18), and a negative upper bound, equivalently $ABC(T_1) < ABC(T)$, follows from direct calculation straightforwardly.

As to the last case $t = 5$ and $s = 1$, we apply the transformation \mathcal{T}_4 illustrated in Fig 14.

After applying \mathcal{T}_4 , the degree of vertex v increases by 4, three children of u in T belonging to a B_2 -branch increase its degrees from 3 to 4, the degree of one child of u in T belonging to another B_2 -branch increases from 3 to 5, the remaining child of u in T belonging to a B_2 -branch decreases its degree from 3 to 2, the degree of u decreases from 9 to 1, and the rest of the vertices do not change their degrees. The change of the ABC index after applying \mathcal{T}_4 is

$$\begin{aligned} ABC(T_1) - ABC(T) &= \sum_{xv \in E(\bar{T})} (f(d_v + 4, d_x) - f(d_v, d_x)) \\ &\quad + 4(f(d_v + 4, 4) - f(9, 3)) + f(d_v + 4, 5) - f(d_v, 9) \\ &\quad + 2f(1, 2) - f(9, 4) - f(9, 3). \end{aligned} \tag{19}$$

Clearly, $f(d_v + 4, d_x) - f(d_v, d_x) < 0$ for $xv \in E(\bar{T})$. So

$$\begin{aligned} ABC(T_1) - ABC(T) &< 4(f(d_v + 4, 4) - f(9, 3)) + f(d_v + 4, 5) - f(d_v, 9) \\ &\quad + 2f(1, 2) - f(9, 4) - f(9, 3) \\ &= f(d_v + 4, 5) - f(d_v + 4, 4) + 5f(d_v + 4, 4) - f(d_v, 9) \\ &\quad - 5f(9, 3) - f(9, 4) + 2f(1, 2). \end{aligned} \tag{20}$$

Note that $d_v \geq d_u = 9$ from Proposition 2, and by Lemma 11, $f(d_v + 4, 5) - f(d_v + 4, 4)$ decreases in $d_v \geq 9$. On the other hand, by Lemma 12, $5f(d_v + 4, 4) - f(d_v, 9)$ decreases in $d_v \geq 9$. So the right-hand side of (20) also decreases in $d_v \geq 9$.

Besides the upper bound about $ABC(T_1) - ABC(T)$ as (20), by considering in (19) the term

$$\sum_{xv \in E(\bar{T})} (f(d_v + 4, d_x) - f(d_v, d_x)),$$

we may get a somewhat stricter upper bound about $ABC(T_1) - ABC(T)$. Note that, from Lemma 10, $f(d_v + 4, d_x) - f(d_v, d_x)$ decreases in d_x , and from Proposition 2, every neighbor of v in \bar{T} has degree at least three, thus

$$\sum_{xv \in E(\bar{T})} (f(d_v + 4, d_x) - f(d_v, d_x)) \leq (d_v - 1)(f(d_v + 4, 3) - f(d_v, 3)).$$

Now together with (19), it follows that

$$\begin{aligned} ABC(T_1) - ABC(T) &\leq (d_v - 1)(f(d_v + 4, 3) - f(d_v, 3)) \\ &\quad + 4(f(d_v + 4, 4) - f(9, 3)) + f(d_v + 4, 5) - f(d_v, 9) \\ &\quad + 2f(1, 2) - f(9, 4) - f(9, 3). \end{aligned} \tag{21}$$

For $d_v \geq 15$, by (20), we have

$$\begin{aligned} ABC(T_1) - ABC(T) &< f(15 + 4, 5) - f(15 + 4, 4) + 5f(15 + 4, 4) - f(15, 9) \\ &\quad - 5f(9, 3) - f(9, 4) + 2f(1, 2) \\ &< 0, \end{aligned}$$

i.e., $ABC(T_1) < ABC(T)$. For the remaining cases $9 \leq d_v \leq 14$, we would turn to use (21), and a negative upper bound, equivalently $ABC(T_1) < ABC(T)$, follows from direct calculation easily.

Combining the above arguments, the result follows.

Our main result is stated next. As we will see, the configuration depicted in Fig 10 is very important since, minimal-ABC trees may contain two B_1 -branches only in two very particular configurations.

Theorem 26. *A minimal-ABC tree cannot contain two B_1 -branches, unless the two B_1 -branches belong to the configuration depicted in Fig 10 with $s = 0, t = 1$, or $s = 0, t = 3$.*

proof. Suppose to the contrary that T is a minimal-ABC tree containing exactly two B_1 -branches. Observe that the two B_1 -branches are attached to the same vertex, say u , otherwise, there are at least two T_k -branches, which is a contradiction to Proposition 8. Moreover, by Proposition 15, u is not the root vertex of T . Denote by v the parent of u .

First, by Proposition 3, u contains no B_k -branch with $k > 4$. Next by Proposition 5, u contains no B_4 -branch, and by Propositions 4 and 7, u contains no B_1^* -branch, no matter u has B_3 -branches or B_2 -branches. Now we may deduce that the branches attached to u must be B_3 -, B_2 - or B_1 -branches, i.e., T is of the structure depicted in Fig 10.

Set s and t for the numbers of B_3 - and B_2 -branches attached to u , respectively. Clearly, $s + t \geq 1$, and $s + t \leq 10$ from Proposition 23.

We apply the transformation \mathcal{T} depicted in Fig 15. And let d_x be the degree of vertex x in T .

After applying \mathcal{T} , the degree of vertex v increases by $s + t$, while the degree of vertex u decreases by $s + t$, and the rest of the vertices do not change their degrees. The change of the

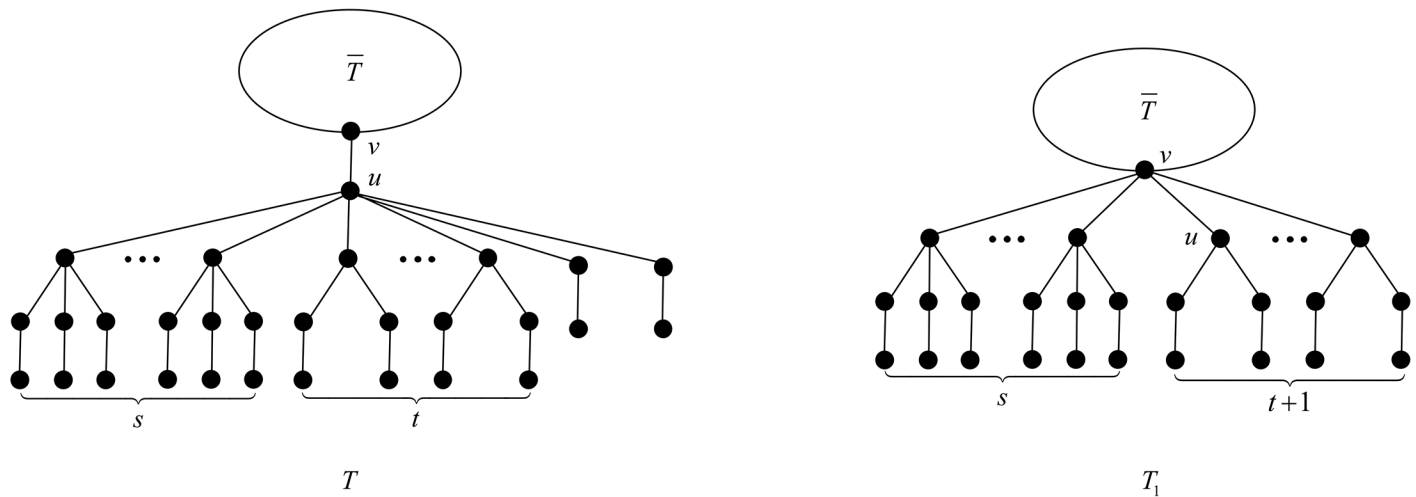


Fig 15. The transformation \mathcal{T} in the proof of Theorem 26.

<https://doi.org/10.1371/journal.pone.0195153.g015>

ABC index after applying \mathcal{T} is

$$\begin{aligned}
 ABC(T_1) - ABC(T) &= \sum_{xv \in E(\bar{T})} (f(d_v + s + t, d_x) - f(d_v, d_x)) \\
 &\quad + s(f(d_v + s + t, 4) - f(s + t + 3, 4)) \\
 &\quad + t(f(d_v + s + t, 3) - f(s + t + 3, 3)) \\
 &\quad + f(d_v + s + t, 3) - f(d_v, s + t + 3).
 \end{aligned} \tag{22}$$

Clearly, $f(d_v + s + t, d_x) - f(d_v, d_x) < 0$ for $xv \in E(\bar{T})$, and thus

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< s(f(d_v + s + t, 4) - f(s + t + 3, 4)) \\
 &\quad + t(f(d_v + s + t, 3) - f(s + t + 3, 3)) \\
 &\quad + f(d_v + s + t, 3) - f(d_v, s + t + 3).
 \end{aligned}$$

On one hand, from Lemma 10, $f(d_v + s + t, 3) - f(d_v, s + t + 3)$ increases in d_v , thus

$$\begin{aligned}
 f(d_v + s + t, 3) - f(d_v, s + t + 3) &\leq \lim_{d_v \rightarrow +\infty} (f(d_v + s + t, 3) - f(d_v, s + t + 3)) \\
 &= \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{s + t + 3}}.
 \end{aligned}$$

So it follows that

$$\begin{aligned}
 ABC(T_1) - ABC(T) &< s(f(d_v + s + t, 4) - f(s + t + 3, 4)) \\
 &\quad + t(f(d_v + s + t, 3) - f(s + t + 3, 3)) \\
 &\quad + \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{s + t + 3}}.
 \end{aligned} \tag{23}$$

Furthermore, note that $d_v \geq d_u = s + t + 3$ from Proposition 2, and both $f(d_v + s + t, 4)$ and $f(d_v + s + t, 3)$ decrease in $d_v \geq s + t + 3$, i.e., the right-hand side of (23) also decreases in $d_v \geq s + t + 3$.

Besides the upper bound about $ABC(T_1) - ABC(T)$ as (23), by considering a bit precisely in (22) for the term

$$\sum_{xv \in E(\bar{T})} (f(d_v + s + t, d_x) - f(d_v, d_x)),$$

we may get a somewhat stricter upper bound about $ABC(T_1) - ABC(T)$. Note that, from Lemma 10, $f(d_v + s + t, d_x) - f(d_v, d_x)$ decreases in d_x , and from Proposition 2, every neighbor of v in \bar{T} has degree at least three, thus

$$\sum_{xv \in E(\bar{T})} (f(d_v + s + t, d_x) - f(d_v, d_x)) \leq (d_v - 1)(f(d_v + s + t, 3) - f(d_v, 3)).$$

Now together with (22), it follows that

$$\begin{aligned} ABC(T_1) - ABC(T) \leq & (d_v - 1)(f(d_v + s + t, 3) - f(d_v, 3)) \\ & + s(f(d_v + s + t, 4) - f(s + t + 3, 4)) \\ & + t(f(d_v + s + t, 3) - f(s + t + 3, 3)) \\ & + f(d_v + s + t, 3) - f(d_v, s + t + 3). \end{aligned} \tag{24}$$

Case 1. $t = 0$.

In this case, note that $1 \leq s \leq 10$, and $d_v \geq s + 3$ from Proposition 2.

By direct calculation, we may deduce that the right-hand side of (23) is negative, equivalently $ABC(T_1) < ABC(T)$, holds for the following cases:

- $s = 1$ and $d_v \geq 13$;
- $s = 2$ and $d_v \geq 17$;
- $s = 3$ and $d_v \geq 21$;
- $s = 4$ and $d_v \geq 25$;
- $s = 5$ and $d_v \geq 30$;
- $s = 6$ and $d_v \geq 35$;
- $s = 7$ and $d_v \geq 41$;
- $s = 8$ and $d_v \geq 47$;
- $s = 9$ and $d_v \geq 54$;
- $s = 10$ and $d_v \geq 61$.

For the remaining cases as follows:

- $s = 1$ and $4 \leq d_v \leq 12$;
- $s = 2$ and $5 \leq d_v \leq 16$;
- $s = 3$ and $6 \leq d_v \leq 20$;
- $s = 4$ and $7 \leq d_v \leq 24$;
- $s = 5$ and $8 \leq d_v \leq 29$;
- $s = 6$ and $9 \leq d_v \leq 34$;
- $s = 7$ and $10 \leq d_v \leq 40$;

- $s = 8$ and $11 \leq d_v \leq 46$;
- $s = 9$ and $12 \leq d_v \leq 53$;
- $s = 10$ and $13 \leq d_v \leq 60$,

we would turn to use (24), and negative upper bounds, equivalently $ABC(T_1) < ABC(T)$, follow from direct calculation easily.

Case 2. $t = 1$.

In this case, note that $0 \leq s \leq 9$, and $d_v \geq s + 4$ from Proposition 2.

By direct calculation, we may deduce that the right-hand side of (23) is negative, equivalently $ABC(T_1) < ABC(T)$, holds for the following cases:

- $s = 1$ and $d_v \geq 46$;
- $s = 2$ and $d_v \geq 38$;
- $s = 3$ and $d_v \geq 39$;
- $s = 4$ and $d_v \geq 43$;
- $s = 5$ and $d_v \geq 49$;
- $s = 6$ and $d_v \geq 55$;
- $s = 7$ and $d_v \geq 61$;
- $s = 8$ and $d_v \geq 68$;
- $s = 9$ and $d_v \geq 76$.

For the remaining cases as follows:

- $s = 1$ and $5 \leq d_v \leq 45$;
- $s = 2$ and $6 \leq d_v \leq 37$;
- $s = 3$ and $7 \leq d_v \leq 38$;
- $s = 4$ and $8 \leq d_v \leq 42$;
- $s = 5$ and $9 \leq d_v \leq 48$;
- $s = 6$ and $10 \leq d_v \leq 54$;
- $s = 7$ and $11 \leq d_v \leq 60$;
- $s = 8$ and $12 \leq d_v \leq 67$;
- $s = 9$ and $13 \leq d_v \leq 75$,

we would turn to use (24), and negative upper bounds, equivalently $ABC(T_1) < ABC(T)$, follow from direct calculation easily.

Case 3. $t = 2$.

In this case, note that $0 \leq s \leq 8$, and $d_v \geq s + 5$ from Proposition 2.

On one hand, the contradiction for $s = 0$ follows from Proposition 25.

On the other hand, by direct calculation, we may deduce that the right-hand side of (23) is negative, equivalently $ABC(T_1) < ABC(T)$, holds for the following cases:

- $s = 1$ and $d_v \geq 1402$;
- $s = 2$ and $d_v \geq 107$;

- $s = 3$ and $d_v \geq 84$;
- $s = 4$ and $d_v \geq 81$;
- $s = 5$ and $d_v \geq 84$;
- $s = 6$ and $d_v \geq 89$;
- $s = 7$ and $d_v \geq 96$;
- $s = 8$ and $d_v \geq 104$.

For the remaining cases as follows:

- $s = 1$ and $6 \leq d_v \leq 1401$;
- $s = 2$ and $7 \leq d_v \leq 106$;
- $s = 3$ and $8 \leq d_v \leq 83$;
- $s = 4$ and $9 \leq d_v \leq 80$;
- $s = 5$ and $10 \leq d_v \leq 83$;
- $s = 6$ and $11 \leq d_v \leq 88$;
- $s = 7$ and $12 \leq d_v \leq 95$;
- $s = 8$ and $13 \leq d_v \leq 103$,

we would turn to use (24), and negative upper bounds, equivalently $ABC(T_1) < ABC(T)$, follow from direct calculation easily.

Case 4. $t = 3$.

In this case, note that $0 \leq s \leq 7$, and $d_v \geq s + 6$ from Proposition 2.

On one hand, the contradiction for $s = 1, 2$ follows from Proposition 25.

On the other hand, by direct calculation, we may deduce that the right-hand side of (23) is negative, equivalently $ABC(T_1) < ABC(T)$, holds for the following cases:

- $s = 3$ and $d_v \geq 290$;
- $s = 4$ and $d_v \geq 193$;
- $s = 5$ and $d_v \geq 170$;
- $s = 6$ and $d_v \geq 163$;
- $s = 7$ and $d_v \geq 165$.

For the remaining cases as follows:

- $s = 3$ and $9 \leq d_v \leq 289$;
- $s = 4$ and $10 \leq d_v \leq 192$;
- $s = 5$ and $11 \leq d_v \leq 169$;
- $s = 6$ and $12 \leq d_v \leq 162$;
- $s = 7$ and $13 \leq d_v \leq 164$,

we would turn to use (24), and negative upper bounds, equivalently $ABC(T_1) < ABC(T)$, follow from direct calculation easily.

Case 5. $t = 4$.

In this case, note that $0 \leq s \leq 6$. The contradiction may be deduced from Proposition 25.

Case 6. $t = 5$.

In this case, note that $0 \leq s \leq 5$. The contradiction for the cases that $s = 0$ and $s = 1, 2, 3, 4, 5$ may be deduced from Propositions 24 and 25, respectively.

Case 7. $t = 6$.

In this case, note that $0 \leq s \leq 4$. The contradiction for the cases that $s = 0$ and $s = 1, 2, 3, 4$ may be deduced from Propositions 24 and 25, respectively.

Case 8. $t = 7$.

In this case, note that $0 \leq s \leq 3$. The contradiction for the cases that $s = 0$ and $s = 1, 2, 3$ may be deduced from Propositions 24 and 25, respectively.

Case 9. $t = 8$.

In this case, note that $s = 0, 1, 2$. The contradiction for the cases that $s = 0$ and $s = 1, 2$ may be deduced from Propositions 24 and 25, respectively.

Case 10. $t = 9$.

In this case, note that $s = 0, 1$. The contradiction for the cases that $s = 0$ and $s = 1$ may be deduced from Propositions 24 and 25, respectively.

Case 11. $t = 10$.

In this case, note that $s = 0$. The contradiction may be deduced from Proposition 24 directly.

Combining the above arguments, the result finally follows.

Discussion

The characterization of minimal-ABC trees is a rather active topic in chemical graph theory these years, which has led to a lot of structural properties and potential conjectures.

It is known that every pendent vertex of minimal-ABC trees belongs to some B_k -branch. As a strengthening, this paper proves that a minimal-ABC tree contains at most two B_1 -branches. Moreover, we claim that a minimal-ABC tree can not contain two B_1 -branches simultaneously, except for two cases that $s = 0$, and $t = 1$ or 3.

During the investigation of this paper, we also considered the two unsolved cases. However, to the best of our knowledge, until now we only get a solution under some particular degree conditions. In future research, the key point is to construct a more perfect graph transformation involve in general cases, which lead to a desired solution finally.

Actually, our ultimate goal is to show that the minimal-ABC trees contain no B_1 -branch, when the order of that tree is large sufficiently.

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References

1. Randić M. Characterization of molecular branching, *J. Am. Chem. Soc.* 97 (1975) 6609–6615. <https://doi.org/10.1021/ja00856a001>
2. Estrada E, Torres L, Rodríguez L, Gutman I. An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes, *Indian J. Chem.* 37A (1998) 849–855.
3. Estrada E. Atom-bond connectivity and the energetic of branched alkanes, *Chem. Phys. Lett.* 463 (2008) 422–425. <https://doi.org/10.1016/j.cplett.2008.08.074>
4. Ke X. Atom-bond connectivity index of benzenoid systems and fluoranthene congeners, *Poly. Arom. Comp.* 32 (2012) 27–35. <https://doi.org/10.1080/10406638.2011.637101>
5. Yang J, Xia F, Cheng H. The atom-bond connectivity index of benzenoid systems and phenylenes, *Inter. Math. Forum* 6 (2011) 2001–2005.
6. Ahmadi MB, Sadeghimehr M. Atom bond connectivity index of an infinite class $NS_1[n]$ of dendrimer nanostars, *Optoelectron. Adv. Mat.* 4 (2010) 1040–1042.
7. Furtula B, Graovac A, Vukičević D. Atom-bond connectivity index of trees, *Discrete Appl. Math.* 157 (2009) 2828–2835. <https://doi.org/10.1016/j.dam.2009.03.004>
8. Ahmadi MB, Hosseini SA, Zarrinderakht M. On large trees with minimal atom-bond connectivity index, *MATCH Commun. Math. Comput. Chem.* 69 (2013) 565–569.
9. Gutman I, Furtula B. Trees with smallest atom-bond connectivity index, *MATCH Commun. Math. Comput. Chem.* 68 (2012) 131–136.
10. Gutman I, Furtula B, Ahmadib MB, Hosseini SA, Nowbandegani PS, Zarrinderakht M. The ABC index conundrum, *Filomat* 27 (2013) 1075–1083. <https://doi.org/10.2298/FIL1306075G>
11. Lin W, Lin X, Gao T, Wu X. Proving a conjecture of Gutman concerning trees with minimal ABC index, *MATCH Commun. Math. Comput. Chem.* 69 (2013) 549–557.
12. Liu J, Chen J. Further properties of trees with minimal atom-bond connectivity index, *Abstr. Appl. Anal.* 2014 (2014) 609208. <https://doi.org/10.1155/2014/609208>
13. Das KC, Mohammed MA, Gutman I, Atan KA, Comparison between atom-bond connectivity indices of graphs, *MATCH Commun. Math. Comput. Chem.* 76 (2016) 159–170.
14. Dimitrov D. Extremal trees with respect to the atom-bond connectivity index, *Bounds in Chemical Graph Theory, Mathematical Chemistry Monographs No.20*, K. C. Das, B. Furtula, I. Gutman, E. I. Milovanović, I. Ž. Milovanović (Eds.), Pages 53–67, 2017.
15. Dimitrov D. On structural properties of trees with minimal atom-bond connectivity index IV: Solving a conjecture about the pendent paths of length three, *Appl. Math. Comput.* 313 (2017) 418–430.
16. Dimitrov D, Ikica B, Škrekovski R. Remarks on maximum atom-bond connectivity index with given graph parameters, *Discrete Appl. Math.* 222 (2017) 222–226. <https://doi.org/10.1016/j.dam.2017.01.019>
17. Gao Y, Shao Y. The smallest ABC index of trees with n pendent vertices, *MATCH Commun. Math. Comput. Chem.* 76 (2016) 141–158.
18. Lin W, Chen J, Ma C, Zhang Y, Chen J, Zhang D, Jia F. On trees with minimal ABC index among trees with given number of leaves, *MATCH Commun. Math. Comput. Chem.* 76 (2016) 131–140.
19. Gutman I, Furtula B, Ivanović M. Notes on trees with minimal atom-bond connectivity index, *MATCH Commun. Math. Comput. Chem.* 67 (2012) 467–482.
20. Wang H. Extremal trees with given degree sequence for the Randić index, *Discrete Math.* 308 (2008) 3407–3411. <https://doi.org/10.1016/j.disc.2007.06.026>
21. Gan L, Liu B, You Z. The ABC index of trees with given degree sequence, *MATCH Commun. Math. Comput. Chem.* 68 (2012) 137–145.

22. Xing R, Zhou B. Extremal trees with fixed degree sequence for atom-bond connectivity index, *Filomat* 26 (2012) 683–688. <https://doi.org/10.2298/FIL1204683X>
23. Dimitrov D. On structural properties of trees with minimal atom-bond connectivity index, *Discrete Appl. Math.* 172 (2014) 28–44. <https://doi.org/10.1016/j.dam.2014.03.009>
24. Du Z, Fonseca CM da, On a family of trees with minimal atom-bond connectivity index, *Discrete Appl. Math.* 202 (2016) 37–49. <https://doi.org/10.1016/j.dam.2015.08.017>
25. Dimitrov D, Du Z, Fonseca CM da, On structural properties of trees with minimal atom-bond connectivity index III: Trees with pendent paths of length three, *Appl. Math. Comput.* 282 (2016) 276–290.
26. Dimitrov D, Du Z, Fonseca CM da, Some forbidden combinations of branches in minimal-ABC trees, *Discrete Appl. Math.* 236 (2018) 165–182. <https://doi.org/10.1016/j.dam.2017.11.003>
27. Dimitrov D. On structural properties of trees with minimal atom-bond connectivity index II—Bounds on B_1 - and B_2 -branches, *Discrete Appl. Math.* 204 (2016) 90–116. <https://doi.org/10.1016/j.dam.2015.10.010>
28. Hosseini SA, Ahmadi MB, Gutman I. Kragujevac trees with minimal atom-bond connectivity index, *MATCH Commun. Math. Comput. Chem.* 71 (2014) 5–20.
29. Dimitrov D. Efficient computation of trees with minimal atom-bond connectivity index, *Appl. Math. Comput.* 224 (2013) 663–670.
30. Lin W, Gao T, Chen Q, Lin X. On the minimal ABC index of connected graphs with given degree sequence, *MATCH Commun. Math. Comput. Chem.* 69 (2013) 571–578.