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The Smallest ABC Index of Trees with n Pendent Vertices*

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Abstract

For a graph G, the atom-bond connectivity index (ABC index) is defined as $ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$, where $d_G(u)$ is the degree of the vertex u. For a integer n, a tree T is an n-optimal tree if T has the smallest ABC index among trees with n pendent vertices (leaves). In [1,2], the authors characterized the n-optimal trees for $n \leq 53$. In [3], the authors characterized the n-optimal trees for $54 \leq n \leq 219$. However, the problem of characterizing the n-optimal trees for any $n \geq 220$ remains open. In this work, we introduce some useful graph transformations, and present some properties of n-optimal trees. For each $n \geq 2$, we give an algorithm to find the n-optimal trees and the smallest ABC index of trees with n pendent vertices. In some sense, the problem to determine the n-optimal trees and the smallest ABC index of trees with n pendent vertices is resolved completely.

1 Introduction

For a graph G, the atom-bond connectivity index (ABC index) is defined as

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

where $d_G(u)$ denotes the degree of the vertex u.

For a integer n, a tree T is an n-optimal tree if T has the smallest ABC index among trees with n pendent vertices.

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The ABC index is a vertex-degree-based graph invariant that found applications in chemistry. It is currently attracting much attention of mathematicians (see [1] and the references cited therein). Most known results can be found in [4] and the references therein. For the developments after [4] see [1–3,6–11]. There exist two elementary problems remain open in study the smallest ABC index [3, 5].

Problem A. Characterize tree(s) with minimal ABC index among the trees of order n.

Problem B. Characterize tree(s) with minimal ABC index among trees with n leaves.

The problem A seems to be hard [5]. For problem B, recent papers [1–3] got some results.

Magnant et al. [1] claimed that, the unique n-optimal tree is the balanced double star if $n \geq 19$. Unfortunately, the proof is wrong. Soon counterexamples were found by Goubko et al. [2] by searching n-optimal trees for $n \leq 53$. Lin et al. [3] presented some properties of k-optimal trees, and computer search k-optimal trees for $n \leq 219$.

In this work, we introduce some useful graph transformations, and present some properties of n-optimal trees. For each $n \geq 2$, we give an algorithm to find the n-optimal trees and calculate their ABC indices. In some sense, the problem to determine the n-optimal trees and the smallest ABC index of trees with n pendent vertices is resolved completely.

2 Some lemmas

Lemma 2.1 *Let* $f(x) = \sqrt{\frac{x+d-2}{xd}}$ *with* $d > 2$. *Then* $f(x)$ *is decreasing for* $x \geq 2$.

Proof. Note $f'(x) = \frac{1}{2\sqrt{\frac{x+d-2}{xd}}}(-\frac{1}{x^2}\frac{d-2}{d}) < 0$. So $f(x)$ is decreasing for $x \geq 2$. ■

Lemma 2.2 *Let* $f(x) = \sqrt{\frac{x+d}{x+2}} - \sqrt{\frac{x+d-1}{x+1}}$ *with* $d > 2$. *Then* $f(x)$ *is increasing for* $x \geq 1$.

Proof. Let $g(x) = (x+1)^2\sqrt{\frac{x+d-1}{x+1}}$. Then $g'(x) = (x+1)^2\sqrt{\frac{x+d-1}{x+1}}(\frac{2}{x+1} + \frac{1}{2(x+d-1)} - \frac{1}{2(x+1)}) > 0$ and $g(x)$ is increasing for $x \geq 1$.

Note that $f'(x) = \frac{d-2}{2}\left(\frac{1}{\sqrt{\frac{x+d-1}{x+1}}}\frac{1}{(x+1)^2} - \frac{1}{(x+2)^2}\frac{1}{\sqrt{\frac{x+d}{x+2}}}\right) = \frac{d-2}{2}(\frac{1}{g(x)} - \frac{1}{g(x+1)}) > 0$. So $f(x)$ is increasing for $x \geq 1$. ■

Lemma 2.3 *Let* $f(x) = (x+1)\sqrt{\frac{x+1}{x+2}} - x\sqrt{\frac{x}{x+1}}$. *Then* $f(x)$ *is increasing for* $x \geq 1$.

Proof. Let $\varphi(x) = \frac{1}{2}\sqrt{\frac{x}{(x+1)^3}} + \sqrt{\frac{x}{x+1}}$. Then $\varphi'(x) = \frac{3}{4(x+1)^2\sqrt{x(x+1)}} > 0$ and $\varphi(x)$ is a increasing function on x.

Note that $f'(x) = \sqrt{\frac{x+1}{x+2}} - \sqrt{\frac{x}{x+1}} + \frac{1}{2}\sqrt{\frac{x+1}{(x+2)^3}} - \frac{1}{2}\sqrt{\frac{x}{(x+1)^3}} = \varphi(x+1) - \varphi(x) > 0$. So $f(x)$ is increasing for $x \geq 1$. ■

Lemma 2.4 ([3]) *Let T be an n-optimal tree. Then T has no vertices of degree* 2.

3 Some useful graph transformations

In this section, we will introduce some useful graph transformations.

3.1 The edge cutting transformation

Let G_1 be the tree as shown in Figure 3.1, where $k \geq 2$, $t \geq 2$, $d_{G_1}(u_i) \geq 3$ for $i = 1, \ldots, k$ and $d_{G_1}(v_i) \geq 3$ for $i = 1, \ldots, t$.

Denote G'_1 to be the tree obtained from G_1 by deleting the vertex u and edges uu_i for $i = 1, \ldots, k$, and adding the edges vu_i for $i = 1, \ldots, k$ (given in Figure 3.2). It is clear that G_1 and G'_1 have the same number of pendent vertices, $d_{G_1}(u_i) = d_{G'_1}(u_i)$ for $i = 1, \ldots, k$ and $d_{G_1}(v_i) = d_{G'_1}(v_i)$ for $i = 1, \ldots, t$.

We say that G'_1 is obtained from G_1 by the edge cutting transformation.

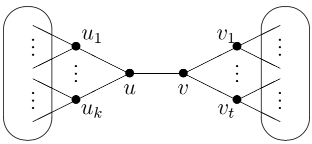

Figure 3.1: Tree G_1

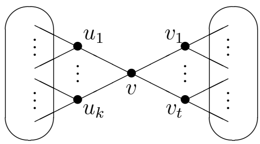

Figure 3.2: Tree G'_1

Lemma 3.1 *Let G'_1 be obtained from G_1 by the edge cutting transformation. Then*

$$ABC(G_1) > ABC(G'_1).$$

Proof. Note that $d_{G_1}(u) = k+1$, $d_{G_1}(v) = t+1$, $d_{G'_1}(v) = k+t$. Denote

$$A = \sqrt{\frac{d_{G_1}(u) + d_{G_1}(v) - 2}{d_{G_1}(u)d_{G_1}(v)}} + \sum_{i=1}^{k}\sqrt{\frac{d_{G_1}(u) + d_{G_1}(u_i) - 2}{d_{G_1}(u)d_{G_1}(u_i)}} + \sum_{i=1}^{t}\sqrt{\frac{d_{G_1}(v) + d_{G_1}(v_i) - 2}{d_{G_1}(v)d_{G_1}(v_i)}},$$

and

$$B = \sum_{i=1}^{k}\sqrt{\frac{d_{G'_1}(v) + d_{G'_1}(u_i) - 2}{d_{G'_1}(v)d_{G'_1}(u_i)}} + \sum_{i=1}^{t}\sqrt{\frac{d_{G'_1}(v) + d_{G'_1}(v_i) - 2}{d_{G'_1}(v)d_{G'_1}(v_i)}}.$$

Then

$$
\begin{aligned}
&ABC(G_1) - ABC(G_1') = A - B \\
&= \sqrt{\frac{k+t}{(k+1)(t+1)}} + \sum_{i=1}^{k} \sqrt{\frac{d_{G_1}(u_i)+k-1}{(k+1)d_{G_1}(u_i)}} + \sum_{i=1}^{t} \sqrt{\frac{d_{G_1}(v_i)+t-1}{(t+1)d_{G_1}(v_i)}} \\
&- \sum_{i=1}^{k} \sqrt{\frac{d_{G_1'}(u_i)+k+t-2}{(k+t)d_{G_1'}(u_i)}} - \sum_{i=1}^{t} \sqrt{\frac{d_{G_1'}(v_i)+k+t-2}{(k+t)d_{G_1'}(v_i)}}.
\end{aligned}
$$

Since $t \geq 2$, $k \geq 2$, by Lemma 2.1, we have

$$
\sqrt{\frac{d_{G_1}(u_i)+k-1}{(k+1)d_{G_1}(u_i)}} > \sqrt{\frac{d_{G_1'}(u_i)+k+t-2}{(k+t)d_{G_1'}(u_i)}}, \quad i = 1, \ldots, k.
$$

$$
\sqrt{\frac{d_{G_1}(v_i)+t-1}{(t+1)d_{G_1}(v_i)}} > \sqrt{\frac{d_{G_1'}(v_i)+k+t-2}{(k+t)d_{G_1'}(v_i)}}, \quad i = 1, \ldots, t.
$$

Note that $\sqrt{\frac{k+t}{(k+1)(t+1)}} > 0$. Then $ABC(G_1) > ABC(G_1')$. ■

3.2 The first kind branches exchanging transformation

Let G_2 be the tree as shown in Figure 3.3, where

(1) $k \geq 1$, $k' \geq 1$, $t \geq 1$, $t' \geq 1$, and $k + k' \geq t + t'$, that is, $d_{G_2}(u) \geq d_{G_2}(v)$;

(2) $d_{G_2}(u_i) \geq 3$ for $i = 1, \ldots, k$, $d_{G_2}(u_i') = 1$ for $i = 1, \ldots, k'$, $d_{G_2}(v_i) \geq 3$ for $i = 1, \ldots, t$, $d_{G_2}(v_i') = 1$ for $i = 1, \ldots, t'$;

(3) G_0 is a tree or empty graph (if G_0 is a empty graph, then $uv \in E(G_2)$).

Denote G_2' to be the tree obtained from G_2 by changing branches uu_1' and vv_1 to vu_1' and uv_1, respectively (as shown in Figure 3.4). It is clear that G_2 and G_2' have the same number of pendent vertices.

We say that G_2' is obtained from G_2 by the first kind branches exchanging transformation.

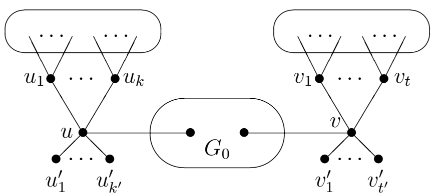

Figure 3.3: Tree G_2

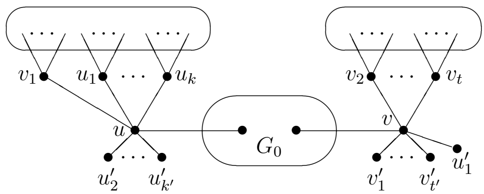

Figure 3.4: Tree G'_2

Lemma 3.2 *Let G'_2 be obtained from G_2 by the first kind branches exchanging transformation. Then*

$$ABC(G_2) \geq ABC(G'_2).$$

Proof. Denote

$$A = \sqrt{\frac{d_{G_2}(u) + d_{G_2}(u'_1) - 2}{d_{G_2}(u)d_{G_2}(u'_1)}} + \sqrt{\frac{d_{G_2}(v) + d_{G_2}(v_1) - 2}{d_{G_2}(v)d_{G_2}(v_1)}},$$

$$B = \sqrt{\frac{d_{G'_2}(u) + d_{G'_2}(v_1) - 2}{d_{G'_2}(u)d_{G'_2}(v_1)}} + \sqrt{\frac{d_{G'_2}(v) + d_{G'_2}(u'_1) - 2}{d_{G'_2}(v)d_{G'_2}(u'_1)}}.$$

Then

$$\begin{aligned} & ABC(G_2) - ABC(G'_2) = A - B \\ = & \sqrt{\frac{d_{G_2}(u) - 1}{d_{G_2}(u)}} + \sqrt{\frac{d_{G_2}(v) + d_{G_2}(v_1) - 2}{d_{G_2}(v)d_{G_2}(v_1)}} - \sqrt{\frac{d_{G'_2}(u) + d_{G'_2}(v_1) - 2}{d_{G'_2}(u)d_{G'_2}(v_1)}} - \sqrt{\frac{d_{G'_2}(v) - 1}{d_{G'_2}(v)}}. \end{aligned}$$

Since $d_{G'_2}(u) = d_{G_2}(u) \geq d_{G_2}(v) = d_{G'_2}(v)$, we have

$$\sqrt{\frac{d_{G_2}(u) - 1}{d_{G_2}(u)}} \geq \sqrt{\frac{d_{G'_2}(v) - 1}{d_{G'_2}(v)}}.$$

Noticing $d_{G_2}(v_1) = d_{G'_2}(v_1) \geq 3$, by Lemma 2.1,

$$\sqrt{\frac{d_{G_2}(v) + d_{G_2}(v_1) - 2}{d_{G_2}(v)d_{G_2}(v_1)}} \geq \sqrt{\frac{d_{G'_2}(u) + d_{G'_2}(v_1) - 2}{d_{G'_2}(u)d_{G'_2}(v_1)}}.$$

So $ABC(G_2) \geq ABC(G'_2)$. ■

3.3 The second kind branches exchanging transformation

Let G_3 be the tree as shown in Figure 3.5, where

(1) $k \geq 1$, $k' \geq 1$, $t \geq 2$, and $k + k' \geq t$ (that is, $d_{G_3}(u) \geq d_{G_3}(v)$);

(2) $d_{G_3}(u_i) \geq 3$ for $i = 1, \ldots, k$, $d_{G_3}(u'_i) = 1$ for $i = 1, \ldots, k'$, and $d_{G_3}(v_i) \geq 3$ for $i = 1, \ldots, t$;

(3) G_0 is a tree or empty graph (if G_0 is a empty graph, then $uv \in E(G_3)$).

Denote G'_3 to be the tree obtained from G_3 by changing branches uu'_1 and vv_1 to vu'_1 and uv_1, respectively (as shown in Figure 3.6). It is clear that G_3 and G'_3 have the same number of pendent vertices.

We say that G'_3 is obtained from G_3 by the second kind branches exchanging transformation.

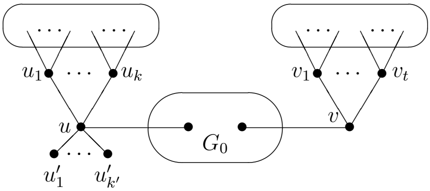

Figure 3.5: Tree G_3

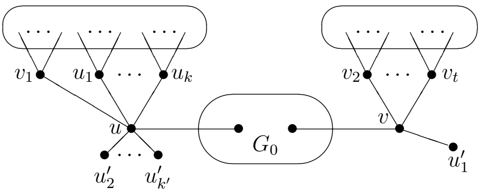

Figure 3.6: Tree G'_3

Lemma 3.3 *Let G'_3 be obtained from G_3 by the second kind branches exchanging transformation. Then*

$$ABC(G_3) \geq ABC(G'_3).$$

Proof. The proof is similar to the proof of Lemma 3.2. We omit it. ■

3.4 The third kind branches exchanging transformation

Let G_4 be the tree as shown in Figure 3.7, where $d_{G_4}(u) \geq 3$, and $d_{G_4}(v_i) = t_i + 1 \geq 3$ for $i = 1, 2$.

Denote G'_4 to be the tree obtained from G_4 by deleting the vertex v_1 and edges v_1u and v_1v_{1i} for $i = 1, \ldots, t_1$, and adding the edges uv_{11} and v_2v_{1i} for $i = 2, \ldots, t_1$ (as shown in Figure 3.8). It is clear that G_4 and G'_4 have the same number of pendent vertices.

We say that G'_4 is obtained from G_4 by the third kind branches exchanging transformation.

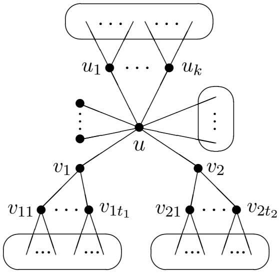

Figure 3.7: Tree G_4

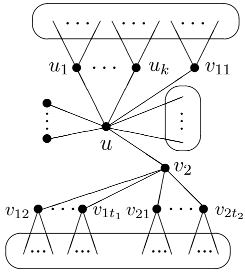

Figure 3.8: Tree G'_4

Lemma 3.4 *Let G'_4 be obtained from G_4 by the third kind branches exchanging transformation. Then*

$$ABC(G_4) > ABC(G'_4).$$

Proof. Denote

$$A = \sqrt{\frac{d_{G_4}(u) + d_{G_4}(v_1) - 2}{d_{G_4}(u)d_{G_4}(v_1)}} + \sum_{i=1}^{t_1} \sqrt{\frac{d_{G_4}(v_1) + d_{G_4}(v_{1i}) - 2}{d_{G_4}(v_1)d_{G_4}(v_{1i})}}$$
$$+\sqrt{\frac{d_{G_4}(u) + d_{G_4}(v_2) - 2}{d_{G_4}(u)d_{G_4}(v_2)}} + \sum_{i=1}^{t_2} \sqrt{\frac{d_{G_4}(v_2) + d_{G_4}(v_{2i}) - 2}{d_{G_4}(v_2)d_{G_4}(v_{2i})}},$$
$$B = \sqrt{\frac{d_{G'_4}(u) + d_{G'_4}(v_{11}) - 2}{d_{G'_4}(u)d_{G'_4}(v_{11})}} + \sqrt{\frac{d_{G'_4}(u) + d_{G'_4}(v_2) - 2}{d_{G'_4}(u)d_{G'_4}(v_2)}}$$
$$+\sum_{i=2}^{t_1} \sqrt{\frac{d_{G'_4}(v_2) + d_{G'_4}(v_{1i}) - 2}{d_{G'_4}(v_2)d_{G'_4}(v_{1i})}} + \sum_{i=1}^{t_2} \sqrt{\frac{d_{G'_4}(v_2) + d_{G'_4}(v_{2i}) - 2}{d_{G'_4}(v_2)d_{G'_4}(v_{2i})}}.$$

Note that $d_{G_4}(u) = d_{G'_4}(u)$. We use d to indicate it, that is, $d_{G_4}(u) = d_{G'_4}(u) = d$. Then

$$ABC(G_4) - ABC(G'_4) = A - B$$
$$= \sqrt{\frac{d + t_1 - 1}{d(t_1+1)}} + \sqrt{\frac{t_1 + d_{G_4}(v_{11}) - 1}{(t_1+1)d_{G_4}(v_{11})}} + \sum_{i=2}^{t_1} \sqrt{\frac{t_1 + d_{G_4}(v_{1i}) - 1}{(t_1+1)d_{G_4}(v_{1i})}}$$
$$+\sqrt{\frac{d + t_2 - 1}{d(t_2+1)}} + \sum_{i=1}^{t_2} \sqrt{\frac{t_2 + d_{G_4}(v_{2i}) - 1}{(t_2+1)d_{G_4}(v_{2i})}} - \sqrt{\frac{d + d_{G'_4}(v_{11}) - 2}{dd_{G'_4}(v_{11})}}$$
$$-\sqrt{\frac{d + t_1 + t_2 - 2}{d(t_1+t_2)}} - \sum_{i=2}^{t_1} \sqrt{\frac{t_1 + t_2 + d_{G'_4}(v_{1i}) - 2}{(t_1+t_2)d_{G'_4}(v_{1i})}} - \sum_{i=1}^{t_2} \sqrt{\frac{t_1 + t_2 + d_{G'_4}(v_{2i}) - 2}{(t_1+t_2)d_{G'_4}(v_{2i})}}.$$

Since that $d \geq 3$, $t_1 \geq 2$, $t_2 \geq 2$, $d_{G_4}(v_{1i}) = d_{G_4'}(v_{1i}) \geq 3$ for $i = 1, \ldots, t_1$, and $d_{G_4}(v_{2i}) = d_{G_4'}(v_{2i}) \geq 3$ for $i = 1, \ldots, t_2$, by Lemma 2.1, we have

$$\sqrt{\frac{t_1 + d_{G_4}(v_{1i}) - 1}{(t_1+1)d_{G_4}(v_{1i})}} > \sqrt{\frac{t_1 + t_2 + d_{G_4'}(v_{1i}) - 2}{(t_1+t_2)d_{G_4'}(v_{1i})}} \text{ for } i = 2, \ldots, t_1,$$

$$\sqrt{\frac{t_2 + d_{G_4}(v_{2i}) - 1}{(t_2+1)d_{G_4}(v_{2i})}} > \sqrt{\frac{t_1 + t_2 + d_{G_4'}(v_{2i}) - 2}{(t_1+t_2)d_{G_4'}(v_{2i})}} \text{ for } i = 1, \ldots, t_2,$$

$$\sqrt{\frac{d + t_2 - 1}{d(t_2+1)}} > \sqrt{\frac{d + t_1 + t_2 - 2}{d(t_1+t_2)}}.$$

Denote $d_{G_4}(v_{11}) = d_1$. It is clear that $d_1 \geq 3$. In the following, we will show

$$\sqrt{\frac{d + t_1 - 1}{d(t_1+1)}} + \sqrt{\frac{t_1 + d_1 - 1}{(t_1+1)d_1}} - \sqrt{\frac{d + d_1 - 2}{dd_1}} > 0,$$

In fact,

$$\frac{d + t_1 - 1}{d(t_1+1)} + \frac{t_1 + d_1 - 1}{(t_1+1)d_1} - \frac{d + d_1 - 2}{dd_1} = \frac{(d-2)d_1 + d(d_1-2) + 2t_1 + 2}{dd_1(t_1+1)} > 0.$$

So

$$(\sqrt{\frac{d + t_1 - 1}{d(t_1+1)}} + \sqrt{\frac{t_1 + d_1 - 1}{(t_1+1)d_1}})^2 > (\sqrt{\frac{d + d_1 - 2}{dd_1}})^2,$$

and

$$\sqrt{\frac{d + t_1 - 1}{d(t_1+1)}} + \sqrt{\frac{t_1 + d_1 - 1}{(t_1+1)d_1}} - \sqrt{\frac{d + d_1 - 2}{dd_1}} > 0.$$

Finally, $ABC(G_4) > ABC(G_4')$. ■

4 The trees with the smallest ABC index

In this section, we will use the graph transformations given in the above section to get the possible n-optimal trees.

Let T be a tree. Suppose T is not a star. By Lemma 2.4, we may assume that T has no vertices of degree 2.

Assume that $v \in V(T)$ is a non-pendent vertex. Denote $N_T(v) = \{u \in V(T) \text{ and } vu \in E(T)\}$, $\widetilde{N}_T(v) = \{u \in N_T(v) \text{ and } d_T(u) = 1\}$, and $\overline{N}_T(v) = \{u \in N_T(v) \text{ and } d_T(u) \geq 3\}$. The non-pendent vertices of T can be divided into the following three types.

- If $|\overline{N}_T(v)| = 1$ and $|\widetilde{N}_T(v)| \geq 2$, then v is called a vertex of Type 1.

- If $|\overline{N}_T(v)| \geq 2$ and $|\widetilde{N}_T(v)| \geq 1$, then v is called a vertex of Type 2.

- If $|\overline{N}_T(v)| \geq 3$ and $|\widetilde{N}_T(v)| = 0$, then v is called a vertex of Type 3.

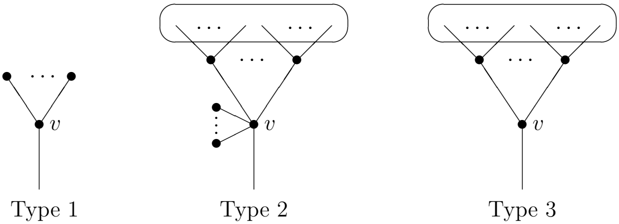

Figure 4.1: Vertices of three types

Denote $\mathbb{T}_n$ to be the set of trees with n pendent vertices. Let $T \in \mathbb{T}_n$ and suppose T is not a star. Now, we will apply some graph transformations to T to get the possible n-optimal trees.

The first step: If T has at least two vertices of Type 2, then by applying the first kind branches exchanging transformation successively, we can get a tree $T' \in \mathbb{T}_n$ such that T' has at most one vertex of Type 2 and $ABC(T) \geq ABC(T')$.

The second step: Suppose T has no vertex of Type 2. By applying the edge cutting transformation successively, we can get a tree $T' \in \mathbb{T}_n$ which is isomorphic to T_1 as shown in Figure 4.2 such that $ABC(T) > ABC(T')$.

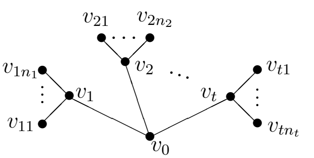

Figure 4.2: Tree T_1

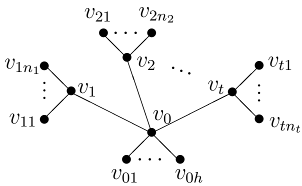

Figure 4.3: Tree T_2

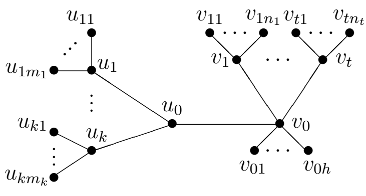

Figure 4.4: Tree T_3 (where $k > t + h$)

Suppose T has exactly one vertex of Type 2. Then either T is isomorphic to a tree T_2

as shown in Figure 4.3, or if necessary, by applying the edge cutting transformation, the second kind branches exchanging transformation, and the third kind branches exchanging transformation, successively, we can get a tree $T' \in \mathbb{T}_n$ which is isomorphic to one of T_1, T_2, and T_3 as shown in Figures 4.2, 4.3, and 4.4, such that $ABC(T) > ABC(T')$.

To sum up, if T is an n-optimal tree, then T is isomorphic to a star or one of T_1, T_2, T_3 as shown in Figures 4.2, 4.3, and 4.4, respectively.

In the following, we consider the trees T_1, T_2 and T_3.

Theorem 4.1 *If T is an n-optimal tree, and is isomorphic to T_2, then $|n_i - n_j| \le 1$ for any $1 \le i < j \le t$.*

Proof. Suppose that there are i, j with $1 \le i < j \le t$ such that $|n_i - n_j| \ge 2$, without loss of generality, we may assume $n_1 = n_2 + 2 + r$, where $r \ge 0$. Then we consider the graph T and the following graph G. Note that $d_G(v_1) = d_T(v_1) - 1$, $d_G(v_2) = d_T(v_2) + 1$ and $d_G(v_i) = d_T(v_i)$ for $i = 0$ and $i = 3, 4, \ldots, t$.

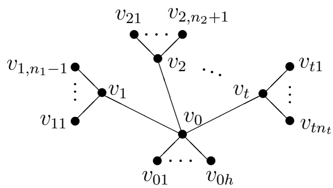

Figure 4.5: Graph G

Denote

$$\begin{aligned}
A =& \sqrt{\frac{d_T(v_0)+d_T(v_1)-2}{d_T(v_0)d_T(v_1)}} + \sqrt{\frac{d_T(v_0)+d_T(v_2)-2}{d_T(v_0)d_T(v_2)}} \\
&+ \sum_{i=1}^{n_1} \sqrt{\frac{d_T(v_1)+d_T(v_{1,i})-2}{d_T(v_1)d_T(v_{1,i})}} + \sum_{i=1}^{n_2} \sqrt{\frac{d_T(v_2)+d_T(v_{2,i})-2}{d_T(v_2)d_T(v_{2,i})}}, \\
B =& \sqrt{\frac{d_G(v_0)+d_G(v_1)-2}{d_G(v_0)d_G(v_1)}} + \sqrt{\frac{d_G(v_0)+d_G(v_2)-2}{d_G(v_0)d_G(v_2)}} \\
&+ \sum_{i=1}^{n_1-1} \sqrt{\frac{d_G(v_1)+d_G(v_{1,i})-2}{d_G(v_1)d_G(v_{1,i})}} + \sum_{i=1}^{n_2+1} \sqrt{\frac{d_G(v_2)+d_G(v_{2,i})-2}{d_G(v_2)d_G(v_{2,i})}}.
\end{aligned}$$

Then $ABC(T) - ABC(G) = A - B$. Noting that $d_T(v_0) = d_G(v_0)$, we indicate it by d, that is, $d_T(v_0) = d_G(v_0) = d$. So

$$A = \sqrt{\frac{d+n_2+r+1}{d(n_2+r+3)}} + \sqrt{\frac{d+n_2-1}{d(n_2+1)}} + (n_2+r+2)\sqrt{\frac{n_2+r+2}{n_2+r+3}} + n_2\sqrt{\frac{n_2}{n_2+1}},$$

$$B = \sqrt{\frac{d+n_2+r}{d(n_2+r+2)}} + \sqrt{\frac{d+n_2}{d(n_2+2)}} + (n_2+r+1)\sqrt{\frac{n_2+r+1}{n_2+r+2}} + (n_2+1)\sqrt{\frac{n_2+1}{n_2+2}}.$$

By Lemmas 2.2 and 2.3, we have

$$\sqrt{\frac{d+n_2+r+1}{n_2+r+3}} - \sqrt{\frac{d+n_2+r}{n_2+r+2}} > \sqrt{\frac{d+n_2}{n_2+2}} - \sqrt{\frac{d+n_2-1}{n_2+1}},$$

and

$$(n_2+r+2)\sqrt{\frac{n_2+r+2}{n_2+r+3}} - (n_2+r+1)\sqrt{\frac{n_2+r+1}{n_2+r+2}} > (n_2+1)\sqrt{\frac{n_2+1}{n_2+2}} - n_2\sqrt{\frac{n_2}{n_2+1}}.$$

Thus

$$\sqrt{\frac{d+n_2+r+1}{d(n_2+r+3)}} + \sqrt{\frac{d+n_2-1}{d(n_2+1)}} > \sqrt{\frac{d+n_2+r}{d(n_2+r+2)}} + \sqrt{\frac{d+n_2}{d(n_2+2)}},$$

and

$$(n_2+r+2)\sqrt{\frac{n_2+r+2}{n_2+r+3}} + n_2\sqrt{\frac{n_2}{n_2+1}} > (n_2+r+1)\sqrt{\frac{n_2+r+1}{n_2+r+2}} + (n_2+1)\sqrt{\frac{n_2+1}{n_2+2}}.$$

In conclusion, we have $A - B > 0$ and Theorem 4.1 holds. ■

For T_1 and T_3, we have the similar results.

Theorem 4.2 *If T is an n-optimal tree, and is isomorphic to T_1, then $|n_i - n_j| \le 1$ for any $1 \le i < j \le t$.*

Theorem 4.3 *If T is an n-optimal tree, and is isomorphic to T_3, then $|m_i - m_j| \le 1$ for any $1 \le i < j \le k$, and $|n_i - n_j| \le 1$ for any $1 \le i < j \le t$.*

5 The smallest ABC index

In this section, we will give an algorithm to find the n-optimal trees and the smallest ABC index of trees with n pendent vertices for each $n \ge 2$.

Denote S_n to be a star with n pendent vertices. From the discussions in the above section, in order to find the n-optimal trees and the smallest ABC index, we only need to compare the ABC indices of trees S_n, T_1, T_2, and T_3, where T_1, T_2, and T_3 are trees with n pendent vertices as shown in Figures 4.2, 4.3, and 4.4, respectively, and T_1, T_2, and T_3 satisfy the following conditions.

- For T_1, $t \geq 3$, $\sum_{i=1}^{t} n_i = n$, and $|n_i - n_j| \leq 1$ for any $1 \leq i < j \leq t$.
- For T_2, $t \geq 1$, $h \geq 1$, $t+h \geq 3$, $h+\sum_{i=1}^{t} n_i = n$, and $|n_i - n_j| \leq 1$ for any $1 \leq i < j \leq t$.
- For T_3, $t \geq 1$, $h \geq 1$, $k > t+h$, $h + \sum_{i=1}^{t} n_i + \sum_{j=1}^{k} m_j = n$, $|m_i - m_j| \leq 1$ for any $1 \leq i < j \leq k$, and $|n_i - n_j| \leq 1$ for any $1 \leq i < j \leq t$.

For S_n, it is known that $ABC(S_n) = \sqrt{n(n-1)}$. In the following three theorems, we will give the ABC indices of trees T_1, T_2, and T_3, respectively.

Theorem 5.1 *Let T_2 be the tree with n pendent vertices as shown in Figure 4.3, where $t \geq 1$, $n_1 = \cdots = n_p = q+1$, $n_{p+1} = \cdots = n_t = q$ and $h = n - tq - p \geq 1$ with $q \geq 2$ and $0 \leq p \leq t-1$. Then*

$$ABC(T_2) = p\sqrt{\frac{h+t+q}{(h+t)(q+2)}} + p(q+1)\sqrt{\frac{q+1}{q+2}} + (t-p)\sqrt{\frac{h+t+q-1}{(h+t)(q+1)}} + (t-p)q\sqrt{\frac{q}{q+1}} + h\sqrt{\frac{h+t-1}{h+t}}.$$

Proof.

$$\begin{aligned} ABC(T_2) = &\sum_{i=1}^{p}\sqrt{\frac{d_{T_2}(v_0)+d_{T_2}(v_i)-2}{d_{T_2}(v_0)d_{T_2}(v_i)}} + \sum_{i=1}^{p}\sum_{j=1}^{q+1}\sqrt{\frac{d_{T_2}(v_i)+d_{T_2}(v_{ij})-2}{d_{T_2}(v_i)d_{T_2}(v_{ij})}} \\ &+ \sum_{i=p+1}^{t}\sqrt{\frac{d_{T_2}(v_0)+d_{T_2}(v_i)-2}{d_{T_2}(v_0)d_{T_2}(v_i)}} + \sum_{i=p+1}^{t}\sum_{j=1}^{q}\sqrt{\frac{d_{T_2}(v_i)+d_{T_2}(v_{ij})-2}{d_{T_2}(v_i)d_{T_2}(v_{ij})}} \\ &+ \sum_{j=1}^{h}\sqrt{\frac{d_{T_2}(v_0)+d_{T_2}(v_{0j})-2}{d_{T_2}(v_0)d_{T_2}(v_{0j})}} \end{aligned}$$

$$\begin{aligned} &= p\sqrt{\frac{h+t+q}{(h+t)(q+2)}} + p(q+1)\sqrt{\frac{q+1}{q+2}} + (t-p)\sqrt{\frac{h+t+q-1}{(h+t)(q+1)}} \\ &\quad + (t-p)q\sqrt{\frac{q}{q+1}} + h\sqrt{\frac{h+t-1}{h+t}}. \end{aligned}$$

The result holds. ■

Note that if $h = 0$, then T_2 becomes T_1. We have the following result for T_1.

Theorem 5.2 *Let T_1 be the tree with n pendent vertices as shown in Figure 4.2, where $t \geq 1$, $n_1 = \cdots = n_p = q+1$ and $n_{p+1} = \cdots = n_t = q$ with $q \geq 2$ and $0 \leq p \leq t-1$. Then*

$$ABC(T_1) = p\sqrt{\frac{t+q}{t(q+2)}} + p(q+1)\sqrt{\frac{q+1}{q+2}} + (t-p)\sqrt{\frac{t+q-1}{t(q+1)}} + (t-p)q\sqrt{\frac{q}{q+1}}.$$

Theorem 5.3 *Let T_3 be the tree with n pendent vertices as shown in Figure 4.4, where $t \geq 1$, $k \geq 2$, $n_1 = \cdots = n_p = q+1$, $n_{p+1} = \cdots = n_t = q$, $m_1 = \cdots = m_r = s+1$, $m_{r+1} = \cdots = m_k = s$, $q \geq 2$, $s \geq 2$, $0 \leq p \leq t-1$, $0 \leq r \leq k-1$, and $h = n - tq - p - ks - r \geq 1$. Then*

$$\begin{aligned} ABC(T_3) = {} & r\sqrt{\frac{k+s+1}{(k+1)(s+2)}} + r(s+1)\sqrt{\frac{s+1}{s+2}} + (k-r)\sqrt{\frac{k+s}{(k+1)(s+1)}} \\ & + s(k-r)\sqrt{\frac{s}{s+1}} + h\sqrt{\frac{h+t}{h+t+1}} + \sqrt{\frac{h+t+k}{(h+t+1)(k+1)}} \\ & + p\sqrt{\frac{h+t+q+1}{(h+t+1)(q+2)}} + p(q+1)\sqrt{\frac{q+1}{q+2}} + (t-p)\sqrt{\frac{h+t+q}{(h+t+1)(q+1)}} \\ & + q(t-p)\sqrt{\frac{q}{q+1}}. \end{aligned}$$

Proof.

$$\begin{aligned} ABC(T_3) = {} & \sum_{i=1}^{r}\sqrt{\frac{d_{T_3}(u_0)+d_{T_3}(u_i)-2}{d_{T_3}(u_0)d_{T_3}(u_i)}} + \sum_{i=1}^{r}\sum_{j=1}^{s+1}\sqrt{\frac{d_{T_3}(u_i)+d_{T_3}(u_{ij})-2}{d_{T_3}(u_i)d_{T_3}(u_{ij})}} \\ & + \sum_{i=r+1}^{k}\sqrt{\frac{d_{T_3}(u_0)+d_{T_3}(u_i)-2}{d_{T_3}(u_0)d_{T_3}(u_i)}} + \sum_{i=r+1}^{k}\sum_{j=1}^{s}\sqrt{\frac{d_{T_3}(u_i)+d_{T_3}(u_{ij})-2}{d_{T_3}(u_i)d_{T_3}(u_{ij})}} \\ & + \sum_{j=1}^{h}\sqrt{\frac{d_{T_3}(v_0)+d_{T_3}(v_{0j})-2}{d_{T_3}(v_0)d_{T_3}(v_{0j})}} + \sqrt{\frac{d_{T_3}(v_0)+d_{T_3}(u_0)-2}{d_{T_3}(v_0)d_{T_3}(u_0)}} \\ & + \sum_{i=1}^{p}\sqrt{\frac{d_{T_3}(v_0)+d_{T_3}(v_i)-2}{d_{T_3}(v_0)d_{T_3}(v_i)}} + \sum_{i=1}^{p}\sum_{j=1}^{q+1}\sqrt{\frac{d_{T_3}(v_i)+d_{T_3}(v_{ij})-2}{d_{T_3}(v_i)d_{T_3}(v_{ij})}} \\ & + \sum_{i=p+1}^{t}\sqrt{\frac{d_{T_3}(v_0)+d_{T_3}(v_i)-2}{d_{T_3}(v_0)d_{T_3}(v_i)}} + \sum_{i=p+1}^{t}\sum_{j=1}^{q}\sqrt{\frac{d_{T_3}(v_i)+d_{T_3}(v_{ij})-2}{d_{T_3}(v_i)d_{T_3}(v_{ij})}} \\ = {} & r\sqrt{\frac{k+s+1}{(k+1)(s+2)}} + r(s+1)\sqrt{\frac{s+1}{s+2}} + (k-r)\sqrt{\frac{k+s}{(k+1)(s+1)}} \\ & + s(k-r)\sqrt{\frac{s}{s+1}} + h\sqrt{\frac{h+t}{h+t+1}} + \sqrt{\frac{h+t+k}{(h+t+1)(k+1)}} \\ & + p\sqrt{\frac{h+t+q+1}{(h+t+1)(q+2)}} + p(q+1)\sqrt{\frac{q+1}{q+2}} + (t-p)\sqrt{\frac{h+t+q}{(h+t+1)(q+1)}} \\ & + q(t-p)\sqrt{\frac{q}{q+1}}. \end{aligned}$$

The result holds. ∎

We now define $T(t,p,q,k,r,s,h) \in \mathbb{T}_n$ to be the tree with seven parameters t, p, q, k, r, s, h.

- If $t = p = q = k = r = s = h = 0$, define $T(t,p,q,k,r,s,h)$ to be the star S_n with n pendent vertices.
- If $k = 0$ and $t > 0$, define $T(t,p,q,k,r,s,h)$ to be the tree T_1 or T_2 as shown in Figure 4.2 or 4.3, where $n_1 = \cdots = n_p = q+1$, $n_{p+1} = \cdots = n_t = q$, and $h = n - tq - p$ with $q \geq 2$, $0 \leq p \leq t-1$, and $h \geq 0$ (if $h = 0$, then $T(t,p,q,k,r,s,h)$ is T_1; if $h \geq 1$, then $T(t,p,q,k,r,s,h)$ is T_2).
- If $k \geq 2$ and $t \geq 1$, define $T(t,p,q,k,r,s,h)$ to be the tree T_3 as shown in Figure 4.4, where $n_1 = \cdots = n_p = q+1$, $n_{p+1} = \cdots = n_t = q$, $m_1 = \cdots = m_r = s+1$, $m_{r+1} = \cdots = m_k = s$, and $h = n - tq - p - ks - r$, with $q \geq 2$, $s \geq 2$, $0 \leq p \leq t-1$, $0 \leq r \leq k-1$, $h \geq 1$, and $k > t+h$.

Now we will give an algorithm to find the n-optimal trees and the smallest ABC index of trees with n pendent vertices for each $n \geq 2$. The main idea is to compare the values of all of $ABC(T(t,p,q,k,r,s,h))$.

Using this algorithm, we can determine the parameters t,p,q,k,r,s,h and get the ABC index of $T = T(t,p,q,k,r,s,h)$ such that $T = T(t,p,q,k,r,s,h)$ has the smallest ABC index among trees with n pendent vertices.

Algorithm. An algorithm for fining the n-optimal trees and the smallest ABC index of trees with n pendent vertices for each $n \geq 2$.

Input The number n of the pendent vertices

Output t,p,q,k,r,s,h and the smallest ABC index

$A = \sqrt{n(n-1)}$; $T = 0$; $P = 0$; $Q = 0$; $K = 0$; $R = 0$; $S = 0$; $H = n$;

for $t = 1$; $t \leq \lfloor \frac{n}{2} \rfloor$; $t++$ **do**

  for $q = 2$; $q \leq \lfloor \frac{n}{t} \rfloor$; $q++$ **do**

    for $p = 0$; $p \leq \min\{t-1, n-tq\}$; $p++$ **do**

      $h = n - tq - p$;

      $x = p\sqrt{\frac{h+t+q}{(h+t)(q+2)}} + p(q+1)\sqrt{\frac{q+1}{q+2}} + (t-p)\sqrt{\frac{h+t+q-1}{(h+t)(q+1)}}$

$+(t-p)q\sqrt{\frac{q}{q+1}}+h\sqrt{\frac{h+t-1}{h+t}}$;

if $x<A$ **do**

$A=x; T=t; P=p; Q=q; H=h;$

end

end

end

end

if $n\geq 7$ **do**

for $l=4;\ l\leq n-3;\ l++$ **do**

for $k=2;\ k\leq\lfloor\frac{l}{2}\rfloor;\ k++$ **do**

$s=\lfloor\frac{l}{k}\rfloor;\ r=l-ks;$

$z=r\sqrt{\frac{k+s+1}{(k+1)(s+2)}}+r(s+1)\sqrt{\frac{s+1}{s+2}}+(k-r)\sqrt{\frac{k+s}{(k+1)(s+1)}}+s(k-r)\sqrt{\frac{s}{s+1}};$

for $t=1;\ t\leq k-1;\ t++$ **do**

for $q=2;\ q\leq\lfloor\frac{n-l-1}{t}\rfloor;\ q++$ **do**

for $p=0;\ p\leq\min\{t-1,n-l-tq-1\};\ p++$ **do**

$h=n-l-tq-p;$

$y=z+h\sqrt{\frac{h+t}{h+t+1}}+\sqrt{\frac{h+t+k}{(h+t+1)(k+1)}}+p\sqrt{\frac{h+t+q+1}{(h+t+1)(q+2)}}$
$+p(q+1)\sqrt{\frac{q+1}{q+2}}+(t-p)\sqrt{\frac{h+t+q}{(h+t+1)(q+1)}}+q(t-p)\sqrt{\frac{q}{q+1}};$

if $y<A$ **do**

$A=y; T=t; P=p; Q=q; K=k; R=r; S=s; H=h;$

end

end

end

end

end

end

end

Output $t=T; p=P; q=Q; k=K; r=R; s=S; h=H;$ the smallest ABC index$=A$.

Example 5.4 *The following Table 1 will give some results for some particular n by this algorithm.*

Table 1: The smallest ABC indices for some particular n

n	t	p	q	k	r	s	h	The smallest ABC index
19	1	0	9	0	0	0	10	18.488380
20	1	0	10	0	0	0	10	19.475810
22	1	0	11	0	0	0	11	21.454264
24	1	0	12	0	0	0	12	23.435299
26	1	0	13	0	0	0	13	25.418443
28	1	0	14	0	0	0	14	27.403337
30	1	0	15	0	0	0	15	29.389702
32	1	0	16	0	0	0	16	31.377316
34	1	0	17	0	0	0	17	33.366003
98	6	0	12	0	0	0	26	96.694917
100	7	0	11	0	0	0	23	98.668638
200	16	11	10	0	0	0	29	197.359789
240	19	0	11	0	0	0	31	236.799027
300	27	0	10	0	0	0	30	295.930534
400	37	0	10	0	0	0	30	394.438032
500	47	1	10	0	0	0	29	492.907920
512	49	48	9	0	0	0	23	504.723697
600	58	0	10	0	0	0	20	591.348708
700	68	0	10	0	0	0	20	689.766291
800	78	1	10	0	0	0	19	788.172425
900	89	0	10	0	0	0	10	886.558802
1000	99	0	10	0	0	0	10	984.939494
2000	200	0	10	0	0	0	0	1968.569319
3000	300	0	10	0	0	0	0	2952.187946

6 Closing remark

We have calculated the results for $2 \leq n \leq 1000$ with the algorithm given in the above section. About the algorithm, we point out some facts as follows.

- The results obtained with our algorithm and the existing results in [1–3] are totally identical.
- With our algorithm, by single PC, to find all n-optimal trees and the smallest ABC indies of trees with n pendent vertices for $19 \leq n \leq 219$ only need about 1 minute 33 seconds. So our algorithm is much more efficient than the algorithm in [3].
- It can be seen from the results in Table 1 that (1) and (2) of Conjecture 4.1 in [3] are negative.

  As an example, for $n = 400$, our calculation results are $t = 37, p = 0, q = 10, k = 0, r = 0, s = 0, h = 30$. According to the notations in [3], $k = 400$, $t = 37$, $d_0 = 67$,

$d_1 = \cdots = d_t = 11$, and the degree sequence $\pi = (67, 11^{37}, 1^{400})$. In this case, $\lfloor \frac{k}{11} \rfloor - 2 = 34 \neq t$, and $d_1 - 1 = 10 < 11$. So both the results (1) and (2) of Conjecture 4.1 in [3] is not established for $k = 400$.

- Looking from the results, we find that

  (1) $10 \leq q \leq 11$ for $99 \leq n \leq 240$;

  (2) $9 \leq q \leq 10$ for $241 \leq n \leq 700$, and $q = 9$ only when $n = 512, 541, 570, 599, 628, 657, 676, 705, 724, 734, 743, 753, 772, 791, 801, 810, 820, 839, 858, 877, 887, 896, 906, 915, 925, 934, 944, 953, 963, 972, 982$;

  (3) The tree T_3 as shown in Figure 4.4 seems never be an n-optimal tree.

At the end of the article, we put forward the following conjectures. They are proposed naturally from the results for $2 \leq n \leq 1000$.

Conjecture 6.1 *T_3 as shown in Figure 4.4 is not an n-optimal tree.*

Conjecture 6.2 *For each $n \geq 241$, if T is an n-optimal tree, then T is isomorphic to one of T_1 and T_2 as shown in Figures 4.2 and 4.3, respectively, where $t \geq 1$, $n_1 = \cdots = n_p = q+1$, $n_{p+1} = \cdots = n_t = q$ and $h = n - tq - p \geq 0$ with $9 \leq q \leq 10$ and $0 \leq p \leq t-1$.*

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