# CHARACTERIZING TREES WITH MINIMAL ABC INDEX WITH COMPUTER SEARCH: A SHORT SURVEY 

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#### Abstract

The atom-bond connectivity $(A B C)$ index of a graph $G=$ $(V, E)$ is defined as $A B C(G)=\sum_{v_{i} v_{j} \in E} \sqrt{\left(d_{i}+d_{j}-2\right) /\left(d_{i} d_{j}\right)}$, where $d_{i}$ denotes the degree of vertex $v_{i}$ of $G$. Due to its interesting applications in chemistry, this molecular structure descriptor has become one of the most actively studied vertex-degree-based graph invariants. Many efforts were made towards the elementary problem of characterizing tree(s) with minimal $A B C$ index, which remains open and was coined as the " $A B C$ index conundrum". Up to date, quite a few significant results have been obtained. In the course of research computer search plays a non-negligible role. In the present paper we review the state of the art of the problem. In addition we intend to demonstrate that, repeating the procedure "searching - conjecturing - proving" can be an applicable paradigm to cope with elusive problems of extremal graph characterization.


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## 1. Introduction

We consider non-trivial connected simple graphs only. Such a graph will be denoted by $G=(V, E)$, where $V=\left\{v_{0}, v_{1}, \cdots, v_{n-1}\right\}$ and are the vertex set and edge set of, respectively. If $v_{i} v_{j} \in E$, then $G-v_{i} v_{j}$ will denote the graph obtained from G by deleting the edge $v_{i} v_{j}$. If, in turn, $v_{i} v_{j} \notin E$, then $G+v_{i} v_{j}$ will denote the graph obtained from $G$ by adding the edge $v_{i} v_{j}$.

[^0]Let $P=u_{0} u_{1} \cdots u_{k-1} u_{k}$ be a path of length $k$ in graph $G$ with $k \geq 1, d\left(u_{0}\right) \geq 3$, $d\left(u_{k}\right) \neq 2$, and $d\left(u_{1}\right)=d\left(u_{2}\right)=\cdots=d\left(u_{k-1}\right)=2$. If $d\left(u_{k}\right) \geq 3$ then $P$ is said to be an internal path of $G$. If $d\left(u_{k}\right)=1$ then $P$ is said to be a pendent path of $G$.
Let $d_{i}=d\left(v_{i}\right)$ be the degree of $v_{i}$, and $\Delta=\Delta(G)$ the maximum degree of $G$. A vertex of degree 1 is called a pendent vertex. $\pi(G)=\left(d_{0}, d_{1}, \cdots, d_{n-1}\right)$ is called the degree sequence of $G$. Given a positive integer sequence $\pi=$ $\left(d_{0}, d_{1}, \cdots, d_{n-1}\right)$, if there exists a connected graph $G$ with $\pi(G)=\pi$, then $\pi$ is said to be a (graphic) degree sequence. In particular, if $G$ is a tree, then $\pi$ is called a tree degree sequence. Let $\mathcal{C}(\pi)=\{G \mid G$ is connected and $\pi(G)=\pi\}$, and $\mathcal{T}(\pi)=\{T \mid T$ is a tree and $\pi(T)=\pi\}$.
The $A B C$ index of graph $G=(V, E)$ is defined [1] as

$$
A B C(G)=\sum_{v_{i} v_{j} \in E} \sqrt{\left(d_{i}+d_{j}-2\right) /\left(d_{i} d_{j}\right)}
$$

This vertex-degree-based topological index turned out to be closely correlated with the heat of formation of alkanes [1], and a quantum-chemical explanation for its descriptive ability was provided in [2]. Gutman et al. [3] later confirmed that the $A B C$ index could reproduce the heat of formation with accuracy comparable to that of high-level ab initio and DFT (MP2, B3LYP) quantum chemical calculations. Recently, a probabilistic interpretation of the generalized $A B C$ index is provided by Estrada 4]. Due to these applications, there is an increased interest in the mathematical properties of the $A B C$ index in the last few years (See [5-36]).
From a mathematical point of view, the first question that needs to answer is for which graphs this index assumes minimal and maximal values. It was proved [5,6] that, the $A B C$ index of a graph strictly increases with addition of edges. Hence among $n$-vertex connected graphs, the complete graph $K_{n}$ uniquely maximizes the $A B C$ index, and a graph with minimal $A B C$ index is a tree. In [7] Furtula proved that, among $n$-vertex trees the star $S_{n}$ uniquely maximizes the $A B C$ index. Xing et al. [8] found some upper bounds for the $A B C$ index in some classes of trees. However, the problem of characterizing $n$-vertex tree(s) with minimal $A B C$ index is more elusive and remains open. In 9 Gutman et al. summarized the known results and coined the problem as the " $A B C$ index conundrum". After [9] there are quite a few significant developments, in both mathematical and computational aspects. In the course of research computer search plays a non-negligible role. Namely, the research paradigm of repeating the procedure "Searching - Conjecturing - Proving" was applied: (a) Computer search for trees with minimal $A B C$ index of order as large as possible by using their known properties; (b) Conjecture their properties based on the search results; (c) Prove or disprove the conjectures; (d) Go to (a). In the present paper, we will review the state of the art of the problem, as an update of 9$]$. In addition we intend to demonstrate that, the paradigm may be applicable to cope with other elusive problems of extremal graph characterization.


Figure 1. The branches in a min- $A B C$ tree.

For convenience, in the rest of the paper, we refer a tree with minimal $A B C$ index as a min- $A B C$ tree, and the problem of characterizing $n$-vertex tree(s) with minimal $A B C$ index as min- $A B C$ tree problem. We also assume $n \geq 10$.

## 2. A brute-force and a heuristic search, and the modulo 7 conjecture

In order to guess the general structure of min- $A B C$ trees, Furtula et al. 10 ] firstly conducted a brute-force computer search. Their algorithm consists of two successive steps: (1) Generating the trees recursively; (2) Computing the $A B C$ index for each generated tree and find its minimum value. Since the number of $n$-vertex trees increases rapidly with $n$, though a computer grid with 400 CPUs was employed, the computation was just performed up to $n=31$. One can refer to 11 for the search results.
Few as the search results obtained in [10 are, some structural properties of min- $A B C$ trees were observed and proved by Gutman et al. in [11].

Lemma 2.1. [12] Let $T$ be an n-vertex min-ABC tree. Then
(1) $T$ has no internal paths of length $\geq 2$;
(2) $T$ has no pendent paths of length $\geq 4$;
(3) T has at most one pendent path of length 3.

It was also conjectured [12] that, such a tree has no pendent paths of length 1. Soon this was confirmed by Lin et al. [13].

Lemma 2.2. [13] Let $T$ be an n-vertex min- $A B C$ tree. Then each pendent path of $T$ is of length 2 or 3.

Lemma 2.2 reveals that, each vertex of degree 1 or 2 of an $n$-vertex min- $A B C$ tree $T$ is contained in a so-called $B_{k^{-}}$or $B_{k}^{*}$-branch (shown in Figure 1). From Lemma 2.1 (3) $T$ has a unique $B_{k}^{*}$-branch if $T$ has a pendent path of length 3. Based on these facts Gutman and Furtula [14] implicitly made the following conjecture.

Conjecture 2.3. Let $T$ be an n-vertex min-ABC tree. Then
(1) $T$ has a single high-degree vertex $v_{0}$;
(2) To $v_{0}$ only $B_{k}$ - or $B_{k}^{*}$-branches, $1 \leq k \leq 5$, are attached.


Figure 2. The counterexample from [15].

Actually, Conjecture 2.3 is somehow natural. Let $T$ be an $n$-vertex min- $A B C$ tree, and $T[\delta]$ the subgraph of $T$ induced by the vertices of degree at least $\delta$. From Lemma 2.1 (2), $T[3]$ is connected and thus is a tree. Moreover, based on the known search results at that time, $T[3]$ is conjectured to be a star (see [13]). With the priori assumptions in Conjecture 2.3, Gutman and Furtula [14] conducted a heuristic incomplete computer search for $n$-vertex min- $A B C$ tree(s) up to $n=700$. This is an easy task, because the key is to find the solution set of the Diophantine equation $n=1+2 x_{1}+5 x_{2}+7 x_{3}+9 x_{4}+11 x_{5}+x_{6}$, where $x_{i} \geq 0$ denotes the number of $B_{k}$-branches, $1 \leq i \leq 5$, and $x_{6} \in\{0,1\}$ is the number of pendent paths of length 3 .
The output of this heuristic search shows that, when $n$ is sufficiently large (e.g., $n \geq 175$ ) the structure of $n$-vertex min- $A B C$ trees present a peculiar modulo 7 regularity. Therefore, the so-called "modulo 7 conjecture" was proposed [14]. Unfortunately, soon later this plausible conjecture was disproved by Ahmad et al. 1516 . In particular, the counterexample (shown in Figure 2) provided in 15 ] violates Conjecture 2.3, and indicates the existence of the so-called $B_{3}^{* *}$-branches (see Figure 1) in a min- $A B C$ tree.
On the other hand, since the trees considered in [14] as candidates with minimal $A B C$ index, have an interesting structure, they were named Kragujevac trees in [17. The modulo 7 conjecture with slight corrections, was shown to be valid for Kragujevac trees.

## 3. Greedy trees and search based on tree degree sequence

Gan et al. 18 and Xing et al. [19] independently proved that, the so-called "greedy tree" minimizes the $A B C$ index in $T(\pi)$. Soon later, Lin et al. 20] generalized this result to connected graphs. One can refer to [20] for the definitions of greedy trees and BFS-graphs.

Lemma 3.1. [20] Let $\pi$ be a degree sequence. Then there exists a BFS-graph $G^{*}$ with minimal $A B C$ index in $\mathcal{C}(\pi)$.

Note that, given the degree sequence of a greedy tree (or equivalently, BFS-tree) $T, A B C(T)$ can be easily computed. With Lemma 3.1 computer search for min$A B C$ trees can be done by enumerating degree sequences of trees. Dimitrov [21] presented the first such algorithm, which consists of three successive steps.

1. Generate all tree degree sequences (recursively);
2. Find corresponding greedy trees for each generated degree sequence;
3. Calculate the $A B C$ index of each greedy tree and select the tree with minimal value.
Comparing with the brute-force algorithm presented in [10, Dimitrov's is much more superior. It avoids generating and storing all $n$-vertex trees, and just needs to generate degree sequences of $n$-vertex trees. The search space is far less. For example, for $n=31$, there are $40,330,829,030$ trees, but only 4565 tree degree sequences. Hence Dimitrov's algorithm is able to find all $n$-vertex min- $A B C$ trees for $n \leq 300$ on a single processor platform in about 15 days.
Later Dimitrov's algorithm was improved by Lin et al. [22,23]. For convenience, we say a non-increasing positive integer sequence $\pi=\left(d_{0}, d_{1}, \cdots, d_{n-1}\right)$ is optimal, if it is the degree sequence of a min- $A B C$ tree. 22] and 23] obtained some features of an optimal tree degree sequence, which can be used to significantly narrow the search space. As reported in [22], for $n=31$ only 49 (about 1\%) tree degree sequences have to be generated. The MPI+OpenMP implement in [23] founds all $n$-vertex min- $A B C$ tree(s) up to $n=400$ in 23 hours on a workstation group with 36 CPU cores. It is worth to remark that, the search results in [22] for the first time disprove Conjecture 2.3, and confirm the existence of $B_{3}^{* *}$-branches in a min- $A B C$ tree.
Based on his search result, Dimitrov modified the modulo 7 conjecture initially proposed in [14]. The modified conjecture is valid for $n \leq 400$. However, this plausible conjecture was shown to be completely false for sufficiently large $n$ by Ahmadi et al. [24]. Hence a much more efficient search algorithm or implementation is still desired to identify large min- $A B C$ trees.

## 4. On branches and search up to order 1100

Let $\pi=\left(\Delta=d_{0}, d_{1}, \cdots, d_{t}, d_{t+1}, \cdots, d_{n-1}\right)\left(d_{t} \geq 3\right.$ and $\left.d_{t+1} \leq 2\right)$ be the (nonincreasing) degree sequence of a min- $A B C$ tree $T, n_{k}$ denotes the number of $k$ 's among $\left\{d_{1}, d_{2}, \cdots, d_{n-1}\right\}$, and $d=\sum_{i=1}^{t} d_{i} / t$. \# $P_{3}=(n-t-1) \bmod 2$ indicates the number of paths of length 3 in $T$.
Since $B_{k}^{(*)}$-branches ( $B_{k^{-}}$or $B_{k}^{*}$-branches) are the main structure of a min- $A B C$ tree $T$, it is meaningful to pay attentions to the number $b_{k}$ of $B_{k}^{(*)}$-branches in $T$. Note please, here a $B_{3}^{* *}$-branch is regarded as one $B_{2}$-branch and two $B_{1}$-branches. In fact, in 2014 Hosseini et al. [17] have considered this task for Kragujevac trees. For general trees, most works were done by Dimitrov et al. and Du et al. in 25$] 30$. We summarize the main results in Theorem 4.1.

Theorem 4.1. [25-30]
(1) $b_{1} \leq 2, b_{2} \leq 11, b_{4} \leq 4$, and $b_{k}=0$ for $k \geq 5$;
(2) $b_{1} b_{4}=b_{2} b_{4}=0$;
(3) If $n>18$ and $\# P_{3}=1$, then $b_{1}=0, b_{2} \leq 2$, and $b_{k}=0$ for $k \geq 4$;
(4) If $n>415$, then $\# P_{3}=0$.

Table 1. The performance of some search algorithms.

| Algorithm | Range of $n$ | Time | Test platform |
| :--- | :--- | :--- | :--- |
| Brute-force search [10] | $n \leq 31$ |  | PC grid, 400 CPUs |
| Dimitrovs algorithm [21] | $30 \leq n \leq 300$ | 15 days | PC, 2 cores, 2.3 GHz |
| Algorithm in [22] | $30 \leq n \leq 350$ | 107.8 hours | PC, 8 cores, 1.8 GHz |
| Algorithm in [23] | $30 \leq n \leq 400$ | 23 hours | PC Group, 36 cores |
| Dimitrovs algorithm [31] | $30 \leq n \leq 800$ |  | PC, 2 cores, 2.3 GHz |
| Algorithm in [11] | $30 \leq n \leq 1100$ | 207.1 hours | PC, 4 cores, 2.2 GHz |

From Theorem 4.1 the features of an optimal tree degree sequence obtained in [22] and [23] were significantly refined in [11] as following.
Theorem 4.2. [11]
(1) $n_{1}=\lfloor(n-t-1) / 2\rfloor, n_{2}=\lceil(n-t-1) / 2\rceil, n_{3}=b_{2} \leq 11$, and $n_{4} \geq b_{3} \geq$ $(2 t-31) / 3$;
(2) $\# P_{3}=0$ if $n \geq 416$, and so $n_{1}=n_{2}=(n-t-1) / 2$;
(3) $(n-9) / 7 \leq t \leq(n+13) / 5$;
(4) $4 \leq \Delta \leq t$ and $\Delta \leq n / 7+3$ if $n \geq 40$;
(5) $2 \Delta+5 t \leq n+21$;
(6) $4-77 /(n-9) \leq d<5$;

By applying Theorem 4.1 Dimitrov 31 conducted a computer search for $n$ vertex min- $A B C$ tree(s) up to $n=800$. Soon later by Theorem 4.2 Lin et al. [11] presented the fastest algorithm so far. The test was performed up to $n=1100$ within 9 days on a single PC. Table 1 shows the performance of the main computer search algorithms.

## 5. Further discussions

As pointed out in [11] that, the fastest algorithm is not yet polynomial time one, and still too powerless for large $n$ (e.g., $n=5000$ ), even a large workstation group is involved. Hence towards the complete solution of the min- $A B C$ tree problem, at this point the main task is to find more properties of (sufficiently large) min- $A B C$ trees. The following are some possible directions in further investigation.
(1) Refine the upper bounds of $b_{1}, b_{2}$, and $b_{4}$. We guess $b_{1}=b_{2}=0$ and $b_{4} \leq 2$.
(2) Obtain a non-trivial lower bound of $\Delta$ on $n$ and/or $t$.
(3) Investigate the behavior of $d=\sum_{i=1}^{t} d_{i} / t$ with $n$ increases, so as to get better bounds of $d$ for large $n$. Better bounds of $d$ can help us refine Theorem 4.2. On the other hand, $d<5$ implies that, the number of high-degree vertices should be small. In fact, we guess the high-degree vertices induce a star.

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## Competing Interests

The authors declare that they have no competing interests.

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