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Computer search for large trees with minimal *ABC* index[☆]

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ABSTRACT

The atom-bond connectivity (*ABC*) index of a graph $G=(V, E)$ is defined as $ABC(G)=\sum_{v_iv_j\in E}\sqrt{(d_i+d_j-2)/(d_id_j)}$, where $V=\{v_0,v_1,\cdots, v_{n-1}\}$ and d_i denotes the degree of vertex v_i of G. This molecular structure descriptor found interesting applications in chemistry, and has become one of the most actively studied vertex-degree-based graph invariants. However, the problem of characterizing n-vertex tree(s) with minimal *ABC* index remains open and was coined as the “*ABC* index conundrum”. In attempts to guess the general structure of such trees, several computer search algorithms were developed and tested up to $n=800$. However, for large n, all current search programs seem too powerless. For example, the fastest one up to date reported recently in [30] costs 2.2 h for $n=800$ on a single PC with two CPU cores. In this paper, we significantly refine the known features of the degree sequence of a tree with minimal *ABC* index. With the refined features a search program was implemented with OpenMP. Our program was tested on a single PC with 4 CPU cores, and identified all n-vertex tree(s) with minimal *ABC* index up to $n=1100$ within 207.1 h. Some observations are made based on the search results, which indicate some possible directions in further investigation of the problem of characterizing n-vertex tree(s) with minimal *ABC* index.

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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 $V=\{v_0,v_1,\cdots, v_{n-1}\}$ and E are the vertex set and edge set of G, respectively. Let $d_i=d(v_i)$ denote the *degree* of vertex v_i, and $\Delta=\Delta(G)$ the *maximum degree* of G. $\pi(G)=(d_0,d_1,\cdots, d_{n-1})$ is called the *degree sequence* of G. The *ABC* index of graph $G=(V, E)$ is defined [1] as $ABC(G)=\sum_{v_iv_j\in E}\sqrt{(d_i+d_j-2)/(d_id_j)}$. For convenience, we call a tree degree sequence is *optimal* if it is the degree sequence of a tree with minimal *ABC* index.

The *ABC* 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 *ABC* index could reproduce the heat of formation with accuracy comparable to that of high-level ab initio and DFT (MP2, B3LYP) quantum chemical calculations. Due to these applications, there is an increased interest in the mathematical properties of the *ABC* index in the last few years (See [4–22,31–33]). However, the problem of characterizing n-vertex tree(s) with minimal *ABC* index remains open and was coined as the “*ABC* index conundrum” [23]. In attempts to guess the general structure of n-vertex tree(s)

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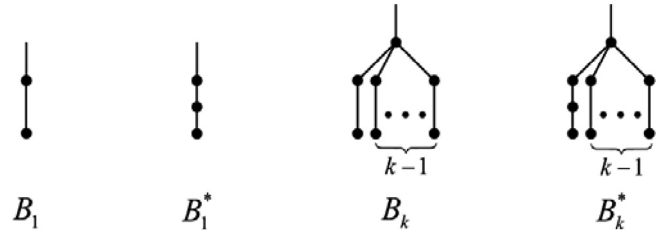

Fig. 1. The $B_k^{(*)}$-branches.

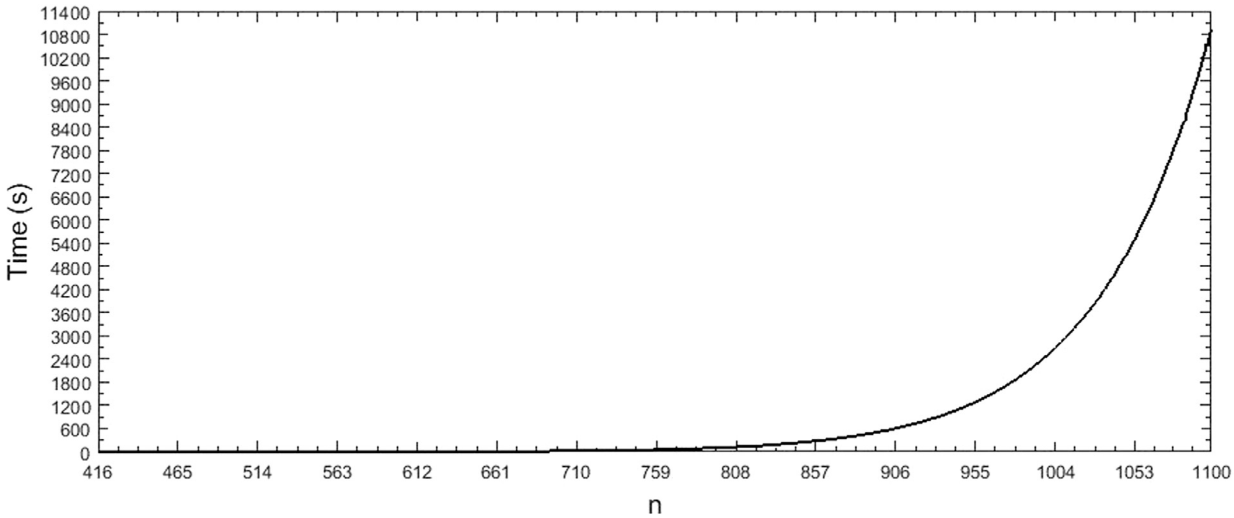

Fig. 2. The elapsed time by our program.

with minimal *ABC* index, several search algorithms were developed. Furtula et al. [24] carried out a brute-force computer search and found n-vertex tree(s) with minimal *ABC* index for $n \leq 31$. Dimitrov [25] presented a search algorithm based on tree degree sequences, which was tested up to $n = 300$. Lin et al. [26, 27] improved Dimitrov's algorithm and tested up to $n = 400$. Recently, by using some recently found structural properties of a tree with minimal *ABC* index (namely, Lemma 2.2 (1) and (4)), Dimitrov and Milosavljević [30] developed the fastest search program up to date, and tested up to $n = 800$.

The current search results ($n \leq 800$) all support the "modulo 7 conjecture", which was initially proposed by Gutman and Furtula [12], and modified by Dimitrov [25]. However, this plausible conjecture was shown to be completely false for sufficiently large n by Ahmadi et al. [28]. Hence a much more efficient search algorithm or implementation is desired to identify large trees with minimal *ABC* index. Obviously, to improve the efficiency of the search algorithm based on tree degree sequences, the key is to refine the features of an optimal tree degree sequence. In the present paper, we significantly refine the results obtained in [26,27,30]. With the main result (Theorem 2.10), a search program was implemented with OpenMP. The performance of our program is quite exciting. It identified all n-vertex tree(s) with minimal *ABC* index up to $n = 1100$ within 207.1 h on a single PC with 4 CPU cores. As a contrast, on a single PC with one Intel Core i5 CPU @2.3 GHz (2 cores), for $n = 800$ our program costs 0.22 h only, while the one presented in [30] costs 2.2 h. Moreover, some observations are made based on the search results, which indicate some possible directions in further investigation of the problem of characterizing n-vertex tree(s) with minimal *ABC* index.

2. More features of an optimal tree degree sequence

For a given non-increasing tree degree sequence $\pi(G) = (d_0, d_1, \cdots, d_{n-1})$, the (unique) *greedy tree* (or equivalently, *BFS-tree*) $T^*(\pi)$ has been shown to be a tree with minimal *ABC* index among trees with degree sequence π (See [13–15]). $T^*(\pi)$ is a rooted tree with vertex set $\{v_0, v_1, \cdots, v_{n-1}\}$ and root v_0 such that $d(v_i) = d_i$, and $i < j$ implies $d_i \geq d_j$, $0 \leq i, j \leq n-1$. To have a better understanding of the properties of a greedy tree, one can refer to the Lemma 3.2 (Switching transformation) and the proof of the Theorem 3.5 in [15].

For convenience, hereafter we always assume $n \geq 10$, $\pi = (\Delta = d_0, d_1, \cdots, d_t, d_{t+1}, \cdots, d_{n-1})$ ($d_t \geq 3$and $d_{t+1} \leq 2$) is optimal, and T is the (unique) greedy tree with degree sequence π. n_k will denote the number of k's among $\{d_1, d_2, \cdots, d_{n-1}\}$ (Note that d_0 is exclusive). Let $d = \sum_{i=1}^{t} d_i/t$, the average of $d_1, d_2, \cdots, d_t$. It is well known that (See [16]), every vertex of degree 1 or 2 of T belongs to a so-called B_k- or B_k^*-branch (shown in Fig. 1), and T has at most one B_k^*-branch. Let $\#P_3$

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