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On Trees with Minimal *ABC* Index among Trees with Given Number of Leaves☆

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Abstract

The atom-bond connectivity (*ABC*) index of a graph $G=(V,E)$ is defined as $ABC(G)=\sum_{v_iv_j\in E}\sqrt{[d(v_i)+d(v_j)-2]/[d(v_i)d(v_j)]}$, where $d(v_i)$ denotes the degree of vertex v_i of G. This recently introduced molecular structure descriptor found interesting applications in chemistry. However, the problem of characterizing trees with minimal *ABC* index among trees with k leaves (k-optimal trees) remains open. In this paper, we present some properties of k-optimal trees, and computer search k-optimal trees for $k \le 220$. Finally, the order of a k-optimal tree is conjectured to be $k+\lfloor \frac{k}{11} \rfloor - 1$ for $k \ge 88$.

1. Introduction and notations

We consider non-trivial connected simple graphs only. Such a graph will be denoted by $G=(V,E)$, where $V=V(G)=\{v_0,v_1,\cdots,v_{n-1}\}$ and $E=E(G)$ are the vertex set and edge set of G, respectively. Let $N_G(v_i)$ denote the set of neighbors of vertex v_i, and $d(v_i)=|N_G(v_i)|$ the degree of v_i. A *leaf* of a tree is a vertex of degree 1. $\pi=\pi(G)=(d(v_0),d(v_1),\cdots,d(v_{n-1}))$ is called the *degree sequence* of G. In particular, if G is a tree, then π is called a tree degree sequence. Let $\mathcal{T}(\pi)=\{T \mid T$ is a tree and $\pi(T)=\pi\}$. We assume, without loss of generality, the degree sequences are non-increasing.

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

$$ABC(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{d(v_i)+d(v_j)-2}{d(v_i)\cdot d(v_j)}}$$

This recently introduced molecular structure descriptor found interesting applications in chemistry, and its mathematical properties has been extensively investigated in the last few years. Most known results can be found in [2] and the references therein. For the developments after [2] see [3-11]. However, the following two elementary problems remain open.

Problem A. Characterize tree(s) with minimal *ABC* index among n-vertex trees.

Problem B. Characterize tree(s) with minimal *ABC* index among trees with k leaves (for convenience, k *-optimal trees*).

Though numerous mathematical results and search algorithms have been developed (see [8-22]), Problem A appears to be elusive still. As for Problem B, Magnant et al. [23] claimed that, the unique k-optimal tree is the balanced double star if $k \geq 19$. Unfortunately, the proof is wrong. Soon counterexamples were found by Goubko et al. [24] by searching k-optimal trees for $k \leq 53$. The algorithm that was used is dynamic programming based (see [25]), and costs too much for large k.

To guess the general structure of k-optimal trees, a more efficient search algorithm is desired. In the present paper, the algorithm based on tree degree sequences that used in [20-22] is modified for this task. In order to improve the efficiency of our algorithm, some properties of k-optimal trees are presented. With these results, the algorithm is implemented to find all k-optimal trees for $k \leq 219$ in about 64 hours on a single PC (personal computer). From the search outcomes, the order of a k-optimal tree is conjectured to be $k + \lfloor \frac{k}{11} \rfloor - 1$ for $k \geq 88$.

2. Search algorithm based on tree degree sequences

Definition 2.1 [26]**.** Suppose that the degrees of the non-leaf vertices are given, the greedy tree is achieved by the following "greedy algorithm":

(i) Label the vertex with the largest degree as v (the root);

(ii) Label the neighbors of v as $v_1, v_2, \cdots$, assign the largest degree available to them such that $d(v_1) \geq d(v_2) \geq \cdots$;

(iii) Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \cdots$ such that they take all the largest degrees available and that $d(v_{11}) \geq d(v_{12}) \geq \cdots$;

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

Lemma 2.2 [14,15,18]**.** Given the degree sequence π, the greedy tree $T^*(\pi)$ minimizes the ABC index in $\mathcal{T}(\pi)$.

The algorithm used to search trees with minimal ABC index among n-vertex trees in [20-22] consists of the following three successive steps:

(1) Generate all tree degree sequences of length n;

(2) Find corresponding greedy tree $T^*(\pi)$ for each generated degree sequence π;

(3) Calculate $ABC(T^*(\pi))$ and select the tree(s) with minimal value.

In order to make the algorithm applicable for searching k-optimal trees, we have to know the lower and upper bounds of the order of a k-optimal tree.

Let $f(x,y) = \sqrt{\frac{x+y-2}{xy}}$, where $x, y \geq 1$. Obviously, $f(x,y) = f(y,x) < 1$.

Lemma 2.3. Let T be a k-optimal tree. Then T has no vertices of degree 2.

Proof. Suppose $v_1v_2v_3$ is a path in T with $d(v_2) = 2$. Let $T' = T - v_1v_2 - v_2v_3 + v_1v_3$. Then

$$ABC(T) - ABC(T') = 2\sqrt{\frac{1}{2}} - f(d(v_1), d(v_3)) > 2\sqrt{\frac{1}{2}} - 1 > 0. \qquad \blacksquare$$

From Lemma 2.3, if $\pi = (d_0, d_1, \cdots, d_t, 1^k)$, where $t \geq 0$ and a^k denotes k successive a's, is the degree sequence of a k-optimal tree, then $d_t \geq 3$.

Corollary 2.4. Let T be a k-optimal tree. Then $n_k = |T| \leq 2k - 2$, and $n_k \geq k + 2$ if $k \geq 19$.

Proof. From the Claim 3 in [23], T is rather than a star if $k \geq 19$, thus the second part holds. Now suppose $\pi(T) = (d_0, d_1, \cdots, d_t, 1^k)$. From Lemma 2.3, we have $d_t \geq 3$. Then it is easily seen that, $2n_k - 2 = 2(k+t+1) - 2 = k + \sum_{i=0}^{t} d_i \geq k + 3(t+1)$, which yields $n_k = k + t + 1 \leq 2k - 2$.

$\blacksquare$

From Corollary 2.4, the algorithm above can be easily modified to search k-optimal trees for $k \geq 19$, just replacing the step (1) as: Generate all tree degree sequences $(d_0, d_1, \cdots, d_t, 1^k)$'s with $d_t \geq 3$ and $1 \leq t \leq k-3$. Though the modified algorithm is already applicable to search k-optimal trees for large k (for example, $k = 120$), we will significantly reduce the number of the tree degree sequences to be generated by finding more properties of k-optimal trees.

3. More properties of *k*-optimal trees

The key result (Theorem 3.6) in this section is that the contracting operation will decrease $ABC(G)$ if it is applied on a cut-edge $e = uv \in E(G)$ with $d(v) \leq 5$. The following lemmas will be used.

Lemma 3.1 [27]**.** Let e be a non-isolated edge of a graph G. Then $ABC(G-e) < ABC(G)$.

Lemma 3.2 [14]**.** $f(x,1)$ strictly increases with x, $f(x,2) = \sqrt{\frac{1}{2}}$, and $f(x,y)$ strictly decreases with x for fixed $y \geq 3$.

Lemma 3.3 [17]**.** If $y \geq 3$, $f(x,y) > \sqrt{\frac{1}{x}}$.

Lemma 3.4 [10]**.** Let $g(x,y) = f(x+\Delta x, y-\Delta y) - f(x,y)$, where $x, y \geq 2$, $\Delta x \geq 0$, and $0 \leq \Delta y < y$. Then $g(x,y)$ increases with x and decreases with y.

Lemma 3.5. Let $h(x) = xf(1,x)$ and $l(x,y) = h(x) - h(x+y)$, $x \geq 2$ and $y > 0$. Then $l(x,y) > -y - \dfrac{y(y+1)}{2(x-1)}$.

Proof. $l(x,y) = xf(1,x) - (x+y)f(1,x+y) = \sqrt{x(x-1)} - \sqrt{(x+y)(x+y-1)}$

$$= -\frac{y(2x+y-1)}{\sqrt{x(x-1)} + \sqrt{(x+y)(x+y-1)}} > -\frac{y(2x+y-1)}{2(x-1)} = -y - \frac{y(y+1)}{2(x-1)}. \qquad \blacksquare$$

Theorem 3.6. Let uv be a non-isolated cut-edge of a graph G, and G_1 the graph obtained from G by contracting edge uv. If $d(v) \leq 5$, then $ABC(G_1) < ABC(G)$.

Proof. If $d(u) = 1$ or $d(v) = 1$, then G_1 is a sub-graph of G, and the result holds from Lemma 3.1. If $d(u) = 2$, the result can be proved analogously to Lemma 2.3. Hence assume $d(u) \geq 3$ and $d(v) \geq 2$. For convenience, denote the degrees of some vertices in G as:

$x = d(u) \geq 3$, $2 \leq y = d(v) \leq 5$, $x_i = d(u_i) \geq 1$ for $u_i \in N_G(u) - \{v\}$, and $y_i = d(v_i) \geq 1$ for $v_i \in N_G(v) - \{u\}$. From Lemmas 3.2-3.5 we have

$$ABC(G) - ABC(G_1) = f(x,y) + \sum_{u_i \in N_G(u)-\{v\}} [f(x_i, x) - f(x_i, x+y-2)]$$

$$+ \sum_{v_i \in N_G(v)-\{u\}} [f(y_i, y) - f(y_i, y+x-2)]$$

$$\geq f(x,y) + (x-1)[f(1,x) - f(1,x+y-2)]$$

$$+(y-1)[f(1,y) - f(1,y+x-2)] \quad \text{(By Lemma 3.4)}$$

$$= f(y,x) + (y-1) f(1,y) + [(x-1) f(1,x) - (x+y-2) f(1,y+x-2)]$$

$$> f(y,x) + (y-1) f(1,y)$$

$$+[(x-1) f(1,x-1) - (x+y-2) f(1,y+x-2)] \quad \text{(By Lemma 3.2)}$$

$$> \sqrt{\tfrac{1}{y}} + (y-1)\sqrt{\tfrac{y-1}{y}} + [h(x-1) - h(x-1+y-1)] \quad \text{(By Lemma 3.3)}$$

$$= \sqrt{\tfrac{1}{y}} + (y-1)\sqrt{\tfrac{y-1}{y}} + l(x-1, y-1)$$

$$> \sqrt{\tfrac{1}{y}} + (y-1)\sqrt{\tfrac{y-1}{y}} - (y-1) - \frac{y(y-1)}{2(x-2)} \triangleq p(x,y) . \quad \text{(By Lemma 3.5)}$$

If $x \geq 404$, then $p(x,5) = 9\sqrt{\tfrac{1}{5}} - 4 - \dfrac{10}{x-2} \geq 9\sqrt{\tfrac{1}{5}} - 4 - \dfrac{10}{404-2} \approx 4.6738 \times 10^{-5} > 0$. On the other hand, it is easily confirmed with computer aid that $p(x,5) > 0$ if $3 \leq x \leq 403$, and $p(x,2) > p(x,3) > p(x,4) > p(x,5)$. Hence $ABC(G) - ABC(G_1) > p(x,5) > 0$.

The proof is thus completed. ■

Theorem 3.7. Let $\pi = (d_0, d_1, \cdots, d_t, 1^k)$ be the degree sequence of a k -optimal tree. If $k \geq 19$, then $d_t \geq 6$ and $1 \leq t \leq \lfloor \frac{k-6}{4} \rfloor$.

Proof. From Theorem 3.6, $d_t \geq 6$ is immediate, and $t \geq 1$ from Corollary 2.4. Finally, $t \leq \lfloor \frac{k-6}{4} \rfloor$ follows immediately from $2k + 2t = k + d_0 + d_1 + \cdots + d_t \geq k + 6(t+1)$. ■

4. Search results and further discussions

From Theorem 3.7, the efficiency of our algorithm for searching k -optimal trees ($k \geq 19$) can be significantly improved, since only the tree degree sequences $(d_0, d_1, \cdots, d_t, 1^k)$'s with $d_t \geq 6$ and $1 \leq t \leq \lfloor \frac{k-6}{4} \rfloor$ have to be generated. Our C implementation (8-threaded) with OpenMP (see [28]) was run on Intel Xeon CPU E5-2403 @1.80GHz (2 processors, 8 cores) with 32.0 GB RAM. All k -optimal trees for $19 \leq k \leq 219$ are found in about 64 hours. Tables 1 and 2 show the search outcomes.

The performance of our program shows the superiority of our algorithm. Analogously to [21], its superiority also can be analyzed theoretically with integer partition theory. However, it still costs about 5.6 hours for $k = 220$. Therefore for larger k , a better algorithm, implementation, or test platform is needed. One may expect that if more properties of k -optimal trees are found, the efficiency of our algorithm can be improved remarkably.

Table 1. Non-leaf degree sequences of k -optimal trees, $54 \leq k \leq 87$.

k	t	d_0	$d_1 - d_t$		k	t	d_0	$d_1 - d_t$		k	t	d_0	$d_1 - d_t$		k	t	d_0	$d_1 - d_t$
54	3	22	$13^2,12$		63	4	23	12^4		72	4	27	$14,13^3$		81	5	28	$13^3,12^2$
55	3	22	13^3		64	4	24	12^4		73	4	27	$14^2,13^2$		82	5	28	$13^4,12$
56	3	23	13^3		65	4	25	12^4		74	4	27	$14^3,13$		83	5	28	13^5
57	3	23	$14,13^2$		66	4	25	$13,12^3$		75	5	26	$12^4,11$		84	5	29	13^5
58	3	23	$14^2,13$		67	4	25	$13^2,12^2$		76	5	26	12^5		85	5	30	13^5
59	3	23	14^3		68	4	25	$13^3,12$		77	5	27	12^5		86	5	30	$14,13^4$
60	3	24	14^3		69	4	25	13^4		78	5	28	12^5		87	6	28	$12^5,11$
61	3	25	14^3		70	4	26	13^4		79	5	28	$13,12^4$					
62	3	25	$15,14^2$		71	4	27	13^4		80	5	28	$13^2,12^3$					

Table 2. Non-leaf degree sequences of k -optimal trees, $88 \leq k \leq 219$.

k	t	d_0	$d_1 - d_t$		k	t	d_0	$d_1 - d_t$		k	t	d_0	$d_1 - d_t$		k	t	d_0	$d_1 - d_t$
88		28	12^6		121		34	$12^6,11^3$		154		39	$12^7,11^5$		187		44	$12^8,11^7$
89		29	12^6		122		34	$12^7,11^2$		155		39	$12^8,11^4$		188		44	$12^9,11^6$
90	6	30	12^6		123	9	34	$12^8,11$		156	12	39	$12^9,11^3$		189	15	44	$12^{10},11^5$
91		30	$13,12^5$		124		34	12^9		157		39	$12^{10},11^2$		190		44	$12^{11},11^4$
92		30	$13^2,12^4$		125		35	12^9		158		39	$12^{11},11$		191		44	$12^{12},11^3$

93		30	$13^3,12^3$		126		36	12^9		159		39	12^{12}		192		44	$12^{13},11^2$
94		30	$13^4,12^2$		127		37	12^9		160		40	12^{12}		193		44	$12^{14},11$
95		30	$13^5,12$		128		37	$13,12^8$		161		41	12^{12}		194		44	12^{15}
96		30	13^6		129		37	$13^2,12^7$		162		42	12^{12}		195		45	12^{15}
97		31	13^6		130		37	$13^3,12^6$		163		42	$13,12^{11}$		196		46	12^{15}
98		32	13^6		131		37	$13^4,12^5$		164		42	$13^2,12^{10}$		197		47	12^{15}
99		30	$12^6,11$		132		36	$12^6,11^4$		165		41	$12^7,11^6$		198		45	$12^9,11^7$
100		30	12^7		133		36	$12^7,11^3$		166		41	$12^8,11^5$		199		45	$12^{10},11^6$
101		31	12^7		134		36	$12^8,11^2$		167		41	$12^9,11^4$		200		45	$12^{11},11^5$
102		32	12^7		135		36	$12^9,11$		168		41	$12^{10},11^3$		201		45	$12^{12},11^4$
103		32	$13,12^6$		136		36	12^{10}		169		41	$12^{11},11^2$		202		45	$12^{13},11^3$
104	7	32	$13^2,12^5$		137	10	37	12^{10}		170	13	41	$12^{12},11$		203	16	45	$12^{14},11^2$
105		33	$13^2,12^5$		138		38	12^{10}		171		41	12^{13}		204		45	$12^{15},11$
106		33	$13^3,12^4$		139		39	12^{10}		172		42	12^{13}		205		45	12^{16}
107		33	$13^4,12^3$		140		39	$13,12^9$		173		43	12^{13}		206		46	12^{16}
108		33	$13^5,12^2$		141		39	$13^2,12^8$		174		44	12^{13}		207		47	12^{16}
109		33	$13^6,12$		142		39	$13^3,12^7$		175		44	$13,12^{12}$		208		48	12^{16}
110		32	$12^6,11^2$		143		37	$12^7,11^4$		176		42	$12^8,11^6$		209		46	$12^{10},11^7$
111		32	$12^7,11$		144		37	$12^8,11^3$		177		42	$12^9,11^5$		210		46	$12^{11},11^6$
112		32	12^8		145		38	$12^8,11^3$		178		42	$12^{10},11^4$		211		46	$12^{12},11^5$
113		33	12^8		146		38	$12^9,11^2$		179		42	$12^{11},11^3$		212		46	$12^{13},11^4$
114		34	12^8		147		38	$12^{10},11$		180		42	$12^{12},11^2$		213		46	$12^{14},11^3$
115	8	35	12^8		148	11	38	12^{11}		181	14	42	$12^{13},11$		214	17	47	$12^{14},11^3$
116		35	$13,12^7$		149		39	12^{11}		182		42	12^{14}		215		47	$12^{15},11^2$
117		35	$13^2,12^6$		150		40	12^{11}		183		43	12^{14}		216		47	$12^{16},11$
118		35	$13^3,12^5$		151		40	$13,12^{10}$		184		44	12^{14}		217		47	12^{17}
119		35	$13^4,12^4$		152		40	$13^2,12^9$		185		45	12^{14}		218		48	12^{17}
120		35	$13^5,12^3$		153		41	$13^2,12^9$		186		45	$13,12^{13}$		219		49	12^{17}

From Table 2, the following conjecture is proposed naturally.

Conjecture 4.1. Let $\pi=(d_0,d_1,\cdots,d_t,1^k)$ be the degree sequence of a k-optimal tree. If $k\geq 88$, then

(1) $t = \lfloor \frac{k}{11} \rfloor - 2$;

(2) $11 \le d_1 - 1 \le d_t \le d_1 \le 13$ and $d_1 - d_t \le 1$;

(3) $k - 11\lfloor \frac{k}{11} \rfloor + 22 \le d_0 \le k - 9\lfloor \frac{k}{11} \rfloor + 18$.

Comparing with Problem A, the complete solution of Problem B seems more promising. Certainly, it is still a challenge in the future, and more theoretic preliminaries are required. We end this paper with the following result.

Lemma 4.2. Let T_k be a k-optimal tree. If $k \ge 72$, then $0.91k \approx \sqrt{\frac{5}{6}}k < ABC(T_k) < k - 1$.

Proof. From Theorem 3.7 and Lemma 3.2, the k pendent edges contribute to $ABC(T_k)$ at least $kf(1,6) = \sqrt{\frac{5}{6}}k$. Hence the first part holds.

With computer aid, it is easily confirmed that the second part holds for $72 \le k \le 106$. Let T be the greedy tree with degree sequence $\pi(T) = (k - 70, 12^7, 1^k)$, where $k \ge 107$. Then from Lemma 3.2,

$$
\begin{aligned}
ABC(T_k) \le ABC(T) &= 77 f(1,12) + 7 f(12, k-70) + (k-77) f(1, k-70) \\
&< 77 f(1,12) + 7 f(12, 107-70) + k - 77 \\
&\approx 75.9994 + k - 77 < k - 1,
\end{aligned}
$$

which completes the proof of the second part. ■

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