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The ABC Index of Trees with Given Degree Sequence*

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Abstract: The atom–bond connectivity index of a graph G is defined as

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

where $E(G)$ is the edge set and $d(u)$, $d(v)$ are the degrees of the vertices u and v in G, respectively. We characterize the trees with given degree sequences, extremal w. r. t. the ABC index.

1 Introduction

Topological indices play a prominent role in chemistry, pharmacology, etc. Among them, one of the best known and widely used is the connectivity index, χ, introduced in 1975 by Randić [8, 9]. Estrada et al. proposed a new index, known as the atom–bond connectivity (ABC) [4]. This index is defined as

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

where $E(G)$ is the edge set and $d(u)$, $d(v)$ are the degrees of u and v in G, respectively.

Furtula et al. [5] showed that the star (S_n) is the unique tree with the maximal ABC index. The characterization of trees with minimal ABC index is still unsolved [7]. Among

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all graphs of order n, the complete graph K_n has maximal ABC index [2]. For other recent studies of the ABC index see [1–3, 6, 7].

Molecular graphs of the practical interest have natural restriction on their degrees corresponding to the valences of the atoms. Therefore it is reasonable to consider a tree with given degree sequence. In this paper we discuss some properties of the extremal trees and construct the trees which have the maximum or minimum ABC index with given degree sequences.

For any vertex $v \in V(T)$, let $d(v)$ denote the degree of v, i. e., the number of edges incident to v. The degree sequence of a tree is the sequence of the degrees (in descending order) of non-leaf vertices. We call a tree maximum (minimum) optimal tree if it maximizes (minimizes) the ABC index among all trees with given degree sequence. In a tree T there is a unique path connecting two vertices u and v, denoted by $P_T(u, v)$. The distance $d_T(u, v)$ between them is the number of edges on the path $P_T(u, v)$. Let T_r be a rooted tree with root r. The height of a vertex v in T_r is $h_T(v) = d_T(r, v)$. In T_r, if the vertex u is adjacent to the vertex v and $d_T(r, u) = d_T(r, v) - 1$, then we call v a child of u. Through this paper, for convenience, we let $\overline{ij} = \sqrt{(i + j - 2)/(ij)}$, where $1 \le i \le j \le \Delta$.

2 Some Lemmas

Lemma 2.1 *Let* $\overline{xy} = \sqrt{\frac{x+y-2}{xy}}$. *If* $x \le y$, *then* $\overline{1x} \le \overline{1y}$.

Proof. If $x \le y$, then $\frac{y-1}{y} - \frac{x-1}{x} = \frac{y-x}{xy} \ge 0$. Hence $\overline{1y} - \overline{1x} = \sqrt{\frac{y-1}{y}} - \sqrt{\frac{x-1}{x}} \ge 0$. □

Lemma 2.2 *(* [11]*) Let*

$$f(x, y) = \sqrt{\frac{x + y - 2}{xy}} = \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}}$$

where $x, y \ge 1$. *If* $y \ge 2$ *is fixed, then* $f(x, y)$ *is decreasing for* x.

Lemma 2.3 *Let* a, b, *and* x *be the positive integers with* $a, b, x \ge 2$. *Denote* $f(x) = \sqrt{\frac{x+a-2}{ax}} - \sqrt{\frac{x+b-2}{bx}}$. *If* $a \le b$, *then* $f(x)$ *is increasing for* x; *if* $a > b$, *then* $f(x)$ *is decreasing for* x.

Proof. Note that

$$f'(x) = \frac{\sqrt{x}}{2x^2}\left(\frac{2 - a}{\sqrt{x + a - 2}\,\sqrt{a}} - \frac{2 - b}{\sqrt{x + b - 2}\,\sqrt{b}}\right)$$

and consider the function $g(y) = \frac{2-y}{\sqrt{x+y-2}\sqrt{y}}$ $(y \geq 2)$. Note that

$$g'(y) = \frac{-xy - 2x - 2y + 4}{2(xy + y^2 - 2y)^{\frac{3}{2}}} < 0\,.$$

Hence, if $a \leq b$, then $g(a) \geq g(b)$. Thus $f'(x) \geq 0$, i. e., $f(x)$ is monotonously increasing for x. Similarly, if $a > b$, then $f(x)$ is decreasing for x. □

3 Tree with given degree sequence with minimum ABC index

For a tree T, suppose that $v_0 v_1 \cdots v_t v_{t+1}$ is a path, where v_0 and v_{t+1} are leaves. Let T' denote a new tree obtained from T by reversing the order of the components attached to $v_i \cdots v_k$. We denote such operation by $J(v_i, v_k)$. (Fig.1 and Fig.2)

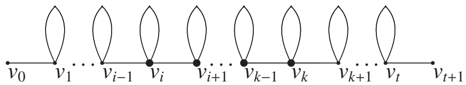

Fig. 1: A path $v_0 v_1 \cdots v_t v_{t+1}$ in T.

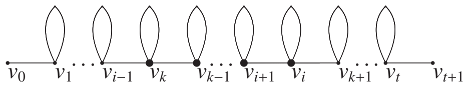

Fig. 2: A new path obtained by $J(v_i, v_k)$ on a path $v_0 v_1 \cdots v_t v_{t+1}$.

Lemma 3.1 *In a minimum optimal tree T, every path $v_0 v_1 \cdots v_t v_{t+1}$, where v_0 and v_{t+1} are leaves, has the properties:*

1) if t is odd, then

$$d(v_1) \leq d(v_t) \leq d(v_2) \leq d(v_{t-1}) \leq \cdots \leq d(v_{\frac{t-1}{2}}) \leq d(v_{\frac{t+3}{2}}) \leq d(v_{\frac{t+1}{2}})$$

2) if t is even, then

$$d(v_1) \leq d(v_t) \leq d(v_2) \leq d(v_{t-1}) \leq \cdots \leq d(v_{\frac{t+4}{2}}) \leq d(v_{\frac{t}{2}}) \leq d(v_{\frac{t+2}{2}})\,.$$

Proof. It clearly suffices to prove that $d(v_i) \leq d(v_{t+1-i}) \leq d(v_k)$, $(i + 1 \leq k \leq t + 1 - i, i = 1, 2, \ldots, \lceil (t + 1)/2 \rceil)$.

By induction on i. For $i = 1$, we should show that $d(v_1) \leq d(v_t) \leq d(v_k)$ $(2 \leq k \leq t)$. By the way of contradiction, suppose that $d(v_k) < d(v_1)$ for some $2 \leq k \leq t$. Then we get T' by using $J(v_1, v_k)$ on T. Note that the edges v_0v_1 and v_kv_{k+1} in T are transformed to the edges v_0v_k and v_1v_{k+1} in T', respectively. Moreover, no other edges are changed. By Lemmas 2.1 and 2.2,

$$ABC(T') - ABC(T) = (\overline{1d(v_k)} - \overline{1d(v_1)}) + (\overline{d(v_1)\,d(v_{k+1})} - \overline{d(v_k)\,d(v_{k+1})}) < 0\ .$$

It is contradicted to the minimum optimality of T. Hence we have $d(v_1) \leq d(v_k)$ $(1 \leq k \leq t)$. At the same time, we easily have $d(v_1) \leq d(v_t)$. Similarly, we can verify the $d(v_t) \leq d(v_k)$. Then we have

$$d(v_1) \leq d(v_t) \leq d(v_k) \quad (2 \leq k \leq t)\ .$$

We now assume Lemma 3.1 holds for any $l \leq i-1$. In other words, we have $d(v_l) \leq d(v_{t+1-l}) \leq d(v_k)$ $\quad (l+1 \leq k \leq t+1-l, l = 1, 2, \ldots, \lfloor (t+1)/2 \rfloor)$. We should prove that $d(v_i) \leq d(v_{t+1-i}) \leq d(v_k)$ $\ (i+1 \leq k \leq t+1-i, i = 1, 2, \ldots, \lfloor (t+1)/2 \rfloor)$. Suppose $d(v_i) > d(v_k)$ for some $i+1 \leq k \leq t+1-i$. We obtain a new T' by applying $J(v_i, v_k)$ on T. Note that the edges $v_{i-1}v_i$ and v_kv_{k+1} in T are transformed to the edges $v_{i-1}v_k$ and v_iv_{k+1} in T', respectively. And no other edges are changed. By the inductive hypothesis, we have $d(v_{i-1}) \leq d(v_{k+1})$. Let

$$f(x) = \sqrt{\frac{x + d(v_{k+1}) - 2}{x d(v_{k+1})}} - \sqrt{\frac{x + d(v_{i-1}) - 2}{x d(v_{i-1})}}\ .$$

By Lemma 2.3, $f(x)$ is decreasing for x. Then,

$$\begin{aligned} ABC(T') - ABC(T) &= \overline{d(v_{i-1})\,d(v_k)} + \overline{d(v_i)\,d(v_{k+1})} - \overline{d(v_{i-1})\,d(v_i)} \\ &- \overline{d(v_k)\,d(v_{k+1})} = f(d(v_i)) - f(d(v_k)) < 0\ . \end{aligned}$$

It is contradicted to the minimum optimality of T. Thus we have $d(v_i) \leq d(v_k)$ $\quad (i+1 \leq k \leq t+1-i)$. Clearly, $d(v_i) \leq d(v_{t+1-i})$. We can also prove that $d(v_{t+1-i}) \leq d(v_k)$ with the same methods present in the former discussion for $i+1 \leq k \leq t+1-i$. Hence, we have $d(v_i) \leq d(v_{t+1-i}) \leq d(v_k)$ $\quad (i \leq k \leq t+1-i)$. □

Definition 3.2 *([10]) Suppose 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 $v_1, v_2, \ldots,$ assign the largest degree available to them such that $d(v_1) \geq d(v_2) \geq \ldots$

3) Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \ldots$ such that they take all the largest *degrees available and that* $d(v_{11}) \geq d(v_{12}) \geq \ldots$ *then do the same for* $v_2, v_3, \ldots$

4) Repeat (3) for all newly labeled vertices, always starting with the neighbors of the labeled vertex with largest whose neighbors are not labeled yet.

Theorem 3.3 *Given the degree sequence, the greedy tree minimizes the ABC index.*

Proof. The greedy tree obviously satisfies the conditions in Lemma 3.1. However, there are many trees for which these conditions hold. Now we only show that the *ABC* index of the greedy tree achieves the minimum among these trees. First, we observe the followings hold: (1) When $d(v_i) > d(v_j)$ and v_i is not adjacent to a leaf, the v_j is also not adjacent to a leaf, for otherwise the *ABC* index decreases. (2) When $d(v_i) > d(v_j) > d(v_k)$ and v_i is not adjacent to v_j, then v_i is not adjacent to v_k, for which $\overline{d(v_i)d(v_j)} < \overline{d(v_i)d(v_k)}$. The tree which possesses the above properties is the greedy tree. Hence, the greedy tree minimizes the *ABC* index. □

Example 1 *We present an example which is a minimum optimal tree obtained by the greedy algorithm with degree sequence* $\pi = (4, 4, 3, 3, 3, 3, 3, 3, 2, 2)$. *Also it is a greedy tree.*

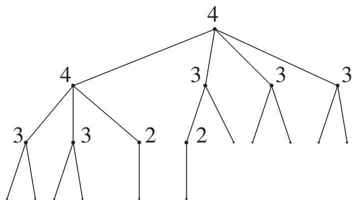

Fig. 3: A greedy tree with degree sequence (4,4,3,3,3,3,3,2,2).

4 Tree with given degree sequence with maximum ABC index

Theorem 4.1 *In a maximum optimal tree, every path* $v_0v_1 \cdots v_tv_{t+1}$, *where* v_0 *and* v_{t+1} *are leaves, has the properties:*

1) if i is odd, then $d(v_i) \geq d(v_{t+1-i}) \geq d(v_k)$ *for* $i \leq k \leq t + 1 - i$;

2) if i is even, then $d(v_i) \leq d(v_{t+1-i}) \leq d(v_k)$ *for* $i \leq k \leq t + 1 - i$.

Proof. By induction on i. For $i = 1$, we prove that $d(v_1) \geq d(v_t) \geq d(v_k)$ $(2 \leq k \leq t)$. By contradiction, suppose that $d(v_k) > d(v_1)$ for some $2 \leq k \leq t$. Then we get T' by using

$J(v_1, v_k)$ on T. Note that the edges v_0v_1 and v_kv_{k+1} in T are transformed to the edges v_0v_k and v_1v_{k+1} in T'. And no other edges are changed. Thus combining Lemmas 2.1 and 2.2, we have

$$ABC(T') - ABC(T) = \overline{1d(v_k)} - \overline{1d(v_1)} + \overline{d(v_1)\, d(v_{k+1})} - \overline{d(v_k)\, d(v_{k+1})} > 0\,.$$

This contradicts to the maximum optimality of T. Hence we have $d(v_1) \geq d(v_k)$ $(2 \leq k \leq t)$. At the same time, we have $d(v_1) \geq d(v_t)$. The proof of $d(v_t) \geq d(v_k)$ is carried out in the same way. Hence we have

$$d(v_1) \geq d(v_t) \geq d(v_k) \quad (1 \leq k \leq t)\,.$$

Now, assume that Lemma 3.1 holds for smaller values. We divide the proof into the next two cases.

Case 1: When $i \geq 2$ is even, we have $d(v_{i-1}) \geq d(v_{t+1-i}) \geq d(v_k)$ $(i + 1 \leq k \leq t + 1 - i)$. By contradiction suppose that $d(v_i) > d(v_k)$ for some $i + 1 \leq k \leq t + 1 - i$. Then we get T' by applying $J(v_i, v_k)$ on T. The edges $v_{i-1}v_i$ and v_kv_{k+1} in T are transformed to the edges $v_{i-1}v_k$ and v_iv_{k+1} in T', respectively. Moreover, no other edges are changed. By the inductive hypothesis, $d(v_{i-1}) \geq d(v_{k+1})$. Let

$$f(x) = \sqrt{\frac{x + d(v_{i-1}) - 2}{xd(v_{i-1})}} - \sqrt{\frac{x + d(v_{k+1}) - 2}{xd(v_{k+1})}}\,.$$

By Lemma 2.3, $f(x)$ is decreasing. We have

$$\begin{aligned} ABC(T') - ABC(T) &= \overline{d(v_{i-1})\, d(v_k)} + \overline{d(v_i)\, d(v_{k+1})} - \overline{d(v_{i-1})\, d(v_i)} \\ &- \overline{d(v_k)\, d(v_{k+1})} = f(d(v_k)) - f(d(v_i)) > 0\,. \end{aligned}$$

This contradicts to the maximum optimality of T. Then we immediately get $d(v_i) \leq d(v_k)$ for any $i \leq k \leq t + 1 - i$. Obviously $d(v_i) \leq d(v_{t+1-i})$. Using the same way, we can prove $d(v_{t+1-i}) \leq d(v_k)$ for $i \leq k \leq t + 1 - i$.

Case 2: When $i \geq 2$ is odd, we can similarly verify $d(v_i) \geq d(v_{t+1-i}) \geq d(v_k)$ by the above argument. $\square$

Operation 1 *Suppose that C is the set of vertices that are adjacent to the leaves in some tree T. Let $d^* = min\{d(u), u \in C\}$. Let C^* be the set of leaves whose adjacent vertices have degree d^* in the tree T. For a tree T_i rooted at r_i, $T^{(i)}$ is obtained from T by identifying the root r_i of T_i with a vertex v in C^*.*

Theorem 4.2 *Let* $\widetilde{C}$ *denote the set of leaves which do not belong to* C^* *in the tree* T*. For a tree* T*, we obtain* T_1^* *and* T_2^* *from* T *by identifying the root* r_i *of* T_i *with* v' *and* v''*, respectively, where* $v' \in C^*, v'' \in \widetilde{C}$*. Then* $ABC(T_1^*) \geq ABC(T_2^*)$*.*

Proof. Suppose v_1 and v_2 are adjacent to v' and v'', respectively. Obviously, $d(v_1) \leq d(v_2)$ holds. By Lemma 2.1, $ABC(T_1^*) - ABC(T_2^*) = \overline{d(v_1)(d(r_i)+1)} + \overline{1d(v_2)} - \overline{1d(v_1)} - \overline{d(v_2)\,(d(r_i)+1)} \geq 0$. $\square$

By Theorem 4.2, the maximum optimal tree is obtained by attaching a tree T_i to a vertex in T. Now we construct the extremal tree of the maximum ABC index with given degree sequence by the following 'adopting algorithm'.

Definition 4.3 *Suppose the degrees of the non-leaf vertices are* $(d_1, d_2, \ldots, d_m)$*. Then the tree with maximum ABC index is obtained by the following 'adopting algorithm'.*

1) We produce some subtrees T_i *as follows:* T_1 *rooted at* r_1 *are assigned* $d_m - 1$ *children whose degrees are* $d_1, d_2, \ldots, d_{d_m-1}$*.* T_2 *rooted at* r_2 *are assigned* $d_{m-1} - 1$ *children whose degrees are* $d_{d_m}, d_{d_m+1}, \ldots, d_{d_m+d_{m-1}-2}$*. Do the same to get* $T_3, T_4, \ldots$*.*

2) Until T_l *rooted at* r_l *with less* $d_{m-l+1} - 1$ *children, or there is no degree available to choose for* T_{l+1}*. Then we get some subtrees* $T_1, T_2, \ldots, T_l$*. Especially, we should have* $d(r_l) = d_{m-l+1}$ *.*

3) Let $r = r_l$ *and* $T = T_l$*. We obtain* $T^{(l-1)}$ *from* T *and* T_{l-1} *rooted at* r_{l-1} *by Operation 1. Then let* $T = T^{(l-1)}$*. We obtain* $T^{(l-2)}$ *from* T *and* T_{l-2} *rooted at* r_{l-2} *. Do the same for* $T_{l-3}, \ldots, T_1$ *.*

4) Let $T = T^1$*. Then* T *is the extremal tree.*

Example 2 *We present an example which are maximum optimal trees with given degree sequence* $(6, 5, 5, 5, 4, 4, 4, 4, 4, 4, 3, 2, 2)$*.*

T and $\widetilde{T}$ are obtained by the 'adopting algorithm'. It is obvious that $ABC(T) = ABC(\widetilde{T})$ *and they are satisfied with Theorem 4.1. They are both maximum trees with degree sequence* $(6, 5, 5, 5, 4, 4, 4, 4, 4, 4, 3, 2, 2)$*. This means that the extremal tree is not unique. But it does if the degrees of non-leaf vertices are different from each other.*

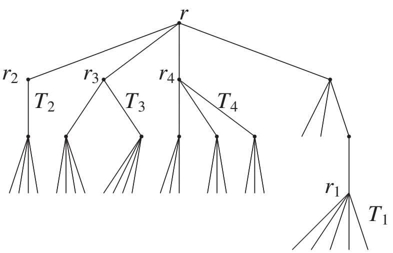

Fig. 4: A maximum optimal tree T with degree sequence (6,5,5,5,4,4,4,4,4,4,3,2,2).

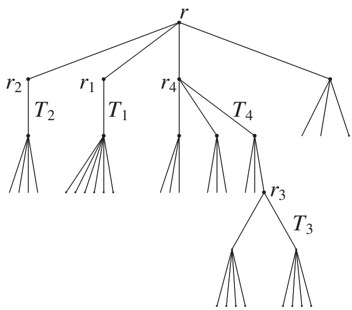

Fig. 5: A maximum optimal tree $\widetilde{T}$ with degree sequence (6,5,5,5,4,4,4,4,4,4,3,2,2).

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