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On The Minimal ABC Index of Connected Graphs with Given Degree Sequence

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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 the vertex v_i of G. This recently introduced molecular structure descriptor found interesting applications in the study of the heats of formation of alkanes. Let $\mathcal{C}(\pi)$ and $\mathcal{T}(\pi)$ denote the sets of connected graphs and trees with degree sequence π, respectively. Gan et al. [*MATCH Commun. Math. Comput. Chem.* **68** (2012)] and Xing et al. [*Filomat* **26** (2012)] proved that, the so-called greedy tree is a tree with minimal ABC index in $\mathcal{T}(\pi)$. In this paper we introduce the breadth-first searching graphs (BFS-graphs for short), and prove that, for any degree sequence π there exists a BFS-graph with minimal ABC index in $\mathcal{C}(\pi)$. This result is applicable to obtain the minimal value or lower bounds of ABC index of connected graphs.

1. Introduction and notations

Molecular descriptors have found wide applications in QSPR/QSAR studies [1]. One of the best known is the Randić index introduced in 1975 by Randić [2], who has shown this index to reflect molecular branching. However, many physic-chemical properties are dependent on factors rather different than branching. In order to take this into account but at the same time to keep the spirit of the Randić index, in 1998 Estrada et al. [3] proposed the *atom-bond connectivity index*.

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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 $E=E(G)$ are the vertex set and edge set of G, respectively. If $v_iv_j\in E$, then $G-v_iv_j$ will denote the graph obtained from G by deleting the edge v_iv_j. If, in turn, $v_iv_j\notin E$, then $G+v_iv_j$ will denote the graph obtained from G by adding the edge v_iv_j. For $v_i\in V$, $N(v_i)$ will denote the set of the neighbors of v_i, and $d(v_i)=|N(v_i)|$ the degree of v_i. The sequence $\pi(G)=(d(v_0),d(v_1),\cdots,d(v_{n-1}))$ is called the degree sequence of G. Let $\Delta=\Delta(G)$ denote the maximum degree of G. If $\Delta(G)\le 4$, then G is said to be a chemical graph.

Given a positive integer sequence $\pi=(d_0,d_1,\cdots,d_{n-1})$, if there exists a connected graph G with $\pi(G)=\pi$, then π is said to be a (graphic) degree sequence. In particular, if G is a tree, then π is also called a tree degree sequence. Let $\mathcal{C}(\pi)=\{G\,|\,G$ is a connected graph and $\pi(G)=\pi\}$, and $\mathcal{T}(\pi)=\{T\,|\,T$ is a tree and $\pi(T)=\pi\}$.

The atom-bond connectivity (ABC) index of a graph $G=(V,E)$ is defined as $ABC(G)=\sum_{v_iv_j\in E}\sqrt{[d(v_i)+d(v_j)-2]/[d(v_i)d(v_j)]}$. This index was shown [3, 4] to be well correlated with the heats of formation of alkanes, and that it thus can serve for predicting their thermodynamic properties. In addition to this, Estrada [5] elaborated a novel quantum-theory-like justification for this topological index, showing that it provides a model for taking into account 1,2-, 1,3-, and 1,4-interactions in the carbon-atom skeleton of saturated hydrocarbons, and that it can be used for rationalizing steric effects in such compounds. These results triggered a number of mathematical investigations of the ABC index [6-24]. The (chemical) trees, unicyclic, bicyclic graph(s) with maximal ABC index were determined [6, 13, 17, 21]. However, the problem of characterizing general connected graph(s) with minimal ABC index appears to be difficult, even in the case of trees.

Molecular graphs of the practical interest have natural restriction on their degrees corresponding to the valences of the atoms. Hence it is reasonable to consider the ABC index of graphs with given degree sequence. Given a tree sequence π, Gan et al. [22] and Xing et al. [23] proved that, the so-called '*greedy tree*' (see Definition 1.1) is a tree with minimal ABC index in $\mathcal{T}(\pi)$.

Definition 1.1 [25]**.** 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.

In order to characterize the graph(s) with minimal *ABC* index in $C(\pi)$, in what follows, we introduce the *breadth-first searching graphs* (BFS-graphs in short), and show that, there is a BFS-graph with minimal *ABC* index in $C(\pi)$.

2. Breadth-first searching graphs

Let $\pi = (d_0, d_1, \cdots, d_{n-1})$ be a non-increasing degree sequence, and $G = (V, E) \in C(\pi)$. We introduce an ordering of the vertices of G induced by *breadth-first search* (BFS for short): Create a sorted list of vertices beginning with v_0, a vertex of degree $d(v_0) = d_0 = \Delta(G)$; append all neighbors $v_1, v_2 \cdots, v_{d_0}$ of v_0 sorted by decreasing degrees; then append all neighbors of v_1 that are not already in the list, also sorted by decreasing degrees; continue recursively with $v_2, v_3, \cdots$, until all vertices of G are processed. In this way we get a *rooted graph* $G' \in C(\pi)$ with root v_0.

For a graph $G = (V, E)$ with root v_0, the distance $dist(v, v_0)$ is called the *height* $h(v)$ of a vertex v, and $h(G) = \max\{h(v) \mid v \in V\}$ the height of G. Since G is non-trivial, $h(G) \geq 1$. Let $V_i = \{v \in V \mid dist(v, v_0) = i\}$, $i = 0, 1, \cdots . h(G$. Then obviously, $V_0 = \{v_0\}$, $V_1 = N(v_0)$, $N(u) \subseteq V_{h(u)-1} V_{h(u)} \bigcup V_{h(u)+1}$ if $1 \leq h(u) \leq h(G) - 1$, and $N(u) \subseteq V_{h(G)-1} \bigcup V_{h(G)}$ if $h(u) = h(G)$. Moreover, for a vertex $v_i \in V_i$, $i \geq 1$, $N(v_i) \bigcap V_{i-1} \neq \varnothing$. We call the least one in $N(v_i) \bigcap V_{i-1}$ in the ordering the parent of v_i.

Definition 2.1 [26, 27]**.** Let $G = (V, E)$ be a connected rooted graph with root v_0. A well-ordering $\prec$ of the vertices is called *breadth-first searching ordering with non-increasing degrees* (BFS-ordering for short) if the following conditions holds for all vertices $u, v \in V$:

(B1) $u \prec v$ implies $h(u) \le h(v)$;

(B2) $u \prec v$ implies $d(u) \ge d(v)$;

(B3) let $uv, xy \in E$ and $uy, xv \notin E$ with $h(u) = h(x) = h(v) - 1 = h(y) - 1$. If $u \prec x$, then $v \prec y$.

A graph having a BFS-ordering of its vertices is called a BFS-graph. If a BFS-graphs is a tree, then it is also called a BFS-tree.

Fact 2.2. (1) Every graph has an ordering of its vertices which satisfies the conditions (B1) and (B3) by using breadth-first search.

(2) Not all connected graphs have an ordering that satisfies the condition (B2). Hence not all connected graphs are BFS-graphs.

(3) Given a degree sequence π, there may exist more than one BFS-graphs in $\mathcal{C}(\pi)$. If π is a tree degree sequence, then there exist a unique BFS-tree in $\mathcal{T}(\pi)$ (under isomorphism).

(4) If π is a tree degree sequence, then T is a greedy tree in $\mathcal{T}(\pi)$ iff T is a BFS-tree in $\mathcal{T}(\pi)$. (See Lemma 2.2 of [25] and note that, both greedy tree and BFS-tree in $\mathcal{T}(\pi)$ are unique under isomorphism.)

One may refer to [26-28] for the above claims and more details of the BFS-graphs.

3. Main results

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

Lemma 3.1 [19]. For fixed $x \ge 2$, $g(x, y) = f(x, y) - f(x-1, y)$ strictly decreases with $y \ge 1$.

Lemma 3.2 (Switching transformation)**.** Let $G = (V, E) \in \mathcal{C}(\pi)$ with $uv, xy \in E$ and $uy, xv \notin E$. Let $G_1 = G - uv - xy + vy + xv$. If $d(u) \ge d(x)$ and $d(v) \le d(y)$, then $ABC(G_1) \le ABC(G)$, with the equality iff $d(u) = d(x)$ or $d(v) = d(y)$.

Proof. From Lemma 3.1,

$$\begin{aligned} ABC(G) - ABC(G_1) &= [f(d(v), d(u)) + f(d(y), d(x))] - [f(d(y), d(u)) + f(d(v), d(x))] \\ &= [f(d(y), d(x)) - f(d(v), d(x))] - [f(d(y), d(u)) - f(d(v), d(u))] \\ &= [g(d(y), d(x)) + g(d(y)-1, d(x)) + \cdots + g(d(v)+1, d(x))] \\ &\quad - [g(d(y), d(u)) + g(d(y)-1, d(u)) + \cdots + g(d(v)+1, d(u))] \\ &\ge 0, \end{aligned}$$

so $ABC(G) \ge ABC(G_1)$, with the equality iff $d(u) = d(x)$ or $d(v) = d(y)$. ■

It is easily seen that, if $G \in \mathcal{C}(\pi)$ and G_1 is obtained from G by switching transformation, then $G_1 \in \mathcal{C}(\pi)$. Hence the following result is immediate from Lemma 3.2.

Corollary 3.3. Let $G=(V,E)$ be a graph with minimal ABC index in $\mathcal{C}(\pi)$, and $u,x \in V$. If $d(u)>d(x)$, then $d(v) \geq d(y)$ for any $v \in N(u)-\{x\}$ and $y \in N(x)-\{u\}$.

Corollary 3.4 [23]**.** Let T be a tree with minimal ABC index in $\mathcal{T}(\pi)$. Then there are no two non-adjacent edges v_1v_2 and v_3v_4 such that $d(v_1)<d(v_3) \leq d(v_4)<d(v_2)$.

Theorem 3.5. Let π be a degree sequence. Then there exists a BFS-graph G^* with minimal ABC index in $\mathcal{C}(\pi)$.

Proof. Let $G=(V,E)$ be a graph with minimal ABC index in $\mathcal{C}(\pi)$. Choose a vertex v_0 of degree $\Delta=\Delta(G)$ as its root. Let $v_0 \prec v_1 \prec \cdots \prec v_{n-1}$ be the well-ordering of the vertices of G induced by BFS beginning with v_0. Notice that, conditions (B1) and (B3) of Definition 2.1 hold for this ordering. If this ordering is not a BFS-ordering, then there exist $i<j$ such that $d(v_i)<d(v_j)$. Choose i and j such that $d(v_0) \geq d(v_1) \geq \cdots \geq d(v_{i-1}) \geq d(v_j) \geq d(v_k)$ and $d(v_j)>d(v_i)$, where $k \geq i$. Then $i \geq 1$ and $h(v_j) \geq h(v_i) \geq 1$ since $d(v_0)=\Delta$. By switching transformation we will construct a graph $G_1 \in \mathcal{C}(\pi)$ from G.

Case 1. $h(v_i)=h(v_j)$.

Since $d(v_0) \geq d(v_1) \geq \cdots \geq d(v_\Delta)$, $v_j \notin V_0 \bigcup V_1$ and hence $h(v_i)=h(v_j) \geq 2$. Let u_i and u_j be the parent of v_i and v_j, respectively. Then $u_i \succ u_j \succ v_i$ and $d(u_i) \geq d(u_j)$, and $u_iv_j, u_jv_i \notin E(G)$. Let $G_1=G-u_iv_i-u_jv_j+u_iv_j+u_jv_i$.

Case 2. $h(v_i)<h(v_j)$.

Let u_i be the parent of v_i and $u_j \in N(v_j)-N(v_i)-\{v_i\}$. u_j is available since $d(v_j)>d(v_i)$ and $u_i \notin N(v_j)$. Obviously, $u_i \in \{v_0, v_1, \cdots, v_{i-1}\}$ and $d(u_i) \geq d(u_j)$, and $u_iv_j, u_jv_i \notin E(G)$. Let $G_1=G-u_iv_i-u_jv_j+u_iv_j+u_jv_i$.

In both cases we have $G_1 \in \mathcal{C}(\pi)$, and $ABC(G_1)=ABC(G)$ from Lemma 3.2. Let $w_0 \prec w_1 \prec \cdots \prec w_{n-1}$ be the well-ordering of the vertices of G_1 induced by BFS beginning with $w_0=v_0$. Then we have $d(w_0) \geq d(w_1) \geq \cdots \geq d(w_i) \geq d(v_k)$, where $k \geq i+1$.

If G_1 is not a BFS-graph yet, we can repeat the switching transformation $G \to G_1$, and finally arrive at a BFS-graph $G^* \in \mathcal{C}(\pi)$ with $ABC(G^*) = ABC(G)$.

The proof is thus completed. ■

Recall that (Fact 2.2. (4)), T is a greedy tree in $\mathcal{T}(\pi)$ iff T is a BFS-tree in $\mathcal{T}(\pi)$. The following result is immediate from Theorem 3.5.

Corollary 3.6 [22, 23]**.** Given a degree sequence π, the greedy tree T^* is a tree with minimal ABC index in $\mathcal{T}(\pi)$.

Remarks. (1) A graph with minimal ABC index in $\mathcal{C}(\pi)$ need not be a BFS-graph, even in the case of trees. For example, let $\pi = (3,3,2,2,1,1,1,1)$, and $T_1, T_2 \in \mathcal{T}(\pi)$ be the two trees shown in Fig. 1. Then T_1 is not a BFS-tree, but both T_1 and T_2 are two trees with minimal ABC index in $\mathcal{T}(\pi)$.

(2) A BFS-graph in $\mathcal{C}(\pi)$ may not be a graph with minimal ABC index in $\mathcal{C}(\pi)$. For example, let $\pi = (4,4,3,3,2,1,1)$, and $G_1, G_2 \in \mathcal{C}(\pi)$ be the two graphs shown in Fig. 2. It is easily seen that both G_1 and G_2 are BFS-graphs, and $ABC(G_1) > ABC(G_2)$. Hence G_1 is a BFS-graph but not a graph with minimal ABC index in $\mathcal{C}(\pi)$.

Fig. 1. Two trees with degree sequence $\pi = (3,3,2,2,1,1,1,1)$.

Fig. 2. Two BFS-graphs with degree sequence $\pi = (4,4,3,3,2,1,1)$.

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