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On the Atom-Bond Connectivity Index of Cacti

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Abstract. The Atom-Bond Connectivity (ABC) index of a connected graph G is defined as $ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$, where $d(u)$ is the degree of vertex u in G. A connected graph G is called a cactus if any two of its cycles have at most one common vertex. Denote by $\mathscr{G}^0(n,r)$ the set of cacti with n vertices and r cycles and $\mathscr{G}^1(n,p)$ the set of cacti with n vertices and p pendent vertices. In this paper, we give sharp bounds of the ABC index of cacti among $\mathscr{G}^0(n,r)$ and $\mathscr{G}^1(n,p)$ respectively, and characterize the corresponding extremal cacti.

1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, the degree of u, denoted by $d(u)$. The Atom-Bond Connectivity (ABC) index of G is defined as [8]

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}. \tag{1}$$

The ABC index was shown to be well correlated with the heats of formation of alkanes, and that it thus can serve for predicting their thermodynamic properties [8]. Various properties of the ABC index have been established, see chemical literature [20][21]. In addition to this, Estrada [7] 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 ABC index [1]- [6], [9]- [17], [22]- [25].

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Let G be a graph. The neighborhood of a vertex $u \in V(G)$ will be denoted by $N(u)$, $\Delta(G) = max\{d(u)|u \in V(G)\}$ and $\delta(G) = min\{d(u)|u \in V(G)\}$. The graph that arises from G by deleting the vertex $u \in V(G)$ will be denoted by $G - u$. Similarly, the graph $G + uv$ arises from G by adding an edge uv between two non-adjacent vertices u and v of G. A pendent vertex of a graph is a vertex with degree 1. If all of blocks of G are either edges or cycles, i.e., any two of its cycles have at most one common vertex, then G is called a cactus. We use $\mathscr{G}^0(n,r)$ to denote the set of cacti with n vertices and r cycles and $\mathscr{G}^1(n,p)$ to denote the set of cacti with n vertices and p pendent vertices. Obviously, $\mathscr{G}^0(n,0)$ are trees, $\mathscr{G}^0(n,1)$ are unicyclic graphs and $\mathscr{G}^1(n,n-1)$ is star. The star with n vertices, denoted by S_n, is the tree with $n-1$ pendent vertices. Let $G(n,r)$ denote the cactus obtained by adding r independent edges to the star S_n (See Fig.1 (a)). Obviously, $G(n,r)$ is a cactus with n vertices, r cycle, and $n-2r-1$ pendent vertices. Note that $G(n,r) \in \mathscr{G}^0(n,r)$ and $G(n,r) \in \mathscr{G}^1(n,n-2r-1)$. $G'(n,p)$ denotes the cactus obtained by adding $(n-p-1)/2$ independent edges to the star S_n if $n-p$ is odd and by adding $(n-p-2)/2$ independent edges to the start S_{n-1} and then inserting a degree 2-vertex in one of those independent edges if $n-p$ is even (See Fig.1(b)). Obviously, $G'(n,p) \in \mathscr{G}^1(n,p)$ and $G'(n,p) \cong G(n,(n-p-1)/2)$ when $n-p$ is odd .

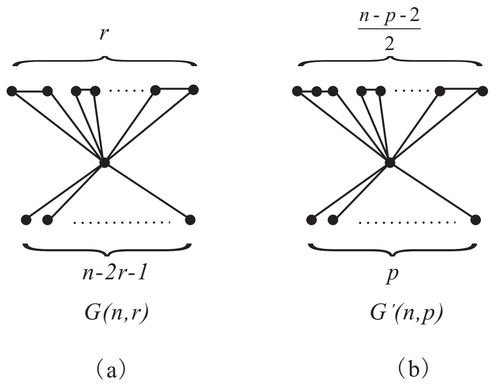

Figure 1: $G(n,r)$ and $G'(n,p)$ for $n-p$ is even

It is straightforward to compute

$$ABC(G(n,r)) = \frac{3r}{\sqrt{2}} + (n-2r-1)\sqrt{\frac{n-2}{n-1}},$$

$$ABC(G'(n,p)) = \begin{cases} \frac{3(n-p-1)}{2\sqrt{2}} + p\sqrt{\frac{n-2}{n-1}} & if\ n-p\ is\ odd, \\ \frac{3(n-p-2)}{2\sqrt{2}} + p\sqrt{\frac{n-3}{n-2}} + \frac{1}{\sqrt{2}} & if\ n-p\ is\ even. \end{cases}$$

For connectivity index of cacti, Lu et al.[19] gave the sharp lower bound on the Randić index of cacti; Lin and Luo [18] gave the sharp lower bound of the Randić index of cacti with fixed pendant vertices. In this paper, we use the techniques in [19] and [18] to give sharp upper bounds on ABC index of cacti among $\mathscr{G}^0(n,r)$ and cacti among $\mathscr{G}^1(n,r)$, and characterize the corresponding extremal graphs, respectively.

For $x, y \geq 1$, let $h(x,y) = \sqrt{\frac{x+y-2}{xy}}$. Obviously, $h(x,y) = h(y,x)$. This lemma will be useful in the following sections.

Lemma 1.1. *[22]* $h(x,1) = \sqrt{\frac{x-1}{x}}$ *is strictly increasing with* x, $h(x,2) = \frac{\sqrt{2}}{2}$ *and* $h(x,y) = \sqrt{\frac{x+y-2}{xy}}$ *is strictly decreasing with* x *for fixed* $y \geq 3$.

2. The Maximum ABC Index of Ccacti with r Cycles

In this section, we will study the sharp upper bound on ABC index of cacti with n vertices and r cycles.

Obviously, $\mathscr{G}^0(n,0)$ are trees with n vertices. Furtula et al [22] proved that the star tree, S_n, has the maximal ABC value among all trees with $n(\geq 2)$ vertices.

Lemma 2.1. *[9] Let* $G \in \mathscr{G}^0(n,0)$ *and* $n \geq 2$, *then* $ABC(G) \leq (n-1)\sqrt{\frac{n-2}{n-1}}$ *with equation if and only if* $G \cong G(n,0) \cong S_n$.

Obviously, $\mathscr{G}^0(n,1)$ are unicyclic graphs. Xing et al [24] gave the upper bound for ABC index of unicyclic graphs and characterized extremal graph.

Lemma 2.2. *[23] Let* $G \in \mathscr{G}^0(n,1)$ *and* $n \geq 3$, *then* $ABC(G) \leq (n-3)\sqrt{\frac{n-2}{n-1}} + \frac{3\sqrt{2}}{2}$ *with equation if and only if* $G \cong G(n,1)$.

Theorem 2.3. *Let* $G \in \mathscr{G}^0(n,r)$, $n \geq 5$. *Then* $ABC(G) \leq F(n,r)$ *with equality if and only if* $G \cong G(n,r)$, *where* $F(n,r) = \frac{3r}{\sqrt{2}} + (n-2r-1)\sqrt{\frac{n-2}{n-1}}$.

Proof. By induction on $n+r$. If $r=0$ or $r=1$, then the theorem holds clearly by Lemma 2.1 and 2.2. Now, we assume that $r \geq 2$, and $n \geq 5$. If $n=5$, then the theorem holds clearly by the facts that there is only one graph $G(5,2)$ in $\mathscr{G}^0(5,2)$ (see Fig. 1).

Let $G \in \mathscr{G}^0(n,r)$, $n \geq 6$ and $r \geq 2$. We consider the following two cases.

Case 1. $\delta(G) = 1$.

Let $u \in V(G)$ with $d(u) = 1$ and $uv \in E(G)$. Denote $d(v) = d$ and $N(v)\backslash\{u\} = \{x_1, x_2, \cdots, x_{d-1}\}$. Then $2 \leq d \leq n-1$. Assume, without loss of generality, that $d(x_1) = d(x_2) = \cdots = d(x_{k-1}) = 1$ and $d(x_i) \geq 2$ for $k \leq i \leq d-1$, where $k \geq 1$. Set $G' = G - u - x_1 - x_2 - \cdots - x_{k-1}$, then $G' \in \mathscr{G}^0(n-k,r)$. By induction assumption and Lemma 1.1 , we have

$$
\begin{aligned}
&ABC(G) = ABC(G') + k\sqrt{\tfrac{d-1}{d}} + \sum_{i=k}^{d-1}[h(d,d(x_i)) - h(d-k,d(x_i))]\\
&\leq ABC(G') + k\sqrt{\tfrac{d-1}{d}} \qquad \text{(by Lemma 1.1)}\\
&\leq F(n-k,r) + k\sqrt{\tfrac{d-1}{d}} \qquad \text{(by inductive assumption)}\\
&= F(n,r) - (n-2r-1)\sqrt{\tfrac{n-2}{n-1}} + (n-2r-1-k)\sqrt{\tfrac{n-k-2}{n-k-1}} + k\sqrt{\tfrac{d-1}{d}}\\
&= F(n,r) + (n-2r-1-k)\Big(\sqrt{\tfrac{n-k-2}{n-k-1}} - \sqrt{\tfrac{n-2}{n-1}}\Big) + k\Big(\sqrt{\tfrac{d-1}{d}} - \sqrt{\tfrac{n-2}{n-1}}\Big)\\
&\leq F(n,r). \qquad \text{(by Lemma 1.1)}
\end{aligned}
$$

The equality $ABC(G) = F(n,r)$ holds if and only if equalities hold throughout the above inequalities, that is, if and only if $d = n-1$, $2r = n-k-1$ and $G' \cong G(n-k,r)$. Thus we have $ABC(G) = F(n,r)$ holds if and only if $G \cong G(n,r)$.

Case 2. $\delta(G) \geq 2$.

By the definition of cactus and $\delta(G) \geq 2$, there exist two edges $u_0u_1, u_0u_2 \in E(G)$ such that $d(u_0) = d(u_1) = 2$ and $d(u_2) = d \geq 3$. We will finish the proof by considering two subcases.

Subcase 1. $u_1u_2 \notin E(G)$.

Let $G' \cong G - u_0 + u_1u_2$. Then $G' \in \mathscr{G}^0(n-1, r)$. By induction assumption and Lemma 1.1, we have

$ABC(G) = ABC(G') + \frac{1}{\sqrt{2}} \leq F(n-1, r) + \frac{1}{\sqrt{2}}$ (by inductive assumption)

$= F(n, r) + \frac{1}{\sqrt{2}} - (n-2r-1)\sqrt{\frac{n-2}{n-1}} + (n-2r-2)\sqrt{\frac{n-3}{n-2}}$

$= F(n, r) + [\frac{1}{\sqrt{2}} - \sqrt{\frac{n-2}{n-1}}] + [(n-2r-2)\sqrt{\frac{n-3}{n-2}} - (n-2r-2)\sqrt{\frac{n-2}{n-1}}]$

$< F(n, r)$. (by Lemma 1.1)

Subcase 2. $u_1u_2 \in E(G)$.

Let $N(u_2)\backslash\{u_0, u_1\} = \{x_1, x_2, \cdots, x_{d-2}\}$. $d(x_i) \geq 2$ for $1 \leq i \leq d-2$, since $\delta(G) \geq 2$. Let $G' = G - u_0 - u_1$. Then $G' \in \mathscr{G}^0(n-2, r-1)$. By inductive assumption and Lemma 1.1, we have

$ABC(G) = ABC(G') + \frac{3}{\sqrt{2}} + \sum_{i=1}^{d-2}[h(d, d(x_i)) - h(d-2, d(x_i))]$

$\leq F(n-2, r-1) + \frac{3}{\sqrt{2}} + \sum_{i=k}^{d-2}[h(d, d(x_i)) - h(d-2, d(x_i))]$ (by inductive assumption)

$= F(n, r) - \frac{3}{\sqrt{2}} - (n-2r-1)\sqrt{\frac{n-2}{n-1}} + (n-2r-1)\sqrt{\frac{n-4}{n-3}} + \frac{3}{\sqrt{2}} + \sum_{i=k}^{d-2}[h(d, d(x_i)) - h(d-2, d(x_i))]$

$= F(n, r) + (n-2r-1)[\sqrt{\frac{n-4}{n-3}} - \sqrt{\frac{n-2}{n-1}}] + \sum_{i=k}^{d-2}[h(d, d(x_i)) - h(d-2, d(x_i))]$

$\leq F(n, r)$. (by Lemma 1.1)

The equality $ABC(G) = F(n, r)$ holds if and only if equalities hold throughout the above inequalities, that is, if and only if $G' \cong G(n-2, r-1)$, $2r = n-1$ and $d(x_i) = 2$ for $i = 1, \cdots, d-2$. Thus we have $ABC(G) = F(n, r)$ holds if and only if $G \cong G(n, r)$. ■

3. The Maximum ABC Index of Cacti with p Pendent Vertices

In this section, we will study the sharp upper bound on ABC index of cacti with n vertices and p pendent vertices.

Denote by $S_{1,n-3}$ the tree obtained by attaching one pendent vertex to a pendent vertex of the star S_{n-1}.

Lemma 3.1. *[25] Let T be a tree with $n \geq 4$ vertices and $T \ncong S_n$, then $ABC(T) \leq (n-3)\sqrt{\frac{n-3}{n-2}} + \sqrt{2}$ with equality holds if and only if $T \cong S_{1,n-3}$.*

Theorem 3.2. *Let $G \in \mathscr{G}^1(n, p)$, $n \geq 4$.*

(1) *If $p = n-1$, then $ABC(G) = (n-1)\sqrt{\frac{n-2}{n-1}}$ and $G \cong S_n$.*

(2) *If $p = n-2$, then $ABC(G) \leq \sqrt{2} + (n-3)\sqrt{\frac{n-3}{n-2}}$ with equality if and only if $G \cong S_{1,n-3}$.*

(3) *If $p \leq n-3$, then $ABC(G) \leq f(n, p)$ with equality if and only if $G \cong G'(n, p)$ where*

$$f(n,p) = \begin{cases} \frac{3(n-p-1)}{2\sqrt{2}} + p\sqrt{\frac{n-2}{n-1}} & if\ n-p \text{ is odd}, \\ \frac{3(n-p-2)}{2\sqrt{2}} + p\sqrt{\frac{n-3}{n-2}} + \frac{1}{\sqrt{2}} & if\ n-p \text{ is even}. \end{cases}$$

Proof.

(1) If $p = n-1$, then $G \cong S_n$. So, the result is obvious.

(2) Since G has $n-2$ pendent vertices, it is a tree and $n \geq 4$. By Lemma 3.1, $S_{1,n-3}$ is the unique graph with the maximum ABC index among trees with $n(\geq 4)$ vertices and $n-2$ pendent vertices. This result follows.

(3) By induction on $n+p$. If $n+p=4$ and $p \leq n-3$, then $n=4$ and $p=0$, that is, $G \cong C_4$. Since $C_4 \cong G'(4,0)$, the theorem holds clearly for $n+p=4$. Now, we assume that $n+p \geq 5$.

Case 1. $p \geq 1$.

Let $u \in V(G)$ with $d(u) = 1$ and $uv \in E(G)$. Denote $d(v) = d$ and $N(v)\backslash\{u\} = \{x_1, x_2, \cdots, x_{d-1}\}$. Then $2 \leq d \leq n-1$. Assume, without loss of generality, that $d(x_1) = d(x_2) = \cdots = d(x_{k-1}) = 1$ and $d(x_i) \geq 2$ for $k \leq i \leq d-1$, where $k \geq 1$. If $\Delta(G) = n-1$, then $d(v) = n-1$ and each block of G is either a triangle or an edge by the definition of cactus. It follows that $G \cong G(n, \frac{n-p-1}{2})$ and $n-p-1$ is even. So, we assume that $\Delta(G) \leq n-2$.

Set $G' = G - u - x_1 - x_2 - \cdots - x_{k-1}$, then $G' \in \mathscr{G}^1(n-k, p-k)$. Note that $n-p$ and $n-k-(p-k)$ have the same parity.

By induction assumption and Lemma 1.1 , we have

$$
\begin{aligned}
& ABC(G) = ABC(G') + k\sqrt{\frac{d-1}{d}} + \sum_{i=k}^{d-1}[h(d, d(x_i)) - h(d-k, d(x_i))] \\
\leq \;& ABC(G') + k\sqrt{\frac{d-1}{d}} \qquad \text{(by Lemma 1.1)} \\
\leq \;& f(n-k, p-k) + k\sqrt{\frac{d-1}{d}} \qquad \text{(by inductive assumption)} \\
= \;& \begin{cases} f(n,p) - p\sqrt{\frac{n-2}{n-1}} + (p-k)\sqrt{\frac{n-k-2}{n-k-1}} + k\sqrt{\frac{d-1}{d}}, & if\ n-p\ is\ odd \\ f(n,p) - p\sqrt{\frac{n-3}{n-2}} + (p-k)\sqrt{\frac{n-k-3}{n-k-2}} + k\sqrt{\frac{d-1}{d}}, & if\ n-p\ is\ even \end{cases} \\
= \;& \begin{cases} f(n,p) + (p-k)(\sqrt{\frac{n-k-2}{n-k-1}} - \sqrt{\frac{n-2}{n-1}}) + k(\sqrt{\frac{d-1}{d}} - \sqrt{\frac{n-2}{n-1}}), & if\ n-p\ is\ odd \\ f(n,p) + (p-k)(\sqrt{\frac{n-k-3}{n-k-2}} - \sqrt{\frac{n-3}{n-2}}) + k(\sqrt{\frac{d-1}{d}} - \sqrt{\frac{n-3}{n-2}}), & if\ n-p\ is\ even \end{cases} \\
\leq \;& f(n,p). \qquad \text{(by Lemma 1.1)}
\end{aligned}
$$

The equality $ABC(G) = f(n,p)$ holds if and only if equalities hold throughout the above inequalities, that is, if and only if $d = n-1$, $p = k$ and $G' \cong G'(n-k, p-k)$. Thus we have $ABC(G) = f(n,p)$ holds if and only if $G \cong G'(n,p)$.

Case 2. $p = 0$.

By the definition of cactus and $p = 0$, there exist two edges $u_0u_1, u_0u_2 \in E(G)$ such that $d(u_0) = d(u_1) = 2$ and $d(u_2) = d \geq 3$. We will finish the proof by considering two subcases.

Subcase 1. $u_1u_2 \notin E(G)$.

Let $G' \cong G - u_0 + u_1u_2$. Then $G' \in \mathscr{G}^1(n-1, 0)$.

If n is odd, then $f(n-1,0) = \frac{3(n-3)}{2\sqrt{2}} + \frac{1}{\sqrt{2}}$ and $f(n,0) = \frac{3(n-1)}{2\sqrt{2}}$. Thus, by inductive assumption, we have $ABC(G) = ABC(G') + \frac{1}{\sqrt{2}} \le f(n-1,0) + \frac{1}{\sqrt{2}} = f(n,0) - \frac{1}{\sqrt{2}} < f(n,0)$.

If n is even, then $f(n-1,0) = \frac{3(n-2)}{2\sqrt{2}}$ and $f(n,0) = \frac{3(n-2)}{2\sqrt{2}} + \frac{1}{\sqrt{2}}$. Thus, by inductive assumption, we have $ABC(G) = ABC(G') + \frac{1}{\sqrt{2}} \le f(n-1,0) + \frac{1}{\sqrt{2}} = f(n,0)$.

The equality $ABC(G') = f(n-1,0)$ holds if and only if $G' \cong G'(n-1,0)$. Hence, $ABC(G) = f(n,0)$ holds if and only if $G \cong G'(n,0)$ for n is even.

Subcase 2. $u_1u_2 \in E(G)$.

Let $N(u_2)\backslash\{u_0,u_1\} = \{x_1, x_2, \cdots, x_{d-2}\}$. $d(x_i) \ge 2$ for $1 \le i \le d-2$, since $\delta(G) \ge 2$. Let $G' = G - u_0 - u_1$. Then $G' \in \mathscr{G}^1(n-2,0)$. By inductive assumption and Lemma 1.1, we have

$$ABC(G) = ABC(G') + \frac{3}{\sqrt{2}} + \sum_{i=1}^{d-2}[h(d,d(x_i)) - h(d-2,d(x_i))]$$

$$\le f(n-2,0) + \frac{3}{\sqrt{2}} + \sum_{i=1}^{d-2}[h(d,d(x_i)) - h(d-2,d(x_i))] \qquad \text{(by inductive assumption)}$$

$$= f(n,0) - \frac{3}{\sqrt{2}} + \frac{3}{\sqrt{2}} + \sum_{i=1}^{d-2}[h(d,d(x_i)) - h(d-2,d(x_i))]$$

$$\le f(n,0). \qquad \text{(by Lemma 1.1)}$$

The equality $ABC(G) = f(n,0)$ holds if and only if equalities hold throughout the above inequalities, that is, if and only if $G' \cong G'(n-2,0)$ and $d(x_i) = 2$ for $i = 1, \cdots, d-2$. Thus we have $ABC(G) = f(n,0)$ holds if and only if $G \cong G'(n,0)$.

■

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