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EXTREMAL ATOM-BOND CONNECTIVITY INDEX OF CACTUS GRAPHS

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Abstract. The atom-bond connectivity index of a graph G (ABC index for short) is defined as the summation of quantities $\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$ over all edges of G. A cactus graph is a connected graph in which every block is an edge or a cycle. The aim of this paper is to obtain the first and second maximum values of the ABC index among all n vertex cactus graphs.

1. Introduction

Suppose G is a simple connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. A block of G is a maximal connected subgraph of G without cut-vertex. A cactus is a connected graph in which every block is an edge or a cycle [18, p. 160]. These are connected graphs in which each edge belongs to at most one cycle. An example of a cactus graph is depicted in Figure 1.

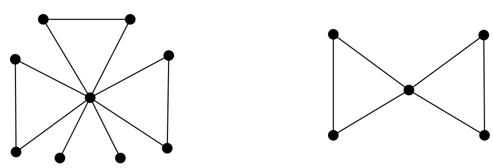

Figure 1. Examples of cactus graphs.

Cactus graphs have several applications in computer science and biology and so it is a topic of interest among many researchers in different scientific disciplines. In [1, 6], it is proved that some graph problems which are NP-hard for general graphs can be solved in polynomial time for cacti. On the other hand, in [15] a number of combinatorial optimization problems are presented

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that may be solved for cactus graphs in polynomial time. We refer the interested readers to Paten et al. [17], for some applications of cacti in examining chromosomal rearrangements.

If G is a connected graph having n vertices and m edges, then $c = m - n + 1$ is called the cyclomatic number of G and conventionally, G is said to be cyclic if $c > 0$. In particular, if $c = 1, 2, 3, 4$, then we call G to be unicyclic, bicyclic, tricyclic and tetracyclic graphs, respectively. The degree, neighbor set of u and minimum degree of the graph G are denoted by $d(u)$, $N_G(u)$ and $\delta(G)$, respectively. For non-adjacent vertices u and v, $G + uv$ is a graph obtained from G by connecting u and v. The complete and star graph on n vertices are denoted by K_n and S_n, respectively.

The ABC index of G is defined as $ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$. This graph invariant was introduced by Estrada et al. [8]. Estrada [7], proved that the ABC index provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes. Recently, several mathematicians spent their time to discover the mathematical properties of this graph invariant.

Chen and Guo [2] characterized the catacondensed hexagonal systems with this graph invariant, and prove that the ABC index of a graph decreases when any edge is deleted. Consequently, they proved that the graph with n vertices and the maximum ABC index is the complete graph K_n. Gutman et al. [14] presented several open questions about minimum ABC index among n vertex trees. Gutman and Furtula [13] determined the structure of trees with a single high-degree vertex and smallest ABC index.

In [11], the authors established some sharp lower and upper bounds on the ABC index in terms of the number of edges, the maximum degree, and the number of pendant vertices, and characterize the corresponding graphs which attain these bounds. They also considered the extremal ABC indices of unicyclic graphs and unicyclic chemical graphs. Xing et al. [19], obtained an upper bound and extremal graphs for the ABC index of molecular graphs with fixed number of vertices and number of edges. They also determined the n vertex unicyclic graphs with the maximum, the second, the third and the fourth maximum ABC indices, and the n vertex bicyclic graphs, $n \geq 5$, with the maximum and the second maximum ABC indices, respectively. The present authors [5], characterized tetracyclic graphs with the maximum and second maximum ABC index.

Gan et al. [12] characterized the trees with given degree sequences, extremal with respect to the ABC index. Furtula et al. [10], studied the extremal problem for the ABC index. They obtained tight upper and lower bounds for the ABC indices of chemical trees. They also proved that, among all trees, the star tree, S_n, has maximal ABC value. Das [3], presented lower and upper bounds for this graph invariant in the classes of graphs and trees. He characterized also the graphs for which these bounds are best possible. Finally, in [9], one of us

(ARA) proved some inequalities for the ABC index of some graph operations. They also proved their bounds are tight.

The aim of this paper is to continue this program by computing the first and second maximum values of ABC index in the class of n vertex cactus graphs, $n \geq 3$. We assume that $G(n,r)$ denotes the set of all cactus graphs containing n vertices and r cycles. Clearly $G(n,0)$, $G(n,1)$ and $G(n,2)$ are trees, unicyclic graphs and bicyclic graphs, respectively. The graph obtained from S_n by connecting two pendants is denoted by $U_{3,n-3}$.

For the sake of completeness we mention here five crucial lemmas as follows:

Lemma 1.1 ([20, Lemma 1]). *Suppose that* $f(x,y) = \sqrt{\frac{x+y-2}{xy}} = \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}}$, $x, y \geq 1$. *Then for a fixed* $y \geq 2$, $f(x,y)$ *is descending for* x.

Lemma 1.2 ([4, Theorem 2.1]). *Suppose that* G *is a simple graph with two non-adjacent vertices* u *and* v. *Then*

$$ABC(G+uv) > ABC(G).$$

Lemma 1.3 ([10, Theorem 2]). *Suppose that* $G \in G(n,0)$, $n \geq 3$. *Then* $ABC(G) \leq \sqrt{(n-1)(n-2)}$. *The equality holds if and only if* $G \cong S_n$.

Lemma 1.4 ([19, Theorem 4.1]). *Suppose* $G \in G(n,1)$, $n \geq 3$. *Then*

$$ABC(G) \leq (n-3)\sqrt{\frac{n-2}{n-1}} + \frac{3\sqrt{2}}{2}.$$

Furthermore, the equality is satisfied if and only if $G \cong U_{3,n-3}$.

Lemma 1.5 ([19, Theorem 5.3]). *Suppose* $G \in G(n,2)$, $n \geq 5$. *Then* $G = S_n^{3,3}$ *has maximum* ABC *index among all bicyclic graphs. Moreover, the* ABC *index of maximum graph is equal to*:

$$ABC(G) = (n-5)\sqrt{\frac{n-2}{n-1}} + 3\sqrt{2},$$

where $S_n^{3,3}$ *is a bicyclic graph obtained from* S_n *by connecting two pairs of pendants in such a way that the resulting graph has exactly* $n-5$ *pendants.*

2. Main results

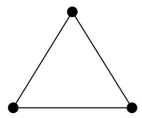
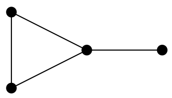
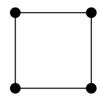
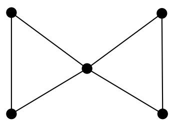
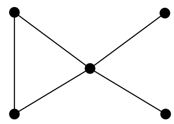
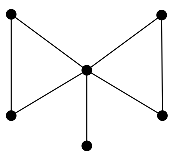
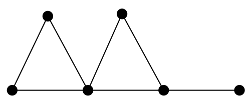
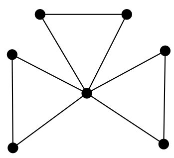
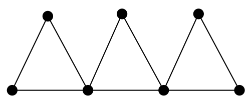
In this section, the maximum and second maximum ABC index among all cactus graphs with n vertices, $n \geq 3$, are calculated. In Table 1, the graphs have the maximum and second maximum of ABC index among n vertex cacti, $3 \leq n \leq 7$, are shown.

The set of all cactus graphs containing r triangles and $n-2r-1$ edges with a common vertex is denoted by $G^0(n,r)$. Let us define

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

where $0 \leq r \leq \left\lfloor \frac{n-1}{2} \right\rfloor$.

TABLE 1. The n vertex cacti, $3 \leq n \leq 7$.

n	**The First Maximum**	**The Second Maximum**
3		
4		
5		
6		
7		

Theorem 2.1. *Suppose $G \in G(n,r)$, $n \geq 3$. Then*

$$ABC(G) \leq h\Big(n, r = \Big\lfloor \frac{n-1}{2} \Big\rfloor\Big).$$

The equality holds if and only if $G \cong G^0\Big(n, \big\lfloor \frac{n-1}{2} \big\rfloor\Big)$.

Proof. If $G \in G^0\Big(n, \big\lfloor \frac{n-1}{2} \big\rfloor\Big)$, then the proof is clear. Suppose $G \notin G^0\Big(n, \big\lfloor \frac{n-1}{2} \big\rfloor\Big)$. In a similar way as in [16, Theorem 3.1], we proceed by induction to prove that $ABC(G) < h\Big(n, r = \big\lfloor \frac{n-1}{2} \big\rfloor\Big)$. If $r = 0, 1$, then by Lemmas 1.3 and 1.4 the proof is clear. So, we can assume that $r \geq 2$ and so $n \geq 5$. If $n = 5$, then $r = 2$ and $G^0(5,2)$ is satisfied our condition. Suppose $n \geq 6$, $r \geq 2$ and $G \in G(n,r)$. Our main proof will consider the following two cases:

Case 1: $\delta(G) = 1$. Let u be a pendant vertex adjacent to vertex v of degree d. So, $N_G(v) \setminus \{u\} = \{y_1, \ldots, y_{d-1}\}$, $2 \le d \le n-1$. Assume that $d(y_1) = d(y_2) = \cdots = d(y_{k-1}) = 1$ and $d(y_i) \ge 2$, when $k \le i \le d-1$. If $k = 1$, then $d(y_i) \ge 2$, $1 \le i \le d-1$, and so it is enough to consider the case that $k > 1$. Define $G' = G - u - y_1 - y_2 - \cdots - y_{k-1}$. Then $G' \in G(n-k, r)$ and so by induction hypothesis,

$$ABC(G') < h(n-k, \lfloor \frac{n-k-1}{2} \rfloor).$$

By applying Lemma 1.2, we have:

$$\begin{aligned}
ABC(G) &= ABC(G') + \sum_{i=1}^{k} f(1,d) + \sum_{i=k}^{d-1} [f(d, d(y_i)) - f(d-k, d(y_i))] \\
&\le ABC(G') + k\sqrt{\frac{d-1}{d}} \\
&< \frac{3\sqrt{2}}{2} r + (n-k-2r-1)\sqrt{\frac{n-k-2}{n-k-1}} + k\sqrt{\frac{d-1}{d}} \\
&< h(n, \lfloor \frac{n-1}{2} \rfloor),
\end{aligned}$$

as desired.

Case 2: $\delta(G) \ge 2$. By definition of cactus graph, there exists an edge $u_0u_1 \in E(G)$ such that $d(u_0) = d(u_1) = 2$, $N_G(u_0) = \{u_1, u_2\}$ and $d(u_2) \ge 3$. Since $n \ge 6$ and $r \ge 2$, it is enough to investigate the following two subcases.

Subcase 2.1: $u_1u_2 \notin E(G)$. Let $G' = G - u_0 + u_1u_2$. So, $G' \in G(n-1, r)$, $r = \lfloor \frac{n-1}{2} \rfloor$ and by induction hypothesis $ABC(G') < h(n-1, \lfloor \frac{n-1}{2} \rfloor - 1)$. So, by Lemma 1.1 we have:

$$\begin{aligned}
ABC(G) &= ABC(G') + \sqrt{\frac{d}{2d}} + \frac{\sqrt{2}}{2} - \sqrt{\frac{d}{2d}} \\
&< \frac{3r\sqrt{2}}{2} + (n-2r-2)\sqrt{\frac{n-3}{n-2}} + \frac{1}{\sqrt{2}} \\
&< h(n, \lfloor \frac{n-1}{2} \rfloor).
\end{aligned}$$

Subcase 2.2: $u_1u_2 \in E(G)$. Suppose $G' = G - u_0 - u_1$. Then $G' \in G(n-2, r-1)$, $r = \lfloor \frac{n-1}{2} \rfloor$ and by induction hypothesis, $ABC(G') < h(n-2, \lfloor \frac{n-1}{2} \rfloor - 1)$. If $N_G(u_2) \setminus \{u_0, u_1\} = \{y_1, \ldots, y_{d-2}\}$, then by Lemma 1.1,

$$\begin{aligned}
ABC(G) &= ABC(G') + 2f(2,d) + f(2,2) + \sum_{i=1}^{d-2} [f(d, d(y_i)) - f(d-2, d(y_i))] \\
&\le ABC(G') + 3f(2,2) \\
&< \frac{3\sqrt{2}}{2}(r-1) + (n-2r-1)\sqrt{\frac{n-4}{n-3}} + 3\sqrt{\frac{2}{4}}
\end{aligned}$$

$$< h(n, \lfloor \frac{n-1}{2} \rfloor).$$

Hence the proof is completed. □

Theorem 2.2. *Among all graphs in $G(n, r)$, $0 \leq r < \lfloor \frac{n-1}{2} \rfloor$, the graph $G^0(n, \lfloor \frac{n-1}{2} \rfloor - 1)$ has the maximum ABC index, and,*

$$ABC\Big(G^0(n, \lfloor \frac{n-1}{2} \rfloor - 1)\Big) = 3(\lfloor \frac{n-1}{2} \rfloor - 1)\frac{\sqrt{2}}{2} + (n - 2\lfloor \frac{n-1}{2} \rfloor + 1)\sqrt{\frac{n-2}{n-1}}$$
$$= h(n, \lfloor \frac{n-1}{2} \rfloor - 1).$$

Proof. Suppose $G \in G(n, r)$. It is enough to prove that $ABC(G) < h(n, \lfloor \frac{n-1}{2} \rfloor - 1)$. We proceed by induction on r and n. If $r = 0, 1, 2$, then by Lemmas 1.3, 1.4 and 1.5 the result holds. It can be assumed that $r \geq 3$ and so $n \geq 9$. If $n = 9$, then $r = 3$ and the only graph with this condition is $G^0(9, 3)$. Assume that $G \in G(n, r)$, where $n \geq 10$ and $r \geq 3$. The following two cases are occurred:

Case 1: $\delta(G) = 1$. Consider a vertex u adjacent to the vertex v of degree d, and assume that $N_G(v) \setminus \{u\} = \{y_1, \ldots, y_{d-1}\}$, $2 \leq d \leq n - 1$. If $G' = G - u$, then $G' \in G(n - 1, r)$. So according to induction hypothesis

$$ABC(G') < h(n - 1, \lfloor \frac{n-1}{2} \rfloor - 1)\,.$$

Therefore, by Lemma 1.1 we have:

$$\begin{aligned} ABC(G) &= ABC(G') + f(1, d) + \sum_{i=1}^{d-1}[f(d, d(y_i)) - f(d - 1, d(y_i))] \\ &\leq ABC(G') + \sqrt{\frac{d-1}{d}} \\ &< \frac{3\sqrt{2}}{2}(r - 1) + (n - 2r)\sqrt{\frac{n-3}{n-2}} + \sqrt{\frac{d-1}{d}} \\ &< h(n, \lfloor \frac{n-1}{2} \rfloor - 1). \end{aligned}$$

Case 2: $\delta(G) \geq 2$. By definition of cactus graph and our assumption, there is an edge $u_0u_1 \in E(G)$ such that $d(u_0) = d(u_1) = 2$, $N_G(u_0) = \{u_1, u_2\}$ and $d(u_2) \geq 3$. Since $n \geq 10$ and $r \geq 3$, we have again two different subcases as follows:

Subcase 2.1: $u_1u_2 \notin E(G)$. Suppose $G' = G - u_0 + u_1u_2$. So, $G' \in G(n-1, r)$ and by induction $ABC(G') < h(n-1, \lfloor \frac{n-1}{2} \rfloor - 1)$. On the other hand, by Lemma 1.1 we have:

$$ABC(G) = ABC(G') + \sqrt{\frac{d}{2d}} + \frac{\sqrt{2}}{2} - \sqrt{\frac{d}{2d}}$$

$$< \frac{3(r-1)\sqrt{2}}{2} + (n-2r)\sqrt{\frac{n-3}{n-2}} + \frac{1}{\sqrt{2}}$$
$$< h(n, \lfloor \frac{n-1}{2} \rfloor - 1).$$

Subcase 2: $u_1u_2 \in E(G)$. Suppose $G' = G - u_0 - u_1$. Then $G' \in G(n-2, r-1)$ and by induction, $ABC(G') < h(n-2, \lfloor \frac{n-1}{2} \rfloor - 2)$. If $N_G(u_2) \setminus \{u_0, u_1\} = \{y_1, \ldots, y_{d-2}\}$, then by Lemma 1.1, we get,

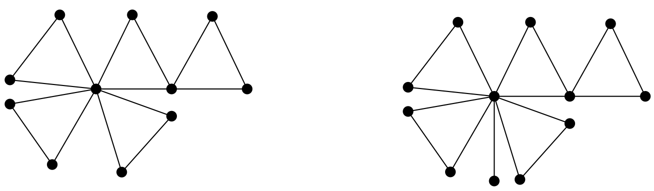
$$\begin{aligned} ABC(G) &= ABC(G') + 2f(2,d) + f(2,2) + \sum_{i=1}^{d-2}[f(d, d(y_i)) - f(d-2, d(y_i))] \\ &\leq ABC(G') + 3f(2,2) \\ &< \frac{3\sqrt{2}}{2}(r-2) + (n-2r+1)\sqrt{\frac{n-4}{n-3}} + 3\sqrt{\frac{2}{4}} \\ &< h(n, \lfloor \frac{n-1}{2} \rfloor - 1). \end{aligned}$$

This completes the proof. □

Suppose $G^1(n,r)$, $n \geq 7$, denotes the set of all cactus graphs obtained from r cycles of length 3 and $n-2r-1$ pendant edges having a common vertex with $r-1$ cycles, where $2 \leq r \leq \lfloor \frac{n-1}{2} \rfloor$, see Figure 2. So,

$$ABC(G^1(n,r)) = (3r-1)\frac{\sqrt{2}}{2} + (n-2r-1)\sqrt{\frac{n-4}{n-3}} + \sqrt{\frac{n-1}{4(n-3)}}.$$

The last expression is denoted by $p(n,r)$.



(a) $G^1(11,5)$ (b) $G^1(12,5)$

FIGURE 2. Some cactus graphs of type $G^1(n,r)$.

Theorem 2.3. *Among all n vertex cactus graphs, $n \geq 7$, the graph $G^1(n, \lfloor \frac{n-1}{2} \rfloor)$ has the second maximum of ABC index.*

Proof. By Theorem 2.1, the graph $G^0(n, \lfloor \frac{n-1}{2} \rfloor)$ has the maximum ABC index. Let A be the set of all cactus graphs with $r = \lfloor \frac{n-1}{2} \rfloor$ cycles except from

$G^0(n, \lfloor \frac{n-1}{2} \rfloor)$. By definition of cactus graphs, members of A has one of the following forms:

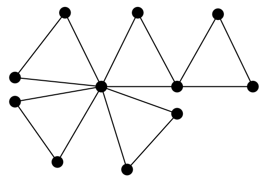
1) The members of A have odd order and their blocks have length three.
2) The members of A have even order and one of the following are satisfied:
   i) All except one block are cycles of length three and the remaining block is a pendant edge,
   ii) All except one block are cycles of length three and the remaining block is a cycle of length four,
   iii) All except one block are cycles of length three and the remaining block is an edge connecting two other blocks.

Note that if the order of an element X of A is odd, then $|E(X)| = 3r$. If its order is even, then $|E(X)| = 3r + 1$. Let B be the set of all Y, $Y \in A$, such that Y has the maximum number of edges with an end vertex of degree two. Then,

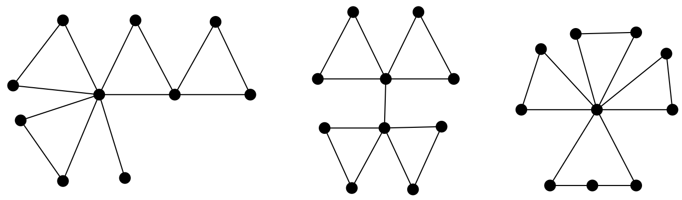
1. If $|Y|$ is odd, then the maximum number of edges that each of them has an end vertex of degree two is $3r - 1$. This happens if the graph Y has $r - 1$ cycles with a common vertex a and another cycle which has a common vertex with one of these $r - 1$ cycles in a vertex b different from a, i.e., $G^1(n, \lfloor \frac{n-1}{2} \rfloor)$, Figure 3(a).
2. The order of Y is even and one of the following are happened:
   (a) Y has an pendant and all other blocks are having length three. In this case, Y has at most $3r - 1$ edges with this property that one of its vertices has degree two, Figure 3(b).
   (b) Y has a unique block of order two that connects other blocks which are triangles. In this case, Y has at most $3r$ edges with this property that one of its vertices has degree two, Figure 3(c).
   (c) All blocks of Y are cycles of lengths three or four. There is one block of order four and so Y has at most $3r + 1$ edges with this property that one of its vertices has degree two, Figure 3(d).

Put $C = A - B$. Clearly, all element of C has $k(\geq 2)$ non-pendant edges such that their endpoints have degree ≥ 3. So, $m - k$ edges are having at least one end vertex of degree two. Obviously $m - k < 3r - 1$. We shall show that ABC index of $G^1(n, \lfloor \frac{n-1}{2} \rfloor)$ is an upper bound for both sets B and C. Since $G^1(n, \lfloor \frac{n-1}{2} \rfloor) \in B$, $B \neq \emptyset$. Suppose $G \in B$. If $G = G^1(n, \lfloor \frac{n-1}{2} \rfloor)$, then the statement holds. Assume that $G \in B$, $G \neq G^1(n, r)$ and its order is odd. Then, G has $3r - 1$ edges in which at least one of end vertices has degree two and only one edge of degree $(n - u, u + 1)$, where $u > 6$ and even. Therefore,

$$
\begin{aligned}
ABC(G) &= (3r-1)\frac{\sqrt{2}}{2} + \sqrt{\frac{n-1}{(n-u+1)(u)}} \\
&\leq (3r-1)\frac{\sqrt{2}}{2} + \sqrt{\frac{n-1}{6(n-5)}}
\end{aligned}
$$



(a) The order of cactus is odd. It has $3r-1$ edges with at least one end vertex of degree 2.



(b) $3r-1$ (c) $3r$ (d) $3r+1$

FIGURE 3. Some elements in B. Graphs with $3r-1$ (left), $3r$ (middle) and $3r+1$ (right) edges such that at least one end vertex has degree 2. The ABC index of all edges are $\frac{\sqrt{2}}{2}$.

$$< (3r-1)\frac{\sqrt{2}}{2} + \sqrt{\frac{n-1}{4(n-3)}} = ABC(G^1(n, \lfloor \frac{n-1}{2} \rfloor))\,.$$

Since $u > 6$ and $n-5 > n-u+1$, $4(n-3) < 6(n-5) \leq (n-u+1)u$. Thus,

$$\sqrt{\frac{n-1}{4(n-3)}} - \sqrt{\frac{n-1}{(n-u+)u)}} > 0\,.$$

Let $G \in B$ has even order and there are $3r-1$ edges that at least one of their end vertices have degree two. Then there exists only one edge of degree $(u, n-u+1)$, $u \geq 6$ and $n \geq 12$, and one pendant edge. Without loss of generality, we assume that the pendant edge is linked to the vertex of maximum degree ($u \geq n-u+1$). Therefore,

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

$$\leq (3r-1)\frac{\sqrt{2}}{2} + \sqrt{\frac{n-1}{6(n-5)}} + \sqrt{\frac{n-4}{n-3}}$$
$$< (3r-1)\frac{\sqrt{2}}{2} + \sqrt{\frac{n-1}{4(n-3)}} + \sqrt{\frac{n-4}{n-3}}$$
$$= ABC(G^1(n, \lfloor\frac{n-1}{2}\rfloor)).$$

Again since $u \geq 6$ and $n-3 > n-5 \geq n-u+1$, $4(n-3) < 6(n-5) \leq u(n-u+1)$. So,

$$\sqrt{\frac{n-1}{4(n-3)}} - \sqrt{\frac{n-1}{u(n-u+1)}} > 0.$$

If the graph G has exactly $3r+1$ edges in which at least one of its end vertices has degree two, then

$$ABC(G) = (3r+1)\frac{\sqrt{2}}{2} < (3r-1)\frac{\sqrt{2}}{2} + \sqrt{\frac{n-1}{4(n-3)}} + \sqrt{\frac{n-4}{n-3}}$$
$$= ABC(G^1(n, \lfloor\frac{n-1}{2}\rfloor)).$$

Define $g(n) = \sqrt{\frac{n-1}{4(n-3}} + \sqrt{\frac{n-4}{n-3}} - \sqrt{2}$. Then for $n > 7$,

$$g'(n) = \frac{\sqrt{n-3}}{2(n-3)^2}\left(\frac{-1}{\sqrt{n-1}} + \frac{1}{\sqrt{n-4}}\right) > 0.$$

Hence, $g(10) > g(8) > 0$.

If the graph G has exactly $3r$ edges in which at least one of its end vertices has degree two and an edge of degree $(n-v, v)$, where $v \geq 3$ is odd then we have:

$$ABC(G) = (3r)\frac{\sqrt{2}}{2} + \sqrt{\frac{n-2}{v(n-v)}} \leq (3r)\frac{\sqrt{2}}{2} + \sqrt{\frac{n-2}{3(n-3)}}$$
$$< (3r-1)\frac{\sqrt{2}}{2} + \sqrt{\frac{n-1}{4(n-3)}} + \sqrt{\frac{n-4}{n-3}}$$
$$= ABC(G^1(n, \lfloor\frac{n-1}{2}\rfloor)).$$

Define $f(n) = \sqrt{\frac{n-1}{4(n-3)}} + \sqrt{\frac{n-4}{n-3}} - \sqrt{\frac{n-2}{3(n-3)}} - \frac{\sqrt{2}}{2}$. Then for each even n, $n > 7$,

$$f'(n) = \frac{\sqrt{n-3}}{2(n-3)^2}\left((\frac{-1}{\sqrt{n-1}} + \frac{1}{\sqrt{n-4}}) + \frac{1}{\sqrt{3(n-2)}}\right) > 0.$$

So, $f(10) > f(8) > 0$ and the statement holds.

Suppose that $G \in C$ has odd order $n, n \geq 8$, degree of one of its k non-pendant edges is greater than three, say $d(x) > 3$, and $\Delta \geq 4$. Notice that there is no graph in C with order seven. Then,

$$\begin{aligned}
ABC(G) &\leq (3r-k)\frac{\sqrt{2}}{2} + (n-2r-1)\sqrt{\frac{\Delta-1}{\Delta}} \\
&+ (k-1)\sqrt{\frac{6}{16}} + \sqrt{\frac{\Delta+2}{4\Delta}} \\
&\leq (3r-k)\frac{\sqrt{2}}{2} + (n-2r-1)\sqrt{\frac{n-4}{n-3}} \\
&+ (k-1)\sqrt{\frac{2}{4}} + \sqrt{\frac{n-1}{4(n-3)}} \\
&= p(n,r).
\end{aligned}$$

Define $J(n) = \sqrt{\frac{n-1}{4(n-3)}} + (k-1)\sqrt{\frac{2}{4}} - k\frac{\sqrt{6}}{4}$. Then $J(n)$ is increasing, when $n \geq 8$. Therefore, for a fixed k, $J(8) > 0$. Thus, for $k \geq 2$, we have:

$$(k-1)\sqrt{\frac{2}{4}} + \sqrt{\frac{n-1}{4(n-3)}} > k\sqrt{\frac{6}{16}} \geq (k-1)\sqrt{\frac{6}{16}} + \sqrt{\frac{\Delta+2}{4\Delta}}.$$

If $G \in C$ has even order and one of the end vertices of at least one non-pendant edge has degree three (such an edge is a block), then we can see that $n = |G| \geq 8$. This implies that

$$\begin{aligned}
ABC(G) &\leq (3r-k)\frac{\sqrt{2}}{2} + \frac{2}{3} + k\frac{\sqrt{6}}{4} \\
&\leq (3r-1)\frac{\sqrt{2}}{2} + \sqrt{\frac{n-1}{4(n-3)}} + \sqrt{\frac{n-4}{n-3}} \\
&= p(n,r).
\end{aligned}$$

To do this, we define:

$$L(n) = \sqrt{\frac{n-1}{4(n-3)}} + \sqrt{\frac{n-4}{n-3}} + (k-1)\frac{\sqrt{2}}{2} - \frac{2}{3} - k\frac{\sqrt{6}}{4}.$$

Then it is clear that $L'(n) > 0$, $n \geq 8$. So, for a fixed k, $L(8) > 0$ which completes the proof. □

Theorem 2.4. *Among all graphs in $G(n,r)$, the cactus graph $G^0(n, \lfloor\frac{n-1}{2}\rfloor - 1)$ has second maximum ABC index, $n \geq 20$. If $7 \leq n \leq 19$, then the cactus graph $G^1(n, \lfloor\frac{n-1}{2}\rfloor)$ has second maximum ABC index. Moreover, the ABC values are as follows*:

$$ABC\Big(G^1(n, \lfloor\frac{n-1}{2}\rfloor)\Big) = p(n, \lfloor\frac{n-1}{2}\rfloor),$$

$$ABC\Big(G^0(n,\lfloor\frac{n-1}{2}\rfloor-1)\Big)=h(n,\lfloor\frac{n-1}{2}\rfloor-1).$$

Proof. By definition,

$$p(n,r)=\begin{cases}\frac{(3n-8)\sqrt{2}}{4}+\sqrt{\frac{n-4}{n-3}}+\sqrt{\frac{n-1}{4(n-3)}}, & n=2i\\ \\ \frac{(3n-5)\sqrt{2}}{4}+\sqrt{\frac{n-1}{4(n-3)}}, & n=2i-1,\ i=4,5,\dots,\end{cases}$$

$$h(n,r-1)=\begin{cases}\frac{(3n-12)\sqrt{2}}{4}+3\sqrt{\frac{n-2}{n-1}}, & n=2i\\ \\ \frac{(3n-9)\sqrt{2}}{4}+2\sqrt{\frac{n-2}{n-1}}, & n=2i-1,\ \ i=4,5,\dots,\end{cases}$$

where $r=\lfloor\frac{n-1}{2}\rfloor$. Define $H(n)=p(n,r)-h(n,r-1)$ then

$$H(n)=\begin{cases}\sqrt{2}+\sqrt{\frac{n-4}{n-3}}+\sqrt{\frac{n-1}{4(n-3)}}-3\sqrt{\frac{n-2}{n-1}}, & n=2i\\ \\ \sqrt{2}+\sqrt{\frac{n-1}{4(n-3)}}-2\sqrt{\frac{n-2}{n-1}}, & n=2i-1.\end{cases}$$

Obviously, we can see that $H'(n)<0$, $n\geq 7$. On the other hand, for $7\leq n\leq 19$, $H(n)>0$ and for $n\geq 20$, $H(n)<0$. This completes the proof. □

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References

[1] B. Ben-Moshe, B. Bhattacharya, and Q. Shi, *Efficient algorithms for the weighted 2-center problem in a cactus graph*, Algorithms and Computation, 16th Int. Symp., ISAAC 2005, Lecture Notes in Computer Science 3827, pp. 693-03, Springer-Verlag, 2005.

[2] J. Chen and X. Guo, *Extreme atom-bond connectivity index of graphs*, MATCH Commun. Math. Comput. Chem. **65** (2011), no. 3, 713–722.

[3] K. C. Das, *Atom-bond connectivity index of graphs*, Discrete Appl. Math. **158** (2010), no. 11, 1181–1188.

[4] K. C. Das, I. Gutman, and B. Furtula, *On atom-bond connectivity index*, Chem. Phys. Lett. **511** (2011), 452–454.

[5] T. Dehghan-Zadeh, A. R. Ashrafi, and N. Habibi, *Maximum values of atom-bond connectivity index in the class of tetra-cyclic graphs*, submitted.

[6] E. El-Mallah and C. Colbourn, *The complexity of some edge deletion problems*, IEEE Trans. Circuits and Systems **35** (1988), no. 3, 354–362.

[7] E. Estrada, *Atom-bond connectivity and the energetic of branched alkanes*, Chem. Phys. Lett. **463** (2008), 422–425.

[8] E. Estrada, L. Torres, L. Rodriguez, and I. Gutman, *An atom-bond connectivity index: modeling the enthalpy of formation of alkanes*, Indian J. Chem. **37A** (1998), 849–855.

[9] G. H. Fath-Tabar, B. Vaez-Zadeh, A. R. Ashrafi, and A. Graovac, *Some inequalities for the atom-bond connectivity index of graph operations*, Discrete Appl. Math. **159** (2011), no. 13, 1323–1330.

[10] B. Furtula, A. Graovac, and D. Vukičević, *Atom-bond connectivity index of trees*, Discrete Appl. Math. **157** (2009), no. 13, 2828–2835.

[11] L. Gan, H. Hou, and B. Liu, *Some results on atom-bond connectivity index of graphs*, MATCH Commun. Math. Comput. Chem. **66** (2011), no. 2, 669–680.

[12] L. Gan, B. Liu, and Z. You, *The ABC index of trees of given degree sequence*, MATCH Commun. Math. Comput. Chem. **68** (2012), no. 1, 137–145.

[13] I. Gutman and B. Furtula, *Trees with smallest atom-bond connectivity index*, MATCH Commun. Math. Comput. Chem. **68** (2012), no. 1, 131–136.

[14] I. Gutman, B. Furtula, and M. Ivanović, *Notes on trees with minimal atom-bond connectivity index*, MATCH Commun. Math. Comput. Chem. **67** (2012), no. 2, 467–482.

[15] N. M. Korneyenko, *Combinatorial algorithms on a class of graphs*, Discrete Appl. Math. **54** (1994), no. 2-3, 215–217.

[16] M. Lu, L. Zhang, and F. Tian, *On the Randić index of cacti*, MATCH Commun. Math. Comput. Chem. **56** (2006), no. 3, 551–556.

[17] B. Paten, M. Diekhans, D. Earl, J. St. John, J. Ma, B. Suh, and D. Haussler, *Cactus graphs for genome comparisons*, J. Comput. Biol. **18** (2011), no. 3, 469–481.

[18] D. B. West, *Introduction to Graph Theory*, Prentice Hall, Upper Saddle River, 2001.

[19] R. Xing, B. Zhou, and F. Dong, *On atom-bond connectivity index of connected graphs*, Discrete Appl. Math. **159** (2011), no. 15, 1617–1630.

[20] R. Xing, B. Zhou, and Z. Du, *Further results on atom-bond connectivity index of trees*, Discrete Appl. Math. **158** (2010), no. 14, 1536–1545.

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