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# The Extremal General Atom–Bond Connectivity Indices of Unicyclic and Bicyclic Graphs*

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**Abstract**

The general atom–bond connectivity index ($ABC_\alpha$) of a graph $G = (V, E)$ is defined as $ABC_\alpha(G) = \sum_{uv \in E(G)} \left(\frac{d_u + d_v - 2}{d_u d_v}\right)^\alpha$, where $uv$ is an edge of $G$, $d_u$ is the degree of the vertex $u$, $\alpha$ is an arbitrary nonzero real number, and $G$ has no isolated $K_2$ if $\alpha < 0$. In this paper, we determine the $n$-vertex ($n \geq 4$) unicyclic graphs with maximal and second-maximal (resp. minimal and second-minimal) $ABC_\alpha$ indices for $\alpha > 0$ (resp. $-3 \leq \alpha < 0$). And the $n$-vertex ($n \geq 4$) bicyclic graphs in which the $ABC_\alpha$ index attains maximal (resp. minimal) value for $\alpha > 0$ (resp. $-1 \leq \alpha < 0$) are also obtained.

## 1 Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V$ and edge set $E$, many topological indices defined in terms of the vertex degrees have been considered in the

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literature [9, 13, 16, 22, 23]. The general form of vertex-degree-based topological indices is $TI(G) = \sum_{uv \in E} \Psi(d_u, d_v)$, where $\Psi$ is a non-negative and real two-variables function, $d_v$ denotes the degree of the vertex $v$. Molecular descriptors are playing a significant role in mathematical chemistry, pharmacology, etc. Among all molecular structure descriptors, topological indices have important applications. One of the most crucial topological indices is the Randić index [16], which is defined by $\Psi(d_u, d_v) = \frac{1}{\sqrt{d_u d_v}}$. The Randić index is aimed at the modelling of the branching of the carbon-atom skeleton of alkanes [16]. Bollobás and Erdös [13] generalized the Randić index by replacing $-\frac{1}{2}$ with arbitrary nonzero real number $\alpha$, called the general Randić index, defined as $\Psi(d_u, d_v) = (d_u d_v)^\alpha$.

In 1998, Estrada, Torres, Rodríguez and Gutman [6] proposed the atom–bond connectivity ($ABC$) index, defined as $\Psi(d_u, d_v) = \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$. They showed that the $ABC$ index correlates well with the heats of formation of alkanes and can therefore serve the purpose of predicting their thermodynamic properties. Its mathematical properties were also extensively investigated, see the recent literature [1–5, 10–12, 14, 15, 17–19] and the references cited therein. Furtula et al. [9] made a generalization of $ABC$ index, defined as $\Psi(d_u, d_v) = \left(\frac{d_u + d_v - 2}{d_u d_v}\right)^\alpha$, where $\alpha > 0$ is a real number. They also defined the augmented Zagreb index ($AZI$) by $\Psi(d_u, d_v) = \left(\frac{d_u + d_v - 2}{d_u d_v}\right)^{-3}$. More generally, Xing and Zhou [20] generalized the $ABC$ index for arbitrary nonzero real number $\alpha$, called the general atom–bond index and denoted by $ABC_\alpha$ index:

$$ABC_\alpha(G) = \sum_{uv \in E} \left(\frac{d_u + d_v - 2}{d_u d_v}\right)^\alpha,$$

where $G$ has no isolated $K_2$ (the complete graph with two vertices) if $\alpha < 0$.

Furtula et al [9] also showed that the $AZI$ index has a better prediction power than the $ABC$ index when studying the heat of formation of octanes and heptanes. Estrada [7, 8] provided a quantum-chemical explanation of the capacity of $ABC$-like indices and a probabilistic interpretation that fits very well with the chemical intuition for understanding the capacity of $ABC$-like indices to describe the energetics of alkanes.

Recall that Zhou et al. [21] determined the $n$-vertex unicyclic and bicyclic graphs with the maximal and second-maximal $ABC$ indices. Zhan et al. [24] considered the $n$-vertex unicyclic graphs with the minimal and second-minimal $AZI$ indices and the $n$-vertex bicyclic graphs with the minimal $AZI$ indices. In this paper, we will determine the $n$-vertex unicyclic graphs with the maximal and second-maximal (resp. minimal and second-minimal) $ABC_\alpha$ indices for $\alpha > 0$ (resp. $-3 \le \alpha < 0$), and characterize corresponding graphs. Also, the $n$-vertex bicyclic graphs in which the $ABC_\alpha$ index attains its maximal (resp. minimal) value for $\alpha > 0$ (resp. $-1 \le \alpha < 0$) are obtained.

## 2 On the extremal $ABC_\alpha$ indices of unicyclic graphs

In this section, we consider the $n$-vertex unicyclic graphs with the maximal and second-maximal (resp. minimal and second-minimal) $ABC_\alpha$ index for $\alpha > 0$ (resp. $-3 \le \alpha < 0$).

For any nonzero real number $\alpha$ and $x, y \ge 1$, let $f(x,y,\alpha) = \left(\frac{x+y-2}{xy}\right)^\alpha$. Note that $f(1,1,\alpha) = 0$, and for $x \ge 1$, $f(x,2,\alpha) = \left(\frac{1}{2}\right)^\alpha$.

**Lemma 2.1** Let $f(x,1,\alpha) = \left(\frac{x-1}{x}\right)^\alpha$.

(i) Given $\alpha > 0$, if $x > 1$ then $f(x,1,\alpha)$ is strictly increasing in $x$; if $y > 2$ and $x \ge 1$, then $f(x,y,\alpha)$ is strictly decreasing in $x$.

(ii) Given $-3 \le \alpha < 0$, if $x > 1$ then $f(x,1,\alpha)$ is strictly decreasing in $x$; if $y > 2$ and $x \ge 1$, then $f(x,y,\alpha)$ is strictly increasing in $x$.

**Proof.** (i) Note that for $\alpha > 0$, $x > 1$, $f_x(x,1,\alpha) = \frac{\alpha(x-1)^{\alpha-1}}{x^{\alpha+1}} > 0$. Hence, $f(x,1,\alpha) = \left(\frac{x-1}{x}\right)^\alpha$ is strictly increasing in $x$.

Given $y > 2$, if $x \ge 1$ then $f_x(x,y,\alpha) = \frac{\alpha(2-y)(x+y-2)^{\alpha-1}}{x^{\alpha+1}y^\alpha} < 0$, implying that $f(x,y,\alpha)$ is strictly decreasing in $x$.

(ii) If $-3 \le \alpha < 0$, in a similar manner as in the proof of $\alpha > 0$, we can show that (ii) holds.

The proof is now complete. ■

Let $\mathcal{U}_n$ be the set of $n$-vertex unicyclic graphs, $U_{n,p}$ be the set of unicyclic graphs with $n$ vertices and $p$ pendent vertices, and $S_{n,p}$ be the unicyclic graph formed by attaching $p$ pendent vertices to a vertex of the cycle $C_{n-p}$, where $0 \le p \le n-3$.

For any vertex $v \in V(C_{n-p})$, $d_v \ge 2$, by Lemma 2.1, we get the graph $S_{n,p}$ has the maximal (resp. minimal) $ABC_\alpha$ index in $U_{n,p}$ for $\alpha > 0$ (resp. $-3 \le \alpha < 0$). So we have the following Lemma 2.2.

**Lemma 2.2** Let $G \in U_{n,p}$, $0 \le p \le n-3$.

(i) If $\alpha > 0$, then $ABC_\alpha(G) \le ABC_\alpha(S_{n,p})$.

(ii) If $-3 \le \alpha < 0$, then $ABC_\alpha(G) \ge ABC_\alpha(S_{n,p})$, where $ABC_\alpha(S_{n,p}) = p\left(\frac{p+1}{p+2}\right)^\alpha + (n-p)\left(\frac{1}{2}\right)^\alpha$.

**Theorem 2.1** Among all graphs in $\mathcal{U}_n$ with $n \ge 3$,

(i) if $\alpha > 0$, then $S_{n,n-3}$ is the unique graph with the maximal $ABC_\alpha$ index;

(ii) if $-3 \le \alpha < 0$, then $S_{n,n-3}$ is the unique graph with the minimal $ABC_\alpha$ index.

**Proof.** Let

$$l(n,p) = p\Big(\frac{p+1}{p+2}\Big)^\alpha + (n-p)\Big(\frac{1}{2}\Big)^\alpha,$$

we obtain

$$l_p(n,p) = \Big(\frac{p+1}{p+2}\Big)^\alpha + p\alpha\Big(\frac{p+1}{p+2}\Big)^{\alpha-1}\frac{1}{(p+2)^2} - \Big(\frac{1}{2}\Big)^\alpha > 0 \text{ , for } \alpha > 0.$$

Then $ABC_\alpha(S_{n,p})$ is strictly increasing in $p$, by Lemma 2.2 (i), Theorem 2.1 (i) holds. Similarly, we have $l_p(n,p) < 0$ for $-3 \le \alpha < 0$.

So Theorem 2.1 holds. ■

**Lemma 2.3** Let $d(x,\alpha) = xf(x+2,1,\alpha) - (x-1)f(x+1,1,\alpha)$, then

(i) given $\alpha > 0$, if $x \ge 1$ then $d(x,\alpha)$ is strictly increasing in $x$;

(ii) given $-3 \le \alpha < 0$, if $x \ge 1$ then $d(x,\alpha)$ is strictly decreasing in $x$.

**Proof.** Let $t(x,\alpha) = xf(x+2,1,\alpha) = x\Big(\frac{x+1}{x+2}\Big)^\alpha$, then $d(x,\alpha) = t(x,\alpha) - t(x-1,\alpha)$. By direct calculation, we have

$$t_x(x,\alpha) = \Big(\frac{x+1}{x+2}\Big)^\alpha + x\alpha\Big(\frac{x+1}{x+2}\Big)^{\alpha-1}\frac{1}{(x+2)^2} = \Big(\frac{x+1}{x+2}\Big)^\alpha\Big[1 + \frac{x\alpha}{(x+1)(x+2)}\Big],$$

and

$$\begin{aligned} t_{xx}(x,\alpha) &= \alpha\Big(\frac{x+1}{x+2}\Big)^{\alpha-1}\frac{1}{(x+2)^2}\Big[1+\frac{x\alpha}{(x+1)(x+2)}\Big] \\ &\quad + \Big(\frac{x+1}{x+2}\Big)^\alpha \frac{\alpha(x+1)(x+2) - \alpha x(2x+3)}{(x+1)^2(x+2)^2} \\ &= \alpha\Big(\frac{x+1}{x+2}\Big)^{\alpha-1}\frac{1}{(x+1)(x+2)^3}[(3+\alpha)x+4]. \end{aligned}$$

Then, (i) for $\alpha > 0$ and $x \ge 1$, $t_{xx}(x,\alpha) > 0$. It follows that $d_x(x,\alpha) = t_x(x,\alpha) - t_x(x-1,\alpha) > 0$. Thus $d(x,\alpha)$ is strictly increasing in $x$.

(ii) If $-3 \le \alpha < 0$ and $x \ge 1$ then $t_{xx}(x,\alpha) < 0$. Hence $d(x,\alpha)$ is strictly decreasing in $x$. ■

**Lemma 2.4** Let $x \ge 1$ and $h(x,y,\alpha) = f(x+1,y,\alpha) - f(x,y,\alpha)$.

(i) If $\alpha > 0$ and $y > 2$ then $h(x,y,\alpha)$ is strictly increasing in $x$.

(ii) If $-1 \le \alpha < 0$ and $y > 2$ or if $-3 \le \alpha < -1$ and $2 < y < x+2$, then $h(x,y,\alpha)$ is strictly decreasing in $x$.

**Proof.** By direct calculation, we have

$$f_x(x,y,\alpha) = \alpha\Big(\frac{x+y-2}{xy}\Big)^{\alpha-1}\frac{xy - y(x+y-2)}{(xy)^2} = \alpha\Big(\frac{x+y-2}{xy}\Big)^{\alpha-1}\frac{2-y}{x^2y},$$

and

$$\begin{aligned} f_{xx}(x,y,\alpha) &= \alpha(\alpha-1)\Big(\frac{x+y-2}{xy}\Big)^{\alpha-2}\Big(\frac{2-y}{x^2y}\Big)^2 + \alpha\Big(\frac{x+y-2}{xy}\Big)^{\alpha-1}\frac{(-2)(2-y)}{x^3y} \\ &= \alpha\Big(\frac{x+y-2}{xy}\Big)^{\alpha-2}\frac{y-2}{x^4y^2}\Big[(\alpha-1)(y-2) + 2(x+y-2)\Big]. \end{aligned}$$

Then, (i) for $\alpha > 0$, $f_{xx}(x,y,\alpha) > \alpha\Big(\dfrac{x+y-2}{xy}\Big)^{\alpha-2}\dfrac{y-2}{x^4y^2}\Big[-(y-2)+2(x+y-2)\Big] > 0$. We obtain

$h_x(x,y,\alpha) = f_x(x+1,y,\alpha) - f_x(x,y,\alpha) > 0$.

(ii) For $-1 \le \alpha < 0$, $(\alpha-1)(y-2)+2(x+y-2) \ge -2(y-2)+2(x+y-2) = 2x > 0$, then $f_{xx}(x,y,\alpha) < 0$. We get $h_x(x,y,\alpha) = f_x(x+1,y,\alpha) - f_x(x,y,\alpha) < 0$.

For $-3 \le \alpha < -1$, $(\alpha-1)(y-2)+2(x+y-2) \ge -4(y-2)+2(x+y-2) = 2x-2y+4$. Hence, if $2 < y < x+2$, then $f_{xx}(x,y,\alpha) < 0$. Thus $h_x(x,y,\alpha) = f_x(x+1,y,\alpha) - f_x(x,y,\alpha) < 0$.

So Lemma 2.4 holds. ■

Label by $v_1, v_2, ..., v_r$ the vertices of $C_r$ consecutively. Let $S_n(n_1, n_2, ..., n_r)$ be the unicyclic graph formed by attaching $n_i - 1$ pendent vertices to $v_i$, where $n_1 \ge n_2 \ge ... \ge n_r \ge 1$ and $\sum_{i=1}^{r} n_i = n$.

**Lemma 2.5** (i) If $\alpha > 0$, then $ABC_\alpha(S_n(n_1,n_2,n_3)) < ABC_\alpha(S_n(n_1+1,n_2-1,n_3))$;

(ii) If $-3 \le \alpha < 0$, then $ABC_\alpha(S_n(n_1,n_2,n_3)) > ABC_\alpha(S_n(n_1+1,n_2-1,n_3))$.

**Proof.** By elementary calculation,

$$\begin{aligned}
&ABC_\alpha(S_n(n_1,n_2,n_3)) - ABC_\alpha(S_n(n_1+1,n_2-1,n_3))\\
&= [(n_1-1)f(1,n_1+1,\alpha) - n_1 f(1,n_1+2,\alpha)] + [(n_2-1)f(1,n_2+1,\alpha) - (n_2-2)f(1,n_2,\alpha)]\\
&\quad + [f(n_1+1,n_3+1,\alpha) - f(n_1+2,n_3+1,\alpha)] + [f(n_2+1,n_3+1,\alpha) - f(n_2,n_3+1,\alpha)]\\
&\quad + [f(n_1+1,n_2+1,\alpha) - f(n_1+2,n_2,\alpha)]\\
&= -d(n_1,\alpha) + d(n_2-1,\alpha) - h(n_1+1,n_3+1,\alpha) + h(n_2,n_3+1,\alpha) + f(n_1+1,n_2+1,\alpha) -\\
&\quad f(n_1+2,n_2,\alpha).
\end{aligned}$$

If $n_3+1 = 2$, then $-h(n_1+1,n_3+1,\alpha) + h(n_2,n_3+1,\alpha) = 0$. Now, for (i), given $\alpha > 0$, note that $n_1 > n_2 - 1$ and $n_3+1 > 2$, by Lemmas 2.3 and 2.4, we have $-d(n_1,\alpha) + d(n_2-1,\alpha) < 0$ and $-h(n_1+1,n_3+1,\alpha) + h(n_2,n_3+1,\alpha) < 0$.

Since $n_2(n_1+2) < (n_1+1)(n_2+1)$

and $f(n_1+1,n_2+1,\alpha) - f(n_1+2,n_2,\alpha) = \Big[\dfrac{n_1+n_2}{(n_1+1)(n_2+1)}\Big]^\alpha - \Big[\dfrac{n_1+n_2}{n_2(n_1+2)}\Big]^\alpha$,

we have $f(n_1+1,n_2+1,\alpha) - f(n_1+2,n_2,\alpha) < 0$.

Thus $ABC_\alpha(S_n(n_1,n_2,n_3)) - ABC_\alpha(S_n(n_1+1,n_2-1,n_3)) < 0$.

(ii) When $-3 \le \alpha < 0$, the result can be obtained similarly as (i). ■

**Lemma 2.6** Given $\alpha > 1$, let $k(x,\alpha) = x^\alpha + (1-x)^\alpha$. If $0 < x < \frac{1}{2}$, then $k(x,\alpha)$ is decreasing in $x$. If $x > \frac{1}{2}$, then $k(x,\alpha)$ is increasing in $x$.

**Proof.** Note that $k_x(x,\alpha) = \alpha[x^{\alpha-1} - (1-x)^{\alpha-1}]$. For $\alpha > 1$, if $0 < x < \frac{1}{2}$, then

$k_x(x,\alpha) < 0$. If $x > \frac{1}{2}$, then $k_x(x,\alpha) > 0$.

The Lemma follows. ■

Now, we determine the graphs in $\mathcal{U}_n$ with the second-maximal $ABC_\alpha$ index for $n \geq 4$ and $\alpha > 0$. Clearly, $S_{4,0}$ is the unique graph with the second-maximal $ABC_\alpha$ index in $\mathcal{U}_4$ for $\alpha > 0$. For $n \geq 5$, we have the following theorem.

**Theorem 2.2** For graphs in $\mathcal{U}_n$ with $n \geq 5$, we have the following result.

(i) For $\alpha \geq 1$, $S_n(n-3,2,1)$ is the unique graph with the second-maximal $ABC_\alpha$ index.

(ii) For $\frac{1}{2} \leq \alpha < 1$, if $5 \leq n \leq 15$, then $S_n(n-3,2,1)$ is the unique graph with the second-maximal $ABC_\alpha$ index. While for $n \geq 16$, the graph with the second-maximal $ABC_\alpha$ index is either $S_n(n-3,2,1)$ or $S_{n,n-4}$.

(iii) For $0 < \alpha < \frac{1}{2}$, if $5 \leq n \leq 10$, then $S_n(n-3,2,1)$ is the unique graph with the second-maximal $ABC_\alpha$ index. If $n \geq 16$, then $S_{n,n-4}$ is the unique graph with the second-maximal $ABC_\alpha$ index. While for $11 \leq n \leq 15$, the graph with the second-maximal $ABC_\alpha$ index is either $S_n(n-3,2,1)$ or $S_{n,n-4}$.

**Proof.** For $\alpha > 0$ and $n \geq 5$, let $G_{sm}$ be the graph with the second-maximal $ABC_\alpha$ index in $\mathcal{U}_n$. By Theorem 2.1, $G_{sm}$ will be achieved in $\mathcal{U}_n \backslash \{S_{n,n-3}\}$. By the monotonicity of $ABC_\alpha(S_{n,p})$ with $0 \leq p \leq n-3$, we conclude that $G_{sm}$ is either $S_{n,n-4}$ or the graph with the maximal $ABC_\alpha$ index in $U_{n,n-3} \backslash \{S_{n,n-3}\}$.

Note that the unicyclic graphs in $U_{n,n-3}$ are of the form $S_n(n_1,n_2,n_3)$ with $n_1+n_2+n_3 = n$. By Lemma 2.5, $S_n(n-3,2,1)$ is the unique graph with the maximal $ABC_\alpha$ index among all graphs in $U_{n,n-3} \backslash \{S_{n,n-3}\}$. Let $Z(n,\alpha) = ABC_\alpha(S_{n,n-4}) - ABC_\alpha(S_n(n-3,2,1)) = 2\left(\frac{1}{2}\right)^\alpha - \left(\frac{2}{3}\right)^\alpha - \left[\frac{n-1}{3(n-2)}\right]^\alpha$.

For (i), if $\alpha = 1$, then $2\left(\frac{1}{2}\right) - \frac{2}{3} - \frac{n-1}{3(n-2)} < 1 - \frac{2}{3} - \frac{1}{3} = 0$. We have $Z(n,1) < 0$.

If $\alpha > 1$, then $Z(n,\alpha) < 2\left(\frac{1}{2}\right)^\alpha - \left(\frac{2}{3}\right)^\alpha - \left(\frac{1}{3}\right)^\alpha$. By Lemma 2.6, we have $2\left(\frac{1}{2}\right)^\alpha - \left(\frac{2}{3}\right)^\alpha - \left(\frac{1}{3}\right)^\alpha < 0$, which gives $Z(n,\alpha) < 0$.

For (ii), if $\frac{1}{2} \leq \alpha < 1$, then $Z(15,\alpha) < 0$ (shown in Fig.1). Notice that for any real number $\alpha > 0$, $Z(n,\alpha)$ is increasing in $n$. We have $Z(n,\alpha) < 0$, for $5 \leq n \leq 15$.

Now given $n = 16$, since $Z(16,\frac{1}{2}) = 2\sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} - \sqrt{\frac{5}{14}} \approx 1.03 \times 10^{-4} > 0$. We have $Z(n,\frac{1}{2}) > 0$ for any $n \geq 16$. But from (i), $Z(n,1) < 0$ for any $n \geq 16$. Clearly, $Z(n,\alpha)$ is continuous for any $\alpha$ and $n \geq 5$. Hence, for $\frac{1}{2} \leq \alpha < 1$ and $n \geq 16$, the relation between $ABC_\alpha(S_{n,n-4})$ and $ABC_\alpha(S_n(n-3,2,1))$ is left undecided.

For (iii), if $0 < \alpha < \frac{1}{2}$, then $Z(16,\alpha) > 0$ (shown in Fig.2). Similarly as above, we have $Z(n,\alpha) > 0$ for $n \geq 16$. From Figs.3-4, we get that $Z(n,\alpha) < 0$ with $5 \leq n \leq 10$. From Figs.5-6, we get that for $11 \leq n \leq 15$, $Z(n,\alpha) > 0$ or $Z(n,\alpha) < 0$ is decided by the value of $\alpha$ and $n$ .

This completes the proof of Theorem 2.2. ■

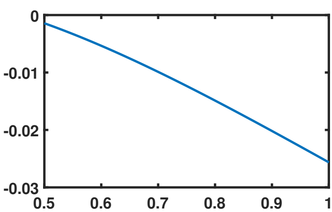


**Fig.1.** The value of Z(15,$\alpha$) for $\alpha \in [0.5, 1]$.

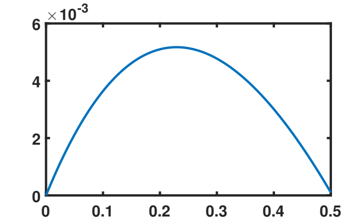


**Fig.2.** The value of Z(16,$\alpha$) for $\alpha \in [0, 0.5]$.

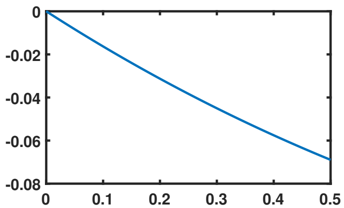


**Fig.3.** The value of Z(5,$\alpha$) for $\alpha \in [0, 0.5]$.

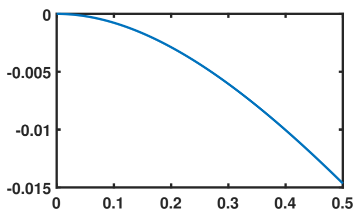


**Fig.4.** The value of Z(10,$\alpha$) for $\alpha \in [0, 0.5]$.

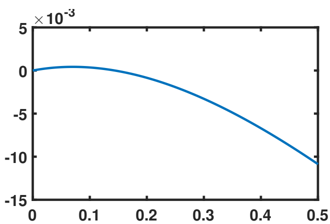


**Fig.5.** The value of Z(11,$\alpha$) for $\alpha \in [0, 0.5]$.

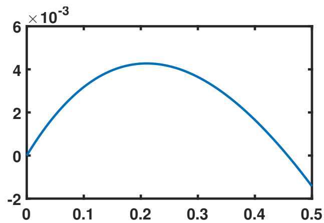


**Fig.6.** The value of Z(15,$\alpha$) for $\alpha \in [0, 0.5]$.

In the following, we consider the graphs in $\mathcal{U}_n$ with the second-minimal $ABC_\alpha$ index for $n \geq 4$ and $-3 \leq \alpha < 0$. It is a trivial case that $S_{4,0}$ is the unique graph with the second-minimal $ABC_\alpha$ index in $\mathcal{U}_4$, where $-3 \le \alpha < 0$. For $n \ge 5$, we have the following theorem.

**Theorem 2.3** Among all graphs in $\mathcal{U}_n$ with $n \ge 5$ and $-3 \le \alpha < 0$,

(i) if $n = 5$, then $S_n(n-3, 2, 1)$ is the unique graph with the second-minimal $ABC_\alpha$ index;

(ii) if $6 \le n \le 9$, then the graph with the second-minimal $ABC_\alpha$ index is either $S_n(n-3, 2, 1)$ or $S_{n,n-4}$;

(iii) if $n \ge 10$, then $S_{n,n-4}$ is the unique graph with the second-minimal $ABC_\alpha$ index.

**Proof.** For $n \ge 5$ and $-3 \le \alpha < 0$, similarly to the proof of Theorem 2.2, we know the graphs with second-minimal $ABC_\alpha$ index in $\mathcal{U}_n$ is either $S_n(n-3, 2, 1)$ or $S_{n,n-4}$.

Recalling that

$$Z(n, \alpha) = ABC_\alpha(S_{n,n-4}) - ABC_\alpha(S_n(n-3, 2, 1)) = 2\left(\frac{1}{2}\right)^\alpha - \left(\frac{2}{3}\right)^\alpha - \left[\frac{n-1}{3(n-2)}\right]^\alpha,$$

we have for $-3 \le \alpha < 0$, $Z(n, \alpha)$ is decreasing in $n$. Thus $Z(5, \alpha) > 0$ (shown in Fig.7.), and $Z(n, \alpha) < 0$ with $n \ge 10$ (shown in Fig.8.). While for $6 \le n \le 9$, we get that $Z(n, \alpha) > 0$ or $Z(n, \alpha) < 0$ is decided by the value of $\alpha$ and $n$ (shown in Figs.9-10.).

This completes the proof of Theorem 2.3. ■

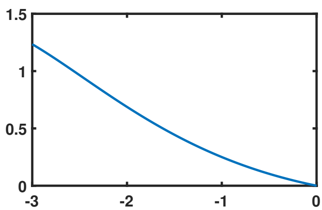


**Fig.7.** The value of Z(5,$\alpha$) for $\alpha \in [-3, 0]$.

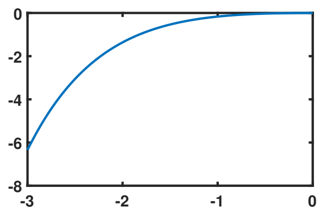


**Fig.8.** The value of Z(10,$\alpha$) for $\alpha \in [-3, 0]$.

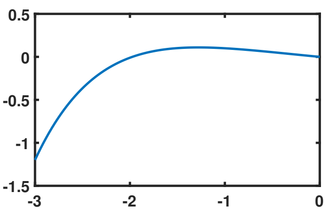


**Fig.9.** The value of Z(6,$\alpha$) for $\alpha \in [-3, 0]$.

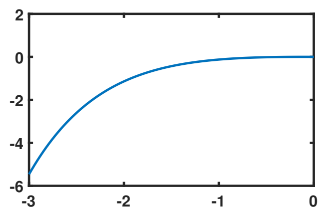


**Fig.10.** The value of Z(9,$\alpha$) for $\alpha \in [-3, 0]$.

# 3 On the extremal $ABC_\alpha$ indices of bicyclic graphs

In this section, the $n$-vertex bicyclic graphs are considered with the maximal (resp. minimal) $ABC_\alpha$ index for $\alpha > 0$ (resp. $-1 \leq \alpha < 0$).

Let $\mathcal{B}_n$ be the set of bicyclic graphs with $n$ vertices, $\mathcal{B}_{n,p}$ be the set of $n-$vertex bicyclic graphs with $p$ pendent vertices for $0 \leq p \leq n-4$, and $C_n^{r,t}$ be the $n$-vertex bicyclic graphs by identifying one vertex of two cycles $C_r$ and $C_t$ and attaching $n+1-r-t$ pendent vertices to the common vertex, where $t \geq r \geq 3$, $r+t \leq n+1$.

For $0 \leq p \leq n-5$, let $\mathcal{C}_{n,p}$ be the set of graphs $C_{n,p} \cong C_n^{r,t}$ with $3 \leq r \leq t \leq n-2-p$ and $r+t = n+1-p$.

Similarly to Lemma 2.2, using Lemma 2.1, we have the following lemma.

**Lemma 3.1** Let $G \in \mathcal{B}_{n,p}$ with $n \geq 5$ and $0 \leq p \leq n-5$,

(i) if $\alpha > 0$, then $ABC_\alpha(G) \leq ABC_\alpha(C_{n,p})$;

(ii) if $-1 \leq \alpha < 0$, then $ABC_\alpha(G) \geq ABC_\alpha(C_{n,p})$, where $ABC_\alpha(C_{n,p}) = \dfrac{n+1}{2^\alpha} + p\Big[\Big(\dfrac{p+3}{p+4}\Big)^\alpha - \Big(\dfrac{1}{2}\Big)^\alpha\Big]$.

**Theorem 3.1** Among all graphs in $\mathcal{B}_{n,p}$ with $n \geq 5$ and $0 \leq p \leq n-5$,

(i) if $\alpha > 0$, then $C_{n,n-5}$ is the unique graph with the maximal $ABC_\alpha$ index;

(ii) if $-1 \leq \alpha < 0$, then $C_{n,n-5}$ is the unique graph with the minimal $ABC_\alpha$ index.

**Proof.** Let

$$T(p,\alpha) = ABC_\alpha(C_{n,p}) = \frac{n+1}{2^\alpha} + p\Big[\Big(\frac{p+3}{p+4}\Big)^\alpha - \Big(\frac{1}{2}\Big)^\alpha\Big].$$

We obtain

$$T_p(p,\alpha) = \Big(\frac{p+3}{p+4}\Big)^\alpha - \Big(\frac{1}{2}\Big)^\alpha + \alpha p\Big(\frac{p+3}{p+4}\Big)^{\alpha-1}\frac{1}{(p+4)^2} > 0, \text{ for } \alpha > 0.$$

Then $ABC_\alpha(C_{n,p})$ is strictly increasing in $p$, by Lemma 3.1 (i), Theorem 3.1 (i) holds.

Similarly, we have $T_p(p,\alpha) < 0$ for $-1 \leq \alpha < 0$.

The theorem follows. ■

Next, we will consider the case of $p = n-4$.

Let $B_4$ be the bicyclic graph obtained by adding an edge to the cycle $C_4$. Label the vertices of $B_4$ by $v_1, v_2, v_3, v_4$ with $d_{v_1} = d_{v_2} = 3$, $d_{v_3} = d_{v_4} = 2$, $B_n(n_1, n_2, n_3, n_4)$ be the graph formed from $B_4$ by attaching $n_i - 1$ pendent vertices to $v_i$, where $n_1 \geq n_2 \geq 1, n_3 \geq n_4 \geq 1$ and $\sum_{i=1}^{4} n_i = n$.

**Lemma 3.2** Let $N(x,\alpha) = xf(x+3,1,\alpha) - (x-1)f(x+2,1,\alpha)$ and $x \geq 1$,

(i) given $\alpha > 0$, then $N(x,\alpha)$ is strictly increasing in $x$;

(ii) given $-1 \leq \alpha < 0$, then $N(x,\alpha)$ is strictly decreasing in $x$.

**Proof.** Let $m(x,\alpha)=xf(x+3,1,\alpha)=x\Big(\dfrac{x+2}{x+3}\Big)^{\alpha}$, then $N(x,\alpha)=m(x,\alpha)-m(x-1,\alpha)$. By direct calculation,

$$m_x(x,\alpha)=\Big(\frac{x+2}{x+3}\Big)^{\alpha}+x\alpha\Big(\frac{x+2}{x+3}\Big)^{\alpha-1}\frac{1}{(x+3)^2}=\Big(\frac{x+2}{x+3}\Big)^{\alpha}\Big[1+\frac{x\alpha}{(x+2)(x+3)}\Big],$$

and

$$\begin{aligned}m_{xx}(x,\alpha)&=\alpha\Big(\frac{x+2}{x+3}\Big)^{\alpha-1}\frac{1}{(x+3)^2}\Big[1+\frac{x\alpha}{(x+2)(x+3)}\Big]+\Big(\frac{x+2}{x+3}\Big)^{\alpha}\frac{\alpha(6-x^2)}{(x+2)^2(x+3)^2}\\&=\alpha\Big(\frac{x+2}{x+3}\Big)^{\alpha-1}\frac{1}{(x+2)(x+3)^3}\Big[(5+\alpha)x+12\Big].\end{aligned}$$

Then (i) for $\alpha>0$ and $x\geq 1$, $m_{xx}(x,\alpha)>0$. It follows that $N_x(x,\alpha)=m_x(x,\alpha)-m_x(x-1,\alpha)>0$, thus $N(x,\alpha)$ is strictly increasing in $x$.

(ii) If $-1\leq\alpha<0$ and $x\geq 1$, then $m_{xx}(x,\alpha)<0$. Thus $N(x,\alpha)$ is strictly decreasing in $x$. ■

**Lemma 3.3** Given $v-u=z-w>0$ and $z>v$,

(i) if $\alpha>0$, then $f(3,u,\alpha)-f(3,v,\alpha)>f(3,w,\alpha)-f(3,z,\alpha)$;

(ii) if $-1\leq\alpha<0$, then $f(3,u,\alpha)-f(3,v,\alpha)<f(3,w,\alpha)-f(3,z,\alpha)$.

**Proof.** Let $g(y)=f(3,y,\alpha)=\Big(\dfrac{y+1}{3y}\Big)^{\alpha}$, it is sufficient to prove $g(u)-g(v)>g(w)-g(z)$ for $v-u=z-w>0$ and $z>v$. By direct calculation,

$$g'(y)=\alpha\Big(\frac{y+1}{3y}\Big)^{\alpha-1}\frac{-1}{3y^2},$$

and

$$\begin{aligned}g''(y)&=\alpha(\alpha-1)\Big(\frac{y+1}{3y}\Big)^{\alpha-2}\Big(\frac{-1}{3y^2}\Big)^2+\alpha\Big(\frac{y+1}{3y}\Big)^{\alpha-1}\frac{2}{3y^3}\\&=\alpha\Big(\frac{y+1}{3y}\Big)^{\alpha-2}\frac{1}{9y^4}\Big[\alpha-1+2(y+1)\Big].\end{aligned}$$

(i) If $\alpha>0$, then $g''(y)>0$. Thus $g'(y)$ is strictly increasing in y. If $v\leq w$, using Lagrange's mean value theorem on the intervals $[w,z]$ and $[u,v]$, then (i) follows directly. If $v>w$, by $v-u=z-w$, then using Lagrange's mean value theorem on the intervals $[v,z]$ and $[u,w]$, the result also holds. Hence, (i) holds.

(ii) For $-1\leq\alpha<0$, in a similar way as in the proof of $\alpha>0$, we can show that (ii) holds. ■

**Lemma 3.4** Let $I(x,\alpha)=\Big(\dfrac{x-2}{x-1}\Big)^{\alpha}+\Big[\dfrac{x}{3(x-1)}\Big]^{\alpha}-2\Big(\dfrac{1}{2}\Big)^{\alpha}$,

(i) given $0<\alpha<1$, if $x\geq 5$ then $I(x,\alpha)$ is increasing in $x$;

(ii) given $-1\leq\alpha\leq -0.3$, if $x\geq 9$ then $I(x,\alpha)$ is increasing in $x$.

**Proof.** Consider the derivative $I(x,\alpha)$ with respect to $x$,

$$\begin{aligned}I_x(x,\alpha)&=\alpha\Big(\frac{x-2}{x-1}\Big)^{\alpha-1}\frac{1}{(x-1)^2}+\alpha\Big[\frac{x}{3(x-1)}\Big]^{\alpha-1}\frac{-1}{3(x-1)^2}\\&=\alpha\Big(\frac{1}{x-1}\Big)^{\alpha-1}\frac{1}{(x-1)^2}\Big[(x-2)^{\alpha-1}-\frac{1}{3}\Big(\frac{x}{3}\Big)^{\alpha-1}\Big].\end{aligned}$$

(i) For $0<\alpha<1$, $\Big[\dfrac{x}{3(x-2)}\Big]^{1-\alpha}>\Big(\dfrac{1}{3}\Big)^{1-\alpha}>\dfrac{1}{3}$. Hence $I_x(x,\alpha)>0$.

(ii) For $x \geq 9$, we have $\dfrac{x}{3(x-2)} \leq \dfrac{3}{7}$. If $-1 \leq \alpha \leq -0.3$, then $\left[\dfrac{x}{3(x-2)}\right]^{1-\alpha} \leq \left(\dfrac{3}{7}\right)^{1-\alpha}$.

Let $q(\alpha) = \left(\dfrac{3}{7}\right)^{1-\alpha} - \dfrac{1}{3}$, Fig.11 shows that $q(\alpha) < 0$. Then $\left[\dfrac{x}{3(x-2)}\right]^{1-\alpha} < \dfrac{1}{3}$ for $-1 \leq \alpha \leq -0.3$. Therefore, $I_x(x,\alpha) > 0$ for $x \geq 9$, the result follows. ■

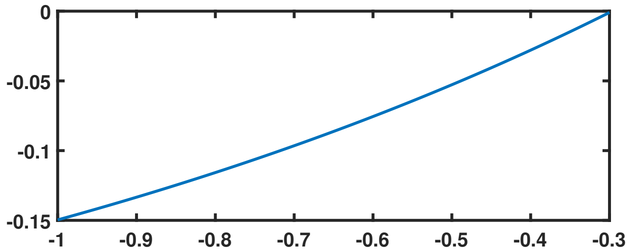


**Fig.11.** The value of $q(\alpha)$ for $\alpha \in [-1,-0.3]$.

**Lemma 3.5** For $n_2 \geq 2$,

(i) if $\alpha > 0$, then $ABC_\alpha(B_n(n_1+1,n_2-1,n_3,n_4)) > ABC_\alpha(B_n(n_1,n_2,n_3,n_4))$;

(ii) if $-1 \leq \alpha < 0$, then $ABC_\alpha(B_n(n_1+1,n_2-1,n_3,n_4)) < ABC_\alpha(B_n(n_1,n_2,n_3,n_4))$.

**Proof.** By direction calculation,

$$ABC_\alpha(B_n(n_1+1,n_2-1,n_3,n_4)) - ABC_\alpha(B_n(n_1,n_2,n_3,n_4))$$
$$= \Big(n_1 f(1,n_1+3,\alpha)+(n_2-2)f(1,n_2+1,\alpha)+f(n_1+3,n_3+1,\alpha)+f(n_2+1,n_3+1,\alpha)+f(n_1+3,n_4+1,\alpha)+f(n_2+1,n_4+1,\alpha)+f(n_1+3,n_2+1,\alpha)\Big) - \Big(\sum_{i=1}^{2}(n_i-1)f(1,n_i+2,\alpha)+f(n_1+2,n_3+1,\alpha)+f(n_2+2,n_3+1,\alpha)+f(n_1+2,n_4+1,\alpha)+f(n_2+2,n_4+1,\alpha)+f(n_1+2,n_2+2,\alpha)\Big)$$
$$= N(n_1,\alpha) - N(n_2-1,\alpha) + h(n_1+2,n_3+1,\alpha) - h(n_2+1,n_3+1,\alpha) + h(n_1+2,n_4+1,\alpha) - h(n_2+1,n_4+1,\alpha) + f(n_1+3,n_2+1,\alpha) - f(n_1+2,n_2+2,\alpha).$$

Then, (i) for $\alpha > 0$, by Lemma 3.2, we have $N(n_1,\alpha) - N(n_2-1,\alpha) > 0$. By Lemma 2.4, we have $h(n_1+2,n_3+1,\alpha) - h(n_2+1,n_3+1,\alpha) > 0$ and $h(n_1+2,n_4+1,\alpha) - h(n_2+1,n_4+1,\alpha) > 0$. Note that $(n_1+3)(n_2+1) < (n_1+2)(n_2+2)$, we get $f(n_1+3,n_2+1,\alpha) - f(n_1+2,n_2+2,\alpha) = \left[\dfrac{n_1+n_2+2}{(n_1+3)(n_2+1)}\right]^\alpha - \left[\dfrac{n_1+n_2+2}{(n_1+2)(n_2+2)}\right]^\alpha > 0$. Thus $ABC_\alpha(B_n(n_1+1,n_2-1,n_3,n_4)) - ABC_\alpha(B_n(n_1,n_2,n_3,n_4)) > 0$.

(ii) For $-1 \leq \alpha < 0$, in a similar manner as above, the result holds. ■

**Lemma 3.6** For $n_4 \geq 2$,

(i) if $\alpha > 0$, then $ABC_\alpha(B_n(n_1,n_2,n_3+1,n_4-1)) > ABC_\alpha(B_n(n_1,n_2,n_3,n_4))$;

(ii) if $-1 \leq \alpha < 0$, then $ABC_\alpha(B_n(n_1, n_2, n_3+1, n_4-1)) < ABC_\alpha(B_n(n_1, n_2, n_3, n_4))$.

**Proof.** By direction calculation,

$ABC_\alpha(B_n(n_1, n_2, n_3+1, n_4-1)) - ABC_\alpha(B_n(n_1, n_2, n_3, n_4))$
$= \Big(n_3 f(1, n_3+2, \alpha) + (n_4-2)f(1, n_4, \alpha) + f(n_1+2, n_3+2, \alpha) + f(n_2+2, n_4, \alpha) + f(n_1+2, n_4, \alpha) + f(n_2+2, n_3+2, \alpha)\Big) - \Big(\sum_{i=3}^{4}(n_i-1)f(1, n_i+1, \alpha) + f(n_1+2, n_3+1, \alpha) + f(n_1+2, n_4+1, \alpha) + f(n_2+2, n_3+1, \alpha) + f(n_2+2, n_4+1, \alpha)\Big)$
$= d(n_3, \alpha) - d(n_4-1, \alpha) + h(n_3+1, n_1+2, \alpha) - h(n_4, n_1+2, \alpha) + h(n_3+1, n_2+2, \alpha) - h(n_4, n_2+2, \alpha)$.

Then, (i) for $\alpha > 0$, using Lemma 2.3, we have $d(n_3, \alpha) - d(n_4-1, \alpha) > 0$. By Lemma 2.4, we have $h(n_3+1, n_1+2, \alpha) - h(n_4, n_1+2, \alpha) > 0$ and $h(n_3+1, n_2+2, \alpha) - h(n_4, n_2+2, \alpha) > 0$. Thus $ABC_\alpha(B_n(n_1, n_2, n_3+1, n_4-1)) - ABC_\alpha(B_n(n_1, n_2, n_3, n_4)) > 0$.

(ii) For $-1 \leq \alpha < 0$, in a similar method as in the proof of $\alpha > 0$, we can show that (ii) holds. ■

**Lemma 3.7** Let $G = B_n(n_1, 1, n_3, 1)$ with $n_1, n_3 \geq 2$ and $n = n_1 + n_3 + 2$,

(i) if $\alpha > 0$, then $ABC_\alpha(G) < ABC_\alpha(B_n(1, 1, n-3, 1)) < ABC_\alpha(B_n(n-3, 1, 1, 1))$;

(ii) if $-1 \leq \alpha < 0$, then $ABC_\alpha(G) > ABC_\alpha(B_n(1, 1, n-3, 1)) > ABC_\alpha(B_n(n-3, 1, 1, 1))$.

**Proof.** By direct calculation,

$ABC_\alpha(B_n(n_1, 1, n_3, 1)) = (n_1-1)f(1, n_1+2, \alpha) + (n_3-1)f(1, n_3+1, \alpha) + f(n_1+2, n_3+1, \alpha) + f(n_1+2, 3, \alpha) + f(n_1+2, 2, \alpha) + f(n_3+1, 3, \alpha) + f(2, 3, \alpha)$,

$ABC_\alpha(B_n(1, 1, n-3, 1)) = ABC_\alpha(B_n(1, 1, n_1+n_3-1, 1))$
$= (n_1+n_3-2)f(1, n_1+n_3, \alpha) + 2f(n_1+n_3, 3, \alpha) + f(3, 3, \alpha) + 2f(3, 2, \alpha)$,

$ABC_\alpha(B_n(n-3, 1, 1, 1)) = (n-4)f(1, n-1, \alpha) + 2f(2, n-1, \alpha) + f(3, n-1, \alpha) + 2f(2, 3, \alpha)$.

Then

$ABC_\alpha(B_n(n_1, 1, n_3, 1)) - ABC_\alpha(B_n(1, 1, n_1+n_3-1, 1))$
$= (n_1-1)[f(1, n_1+2, \alpha) - f(1, n_1+n_3, \alpha)] + (n_3-1)[f(1, n_3+1, \alpha) - f(1, n_1+n_3, \alpha)] + [f(n_1+2, 3, \alpha) - f(n_1+n_3, 3, \alpha)] - [f(3, 3, \alpha) - f(n_3+1, 3, \alpha)] + f(n_1+2, n_3+1, \alpha) - f(n_1+n_3, 3, \alpha)$.

(i) For $\alpha > 0$ and $n_1, n_3 \geq 2$, by Lemma 2.1, we have $f(1, n_1+2, \alpha) - f(1, n_1+n_3, \alpha) < 0$ and $f(1, n_3+1, \alpha) - f(1, n_1+n_3, \alpha) < 0$. By Lemma 3.3, we have $[f(n_1+2, 3, \alpha) - f(n_1+n_3, 3, \alpha)] - [f(3, 3, \alpha) - f(n_3+1, 3, \alpha)] < 0$. Notice that $(n_1+2)(n_3+1) - 3(n_1+n_3) = (n_1-1)(n_3-2) > 0$, we get

$$f(n_1+2,n_3+1,\alpha)-f(n_1+n_3,3,\alpha)=\Big[\frac{n_1+n_3+1}{(n_1+2)(n_3+1)}\Big]^\alpha-\Big[\frac{n_1+n_3+1}{3(n_1+n_3)}\Big]^\alpha<0.$$

Thus $ABC_\alpha(B_n(n_1,1,n_3,1))-ABC_\alpha(B_n(1,1,n-3,1))<0$.

On the other hand, $ABC_\alpha(B_n(n-3,1,1,1))-ABC_\alpha(B_n(1,1,n-3,1))=(n-4)[f(1,n-1,\alpha)-f(1,n-2,\alpha)]+[f(2,3,\alpha)-f(n-2,3,\alpha)]-[f(3,3,\alpha)-f(n-1,3,\alpha)]+f(2,n-1,\alpha)-f(3,n-2,\alpha)$.

Similarly as above, we have $ABC_\alpha(B_n(n-3,1,1,1))-ABC_\alpha(B_n(1,1,n-3,1))>0$.

(ii) For $-1\le\alpha<0$, in a similar method as in the proof of $\alpha>0$, we can show that (ii) holds. ■

From Lemmas 3.5-3.7, we have the following Lemma 3.8.

**Lemma 3.8** Among the graphs in $\mathcal{B}_{n,n-4}$ with $n\ge5$,

(i) if $\alpha>0$, then $B_n(n-3,1,1,1)$ is the unique graph with the maximal $ABC_\alpha$ index, and $B_n(1,1,n-3,1)$ is the unique graph with the second-maximal $ABC_\alpha$ index;

(ii) if $-1\le\alpha<0$, then $B_n(n-3,1,1,1)$ is the unique graph with the minimal $ABC_\alpha$ index, and $B_n(1,1,n-3,1)$ is the unique graph with the second-minimal $ABC_\alpha$ index.

**Theorem 3.2** Among all graphs in $\mathcal{B}_n$ with $n\ge4$ and $\alpha>0$, $B_n(n-3,1,1,1)$ is the unique graph with the maximal $ABC_\alpha$ index.

**Proof.** The case of $n=4$ is trivial. Suppose that $n\ge5$.

By Theorem 3.1, among all graphs in $\mathcal{B}_{n,p}$ with $0\le p\le n-5$, $C_{n,n-5}$ is the unique graph with the maximal $ABC_\alpha$ index. By Lemma 3.8, $B_n(n-3,1,1,1)$ is the unique graph with the maximal $ABC_\alpha$ index in $\mathcal{B}_{n,n-4}$. Then the graphs in $\mathcal{B}_n$ which has the maximal $ABC_\alpha$ index is either $B_n(n-3,1,1,1)$ or $C_{n,n-5}$. Furthermore,

$ABC_\alpha(B_n(n-3,1,1,1))-ABC_\alpha(C_{n,n-5})=\Big(\frac{n-2}{n-1}\Big)^\alpha+\Big[\frac{n}{3(n-1)}\Big]^\alpha-2\Big(\frac{1}{2}\Big)^\alpha=I(n,\alpha)$.

We have $I(n,\alpha)>\Big(\frac{n-2}{n-1}\Big)^\alpha+\Big(\frac{1}{n-1}\Big)^\alpha-2\Big(\frac{1}{2}\Big)^\alpha$. It is clear that $I(n,1)>0$.

For $\alpha>1$, by Lemma 2.6, we get $\Big(\frac{n-2}{n-1}\Big)^\alpha+\Big(\frac{1}{n-1}\Big)^\alpha-2\Big(\frac{1}{2}\Big)^\alpha>0$.

For $0<\alpha<1$, by Lemma 3.4, we have $\Big(\frac{n-2}{n-1}\Big)^\alpha+\Big[\frac{n}{3(n-1)}\Big]^\alpha-2\Big(\frac{1}{2}\Big)^\alpha\ge\Big(\frac{3}{4}\Big)^\alpha+\Big(\frac{5}{12}\Big)^\alpha-2\Big(\frac{1}{2}\Big)^\alpha=I(5,\alpha)>0$ (shown in Fig.12).

This completes the proof of Theorem 3.2. ■

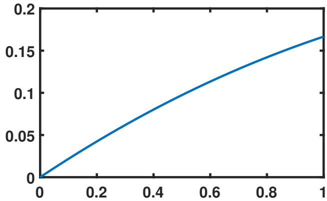


**Fig.12.** The value of I(5,$\alpha$) for $\alpha \in [0, 1]$.

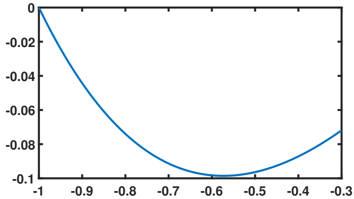


**Fig.13.** The value of L($\alpha$) for $\alpha \in [-1, -0.3]$.

**Theorem 3.3** Among all graphs in $\mathcal{B}_n$ with $n \geq 4$ and $-1 \leq \alpha < 0$, $B_n(n-3, 1, 1, 1)$ is the unique graph with the minimal $ABC_\alpha$ index.

**Proof.** The case of $n = 4$ is trivial. In the following, we suppose that $n \geq 5$.

Similarly to the proof of Theorem 3.2, we get that the graphs in $\mathcal{B}_n$ which has the minimal $ABC_\alpha$ is either $B_n(n-3, 1, 1, 1)$ or $C_{n,n-5}$.

By the proof of Theorem 3.2,

$I(n, \alpha) = ABC_\alpha(B_n(n-3, 1, 1, 1)) - ABC_\alpha(C_{n,n-5}) = \left(\frac{n-2}{n-1}\right)^\alpha + \left[\frac{n}{3(n-1)}\right]^\alpha - 2\left(\frac{1}{2}\right)^\alpha$.

Then we distinguish between the following two cases.

**Case 1.** $-1 \leq \alpha \leq -0.3$.

For $n = 5, 6, 7, 8$ by direct calculation, we have $I(n, \alpha) < 0$. Furthermore, $I(n, \alpha) \to 1+\left(\frac{1}{3}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha$, as $n \to \infty$. Let $L(\alpha) = 1+\left(\frac{1}{3}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha$, Fig.13 shows that $L(\alpha) < 0$. Then for $n \geq 9$, by Lemma 3.4, we have $I(n, \alpha) < 0$.

Combining all above, for any $n \geq 5$ and $-1 \leq \alpha \leq -0.3$, we have $I(n, \alpha) < 0$ .

**Case 2.** $-0.3 < \alpha < 0$.

If $n = 5$, then we have $I(5, \alpha) = \left(\frac{3}{4}\right)^\alpha + \left(\frac{5}{12}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha < 0$ (as shown in Fig.14). Since $\left(\frac{n-2}{n-1}\right)^\alpha$ is decreasing in $n$ and $\left[\frac{n}{3(n-1)}\right]^\alpha$ is increasing in $n$. If $n \geq 6$, then $I(n, \alpha) \leq \left(\frac{4}{5}\right)^\alpha + \left(\frac{1}{3}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha$. Let $R(\alpha) = \left(\frac{4}{5}\right)^\alpha + \left(\frac{1}{3}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha$, we have $R(\alpha) < 0$ (shown in Fig.15). Then the result follows. ■

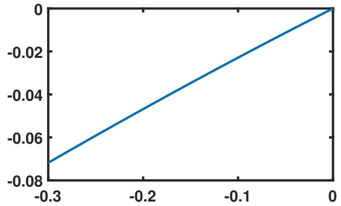


**Fig.14.** The value of I(5,$\alpha$) for $\alpha \in [-0.3, 0]$.

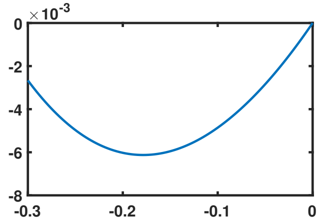


**Fig.15.** The value of $R(\alpha)$ for $\alpha \in [-0.3, 0]$.

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