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Bounds on the General Atom–Bond Connectivity Indices*

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Abstract

The general atom-bond connectivity index (ABC_α) of a graph $G = (V, E)$ is defined as $ABC_\alpha(G) = \sum\limits_{uv \in E} \left(\frac{d_u + d_v - 2}{d_u d_v} \right)^\alpha$, where uv is an edge of G, d_u is the degree of the vertex u, α is an arbitrary nonzero real number, and G has no isolated K_2 if $\alpha < 0$. In this paper, we will determine the upper bound (resp. the lower bound) of ABC_α index for $\alpha \in (0, 1]$ (resp. for $\alpha \in (-\infty, 0)$) among all connected graphs with fixed maximum degree, and characterize the corresponding extremal graphs.

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1 Introduction

For a molecular graph $G = (V, E)$, a large number of topological indices, defined in terms of the vertex degrees, have been considered in the literature [11, 14, 18, 26, 27]. The general form of vertex-degree-based topological indices is $TI(G) = \sum_{uv \in E} \Psi(d_u, d_v)$, where Ψ is a non-negative and real two-variables function, d_v denotes the degree of the vertex v. Topological indices are playing a significant role in mathematical chemistry, pharmacology, etc.

In 1998, Estrada, Torres, Rodríguez and Gutman [8, 9] 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 [1–7, 12, 13, 15–17, 19, 20, 28] and the references cited therein. Furtula et al. [11] 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 [23] generalized the ABC index for arbitrary nonzero real number α, called the general atom-bond connectivity index and denoted as:

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

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

Furtula et al. [11] 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 [9, 10] 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. Moreover, the work would also allow further investigations of more general scenarios outside molecular sciences, such as the study of random walks on graphs.

Zhou et al. [25] determined the upper bound on the ABC index of trees with fixed maximum degree. Xing et al. [24] investigated the upper bound on the ABC index of connected graphs with fixed maximum degree. Liu et al. [22] considered the lower bound on the AZI index of connected graphs with fixed maximum degree. In this paper, we obtain the upper bound (resp. the lower bound) of the ABC_α index for $\alpha \in (0,1]$ (resp. for $\alpha < 0$) among all connected graphs with fixed maximum degree, and characterize the corresponding extremal graphs.

2 Lower bound of ABC_α indices for $\alpha < 0$ among connected graphs with fixed maximum degree

For any connected graph G of order n ($n \geq 3$) with maximum degree Δ, we now investigate the lower bound of $ABC_\alpha(G)$ for $\alpha < 0$ and characterize the corresponding extremal graphs. At first, we need some useful lemmas:

Lemma 2.1 Let $h(x,\alpha) = \dfrac{\alpha(2-x)}{x}\left(\dfrac{2x-2}{x^2}\right)^{\alpha-1}$, where $x \geq 3$ and $\alpha < 0$. Then $h(x,\alpha)$ is strictly increasing in x.

Proof. Note that for $x \geq 3$ and $\alpha < 0$, the partial derived function

$$h_x(x,\alpha) = \alpha\left(\frac{2x-2}{x^2}\right)^{\alpha-1}\frac{2}{x^2}\left[\frac{(\alpha-1)(2-x)^2}{2x-2} - 1\right] > 0,$$

implying that $h(x,\alpha)$ is strictly increasing in x. ■

Lemma 2.2 Let $\Delta \geq 3$ and $\alpha \leq -1.5$, then $-\dfrac{3\alpha}{4}\left(\dfrac{4}{9}\right)^\alpha + 2\left(\dfrac{\Delta-1}{\Delta}\right)^\alpha - 2\left(\dfrac{1}{2}\right)^\alpha > 0.$

Proof. If $\alpha \leq -3$, then $\dfrac{-3\alpha}{4} > 2$. We have

$$\begin{aligned}-\frac{3\alpha}{4}\left(\frac{4}{9}\right)^\alpha + 2\left(\frac{\Delta-1}{\Delta}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha &> 2\left(\frac{4}{9}\right)^\alpha + 2\left(\frac{\Delta-1}{\Delta}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha \\ &> 2\left(\frac{4}{9}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha > 0.\end{aligned}$$

If $\alpha \in (-3,-1.5]$, then $\left(\dfrac{\Delta-1}{\Delta}\right)^\alpha > 1$. We obtain

$$-\frac{3\alpha}{4}\left(\frac{4}{9}\right)^\alpha + 2\left(\frac{\Delta-1}{\Delta}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha > 2 - \frac{3\alpha}{4}\left(\frac{4}{9}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha.$$

Let $D_1(\alpha) = 2 - \dfrac{3\alpha}{4}\left(\dfrac{4}{9}\right)^\alpha - 2\left(\dfrac{1}{2}\right)^\alpha$, by a direct calculation, we have $D_1(-3) \approx 11.63 > 0$ and $D_1(-1.5) \approx 0.14 > 0$. Moreover, with help of software Matlab, we have $D_1'(\alpha) < 0$ for $\alpha \in (-3,-1.5]$ (shown in Fig.1). Then $D_1(\alpha) > 0$ for $\alpha \in (-3,-1.5]$.

So Lemma 2.2 holds. ■

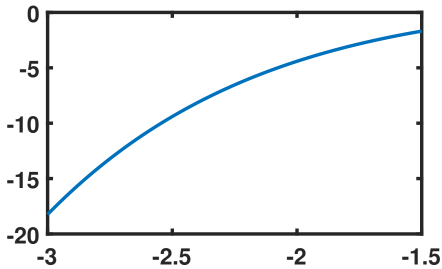

Fig.1. The value of $D_1'(\alpha)$ for $\alpha \in [-3, -1.5]$.

Lemma 2.3 Let $0 < x < 0.5 < y \le 1$, $\alpha < 0$ and $0 < \beta < 1$. If $\frac{\ln 2x}{\ln 2y} < -\beta$, then $x^\alpha + \beta y^\alpha - (1+\beta)\left(\frac{1}{2}\right)^\alpha > 0$.

Proof. It suffices to verify that $\frac{(2x)^\alpha + \beta(2y)^\alpha}{1+\beta} > 1$.

Let $K(x,y,\alpha,\beta) = \frac{(2x)^\alpha+\beta(2y)^\alpha}{1+\beta}$, then $K_{\alpha\alpha}(x,y,\alpha,\beta) = \frac{(2x)^\alpha(\ln 2x)^2+\beta(2y)^\alpha(\ln 2y)^2}{1+\beta} > 0$. We have $K_\alpha(x,y,\alpha,\beta)$ is strictly increasing in α.

If $\frac{\ln 2x}{\ln 2y} < -\beta$, then $K_\alpha(x,y,0,\beta) = \frac{\ln 2x + \beta \ln 2y}{1+\beta} < 0$. We get $K_\alpha(x,y,\alpha,\beta) < 0$ for $\alpha < 0$.

Hence, $K(x,y,\alpha,\beta) = \frac{(2x)^\alpha + \beta(2y)^\alpha}{1+\beta} > K(x,y,0,\beta) = 1$. We obtain $x^\alpha + \beta y^\alpha - (1+\beta)\left(\frac{1}{2}\right)^\alpha > 0$ for $\alpha < 0$. ■

For positive integers x, y, Δ with $1 \le x \le y \le \Delta$, $\Delta \ge 3$, let α be an arbitrary nonzero real number and let

$$f(x,y,\Delta,\alpha) = \left(\frac{x+y-2}{xy}\right)^\alpha + 2\left[\left(\frac{1}{2}\right)^\alpha - \left(\frac{\Delta-1}{\Delta}\right)^\alpha\right]\left(\frac{1}{x}+\frac{1}{y}-\frac{1}{2}-\frac{1}{\Delta}\right) - \left(\frac{1}{2}\right)^\alpha,$$

where $x+y \ne 2$ if $\alpha < 0$. We first prove the following lemma.

Lemma 2.4 Let x, y and Δ be positive integers with $3 \le x \le y \le \Delta$. Then $f(x,y,\Delta,\alpha) > 0$ for $\alpha \le -1.5$.

Proof. Note that $3 \le x \le y \le \Delta$ and

$$f_y(x,y,\Delta,\alpha) = \frac{1}{y^2}\left[\alpha\left(\frac{x+y-2}{xy}\right)^{\alpha-1}\frac{2-x}{x} + 2\left(\frac{\Delta-1}{\Delta}\right)^\alpha - 2\left(\frac{1}{2}\right)^\alpha\right].$$

Let $k(x,y) = \frac{x+y-2}{xy}$. Then $k_y(x,y) = \frac{2-x}{xy^2} < 0$ for $x \ge 3$.

Hence $\left(\frac{x+y-2}{xy}\right)^{\alpha-1} \ge \left(\frac{2x-2}{x^2}\right)^{\alpha-1}$ for $\alpha \le -1.5$, and

$$f_y(x,y,\Delta,\alpha) \geq \frac{1}{y^2}\left[\frac{\alpha(2-x)}{x}\left(\frac{2x-2}{x^2}\right)^{\alpha-1} + 2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}\right]$$
$$= \frac{1}{y^2}\left[h(x,\alpha) + 2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}\right].$$

By Lemma 2.1, we have $h(x,\alpha) \geq h(3,\alpha)$ and then

$$f_y(x,y,\Delta,\alpha) \geq \frac{1}{y^2}\left[h(3,\alpha) + 2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}\right]$$

$$= \frac{1}{y^2}\left[-\frac{3\alpha}{4}\left(\frac{4}{9}\right)^{\alpha} + 2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}\right].$$

By Lemma 2.2, we have $f_y(x,y,\Delta,\alpha) > 0$ for $\alpha \leq -1.5$ and $x \geq 3$. It follows that

$$f(x,y,\Delta,\alpha) \geq f(x,x,\Delta,\alpha) =$$
$$\left(\frac{2x-2}{x^2}\right)^{\alpha} + 2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{2}{x} - \frac{1}{2} - \frac{1}{\Delta}\right) - \left(\frac{1}{2}\right)^{\alpha}.$$

And

$$f_x(x,x,\Delta,\alpha) = \frac{2}{x^2}\left[\frac{\alpha(2-x)}{x}\left(\frac{2x-2}{x^2}\right)^{\alpha-1} + 2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}\right]$$
$$= \frac{2}{x^2}\left[h(x,\alpha) + 2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}\right]$$
$$\geq \frac{2}{x^2}\left[h(3,\alpha) + 2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}\right]$$
$$= \frac{2}{x^2}\left[-\frac{3\alpha}{4}\left(\frac{4}{9}\right)^{\alpha} + 2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}\right] > 0. \text{ (By}$$

Lemma 2.2)

Then

$$f(x,y,\Delta,\alpha) \geq f(x,x,\Delta,\alpha) \geq f(3,3,\Delta,\alpha)$$
$$= \left(\frac{4}{9}\right)^{\alpha} - \left(\frac{1}{2}\right)^{\alpha} + 2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{1}{6} - \frac{1}{\Delta}\right)$$

Clearly $\left(\frac{4}{9}\right)^{\alpha} - \left(\frac{1}{2}\right)^{\alpha} > 0$ for $\alpha \leq -1.5$.

If $\Delta \geq 6$ then $2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{1}{6} - \frac{1}{\Delta}\right) > 0$. Hence $f(x,y,\Delta,\alpha) \geq f(x,x,\Delta,\alpha) \geq f(3,3,\Delta,\alpha) > 0$.

If $\Delta = 3,4,5$ and $\alpha \leq -1.5$, then by Lemma 2.3, we have

- $f(3,3,3,\alpha) = \left(\frac{4}{9}\right)^{\alpha} + \frac{1}{3}\left(\frac{2}{3}\right)^{\alpha} - \frac{4}{3}\left(\frac{1}{2}\right)^{\alpha} > 0,$
- $f(3,3,4,\alpha) = \left(\frac{4}{9}\right)^{\alpha} + \frac{1}{6}\left(\frac{3}{4}\right)^{\alpha} - \frac{7}{6}\left(\frac{1}{2}\right)^{\alpha} > 0,$

- $f(3,3,5,\alpha) = \left(\frac{4}{9}\right)^{\alpha} + \frac{1}{15}\left(\frac{4}{5}\right)^{\alpha} - \frac{16}{15}\left(\frac{1}{2}\right)^{\alpha} > 0.$

This proves $f(x,y,\Delta,\alpha) > 0$ for $3 \leq x \leq y \leq \Delta$ and $\alpha \leq -1.5$. ■

Lemma 2.5 Let y and Δ be positive integers with $3 \leq y \leq \Delta$. Then $f(3,y,\Delta,\alpha) > 0$ for $\alpha \in (-1.5, 0)$.

Proof. Note that

$$f(3,y,\Delta,\alpha) = \left(\frac{y+1}{3y}\right)^{\alpha} + 2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{1}{y} - \frac{1}{6} - \frac{1}{\Delta}\right) - \left(\frac{1}{2}\right)^{\alpha}.$$

We consider the following four cases:

Case.1 $y = 3$.

Note that $f(3,3,\Delta,\alpha) = \left(\frac{4}{9}\right)^{\alpha} - \left(\frac{1}{2}\right)^{\alpha} + 2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{1}{6} - \frac{1}{\Delta}\right)$, and $\left(\frac{4}{9}\right)^{\alpha} - \left(\frac{1}{2}\right)^{\alpha} > 0$ for $\alpha \in (-1.5, 0)$.

If $\Delta \geq 6$, then $2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{1}{6} - \frac{1}{\Delta}\right) > 0$. We have $f(3,3,\Delta,\alpha) > 0$.

If $\Delta = 3, 4, 5$ and $\alpha \in (-1.5, 0)$, then by Lemma 2.3,

- $f(3,3,3,\alpha) = \left(\frac{4}{9}\right)^{\alpha} + \frac{1}{3}\left(\frac{2}{3}\right)^{\alpha} - \frac{4}{3}\left(\frac{1}{2}\right)^{\alpha} > 0,$
- $f(3,3,4,\alpha) = \left(\frac{4}{9}\right)^{\alpha} + \frac{1}{6}\left(\frac{3}{4}\right)^{\alpha} - \frac{7}{6}\left(\frac{1}{2}\right)^{\alpha} > 0,$
- $f(3,3,5,\alpha) = \left(\frac{4}{9}\right)^{\alpha} + \frac{1}{15}\left(\frac{4}{5}\right)^{\alpha} - \frac{16}{15}\left(\frac{1}{2}\right)^{\alpha} > 0.$

Hence $f(3,3,\Delta,\alpha) > 0$ for $\alpha \in (-1.5, 0)$.

Case.2 $y = 4$.

For $\Delta = 4$, we have $f(3,4,4,\alpha) = \left(\frac{5}{12}\right)^{\alpha} + \frac{1}{3}\left(\frac{3}{4}\right)^{\alpha} - \frac{4}{3}\left(\frac{1}{2}\right)^{\alpha}$. By Lemma 2.3, we have $f(3,4,4,\alpha) > 0$, for $\alpha \in (-1.5, 0)$.

If $\Delta \geq 5$, then

$$\begin{aligned} f(3,4,\Delta,\alpha) &= \left(\frac{5}{12}\right)^{\alpha} + 2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{1}{12} - \frac{1}{\Delta}\right) - \left(\frac{1}{2}\right)^{\alpha} \\ &\geq \left(\frac{5}{12}\right)^{\alpha} - \frac{7}{30}\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right] - \left(\frac{1}{2}\right)^{\alpha} \\ &> \left(\frac{5}{12}\right)^{\alpha} + \frac{7}{30} - \frac{37}{30}\left(\frac{1}{2}\right)^{\alpha}. \end{aligned}$$

By Lemma 2.3, we get $\left(\frac{5}{12}\right)^{\alpha} + \frac{7}{30} - \frac{37}{30}\left(\frac{1}{2}\right)^{\alpha} > 0$. Then $f(3,4,\Delta,\alpha) > 0$ for $\alpha \in (-1.5, 0)$.

Case.3 $y = 5$.

For $\Delta=5$, we have $f(3,5,5,\alpha)=\left(\frac{2}{5}\right)^{\alpha}+\frac{1}{3}\left(\frac{4}{5}\right)^{\alpha}-\frac{4}{3}\left(\frac{1}{2}\right)^{\alpha}$. By Lemma 2.3, we obtain $f(3,5,5,\alpha)>0$ for $\alpha\in(-1.5,0)$.

If $\Delta\geq 6$, then

$$\begin{aligned}f(3,5,\Delta,\alpha)&=\left(\frac{2}{5}\right)^{\alpha}+2\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{1}{30}-\frac{1}{\Delta}\right)-\left(\frac{1}{2}\right)^{\alpha}\\&\geq\left(\frac{2}{5}\right)^{\alpha}-\frac{4}{15}\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]-\left(\frac{1}{2}\right)^{\alpha}\\&>\left(\frac{2}{5}\right)^{\alpha}+\frac{4}{15}-\frac{19}{15}\left(\frac{1}{2}\right)^{\alpha}.\end{aligned}$$

By Lemma 2.3, we get $f(3,5,\Delta,\alpha)>0$ for $\alpha\in(-1.5,0)$.

Case.4 $y\geq 6$.

Recall that $y\leq\Delta$, then

$$\begin{aligned}f(3,y,\Delta,\alpha)&\geq\left(\frac{y+1}{3y}\right)^{\alpha}+2\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(-\frac{1}{6}\right)-\left(\frac{1}{2}\right)^{\alpha}\\&>\left(\frac{y+1}{3y}\right)^{\alpha}+\frac{1}{3}-\frac{4}{3}\left(\frac{1}{2}\right)^{\alpha}\\&\geq\left(\frac{7}{18}\right)^{\alpha}+\frac{1}{3}-\frac{4}{3}\left(\frac{1}{2}\right)^{\alpha}.\end{aligned}$$

Similarly, by Lemma 2.3, we have $f(3,y,\Delta,\alpha)>0$ for $\alpha\in(-1.5,0)$.

Hence $f(3,y,\Delta,\alpha)>0$ for $3\leq y\leq\Delta$ and $\alpha\in(-1.5,0)$. The Lemma follows. ■

Lemma 2.6 Let y and Δ be positive integers with $4\leq y\leq\Delta$. Then $f(4,y,\Delta,\alpha)>0$ for $\alpha\in(-1.5,0)$.

Proof. Note that

$$f(4,y,\Delta,\alpha)=\left(\frac{y+2}{4y}\right)^{\alpha}+2\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{1}{y}-\frac{1}{4}-\frac{1}{\Delta}\right)-\left(\frac{1}{2}\right)^{\alpha}.$$

We consider the following three cases:

Case.1 $y=4$.

Note that $f(4,4,\Delta,\alpha)=\left(\frac{3}{8}\right)^{\alpha}+2\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(-\frac{1}{\Delta}\right)-\left(\frac{1}{2}\right)^{\alpha}$.
If $\Delta=4,5$, by Lemma 2.3, we have $f(4,4,4,\alpha)>0$ and $f(4,4,5,\alpha)>0$ for $\alpha\in(-1.5,0)$.

If $\Delta\geq 6$, then

$$\begin{aligned}f(4,4,\Delta,\alpha)&\geq\left(\frac{3}{8}\right)^{\alpha}-\frac{1}{3}\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]-\left(\frac{1}{2}\right)^{\alpha}\\&>\left(\frac{3}{8}\right)^{\alpha}+\frac{1}{3}-\frac{4}{3}\left(\frac{1}{2}\right)^{\alpha}.\end{aligned}$$

By Lemma 2.3, we have $f(4,4,\Delta,\alpha)>0$ for $\alpha\in(-1.5,0)$.

Case.2 $y=5$.

Note that

$$f(4,5,\Delta,\alpha)=\left(\frac{7}{20}\right)^{\alpha}+2\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(-\frac{1}{20}-\frac{1}{\Delta}\right)-\left(\frac{1}{2}\right)^{\alpha}.$$

If $\Delta = 5$, then $f(4,5,5,\alpha) = \left(\frac{7}{20}\right)^{\alpha} + \frac{1}{2}\left(\frac{4}{5}\right)^{\alpha} - \frac{3}{2}\left(\frac{1}{2}\right)^{\alpha} > 0$ (by Lemma 2.3).
If $\Delta \geq 6$, then

$$\begin{aligned} f(4,5,\Delta,\alpha) &\geq \left(\frac{7}{20}\right)^{\alpha} - \frac{13}{30}\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right] - \left(\frac{1}{2}\right)^{\alpha} \\ &> \left(\frac{7}{20}\right)^{\alpha} + \frac{13}{30} - \frac{43}{30}\left(\frac{1}{2}\right)^{\alpha}. \end{aligned}$$

By Lemma 2.3, we have $f(4,5,\Delta,\alpha) > 0$ for $\alpha \in (-1.5, 0)$ and $\Delta \geq 6$.

Case.3 $y \geq 6$.

We consider

$$\begin{aligned} f(4,y,\Delta,\alpha) &= \left(\frac{y+2}{4y}\right)^{\alpha} + 2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{1}{y} - \frac{1}{4} - \frac{1}{\Delta}\right) - \left(\frac{1}{2}\right)^{\alpha} \\ &\geq \left(\frac{y+2}{4y}\right)^{\alpha} + 2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(-\frac{1}{4}\right) - \left(\frac{1}{2}\right)^{\alpha} \\ &> \left(\frac{y+2}{4y}\right)^{\alpha} + \frac{1}{2} - \frac{3}{2}\left(\frac{1}{2}\right)^{\alpha} \\ &\geq \left(\frac{1}{3}\right)^{\alpha} + \frac{1}{2} - \frac{3}{2}\left(\frac{1}{2}\right)^{\alpha}. \end{aligned}$$

Using Lemma 2.3, we have $\left(\frac{1}{3}\right)^{\alpha} + \frac{1}{2} - \frac{3}{2}\left(\frac{1}{2}\right)^{\alpha} > 0$.

Hence $f(4,y,\Delta,\alpha) > 0$ for $4 \leq y \leq \Delta$ and $\alpha \in (-1.5, 0)$.

The Lemma follows. ■

Lemma 2.7 Let x, y, Δ be positive integers with $x \leq y \leq \Delta$ and $\Delta \geq 3$. Then $f(x,y,\Delta,\alpha) > 0$ for $\alpha < 0$ and $(x,y) \notin \{(1,\Delta),(2,\Delta)\}$.

Proof. Note that if $x = 1, 2$ then $y < \Delta$. Let $g(y,\alpha) = \left(\frac{y-1}{y}\right)^{\alpha}$, then $g(2,\alpha) = \left(\frac{1}{2}\right)^{\alpha}$ and $g(y,\alpha)$ is strictly decreasing in y, where $y \geq 2$ and $\alpha < 0$. It follows that

$$\begin{aligned} f(1,y,\Delta,\alpha) &= \left(\frac{y-1}{y}\right)^{\alpha} + 2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{1}{y} + \frac{1}{2} - \frac{1}{\Delta}\right) - \left(\frac{1}{2}\right)^{\alpha} \\ &= \left(\frac{y-1}{y}\right)^{\alpha} + \left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{2}{y} + 1 - \frac{2}{\Delta}\right) - \left(\frac{1}{2}\right)^{\alpha} \\ &= \left(\frac{y-1}{y}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha} + \left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{2}{y} - \frac{2}{\Delta}\right) > 0, \end{aligned}$$

and

$$f(2,y,\Delta,\alpha) = \left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{2}{y} - \frac{2}{\Delta}\right) > 0.$$

If $x \geq 3$ then the proof of the case $\alpha \leq -1.5$ is completed in Lemma 2.4. For $\alpha \in (-1.5, 0)$, if $x = 3,\ 4$ then we get the result by Lemmas 2.5, 2.6. Now we may suppose that $x \geq 5$, in a similar manner as in the proof of Lemma 2.4, we have

$$\begin{aligned} f_y(x,y,\Delta,\alpha) &\geq \frac{1}{y^2}\left[\frac{\alpha(2-x)}{x}\left(\frac{2x-2}{x^2}\right)^{\alpha-1} + 2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}\right] \\ &= \frac{1}{y^2}\left[h(x,\alpha) + 2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - 2\left(\frac{1}{2}\right)^{\alpha}\right] \end{aligned}$$

$$\geq \frac{1}{y^2}\left[h(5,\alpha)+2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}\right]$$
$$=\frac{1}{y^2}\left[-\frac{15\alpha}{8}\left(\frac{8}{25}\right)^{\alpha}+2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}\right]$$
$$>\frac{1}{y^2}\left[2-\frac{15\alpha}{8}\left(\frac{8}{25}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}\right].$$

Let $D_2(\alpha)=2-\frac{15\alpha}{8}\left(\frac{8}{25}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}$, by direct calculation, we have $D_2(-1.5)\approx 11.88>0$ and $D_2(0)=0$. Moreover, we have $D_2'(\alpha)<0$ for $\alpha\in(-1.5,0)$ (shown in Fig.2). Then $D_2(\alpha)>0$ for $\alpha\in(-1.5,0)$. Hence $f_y(x,y,\Delta,\alpha)>0$ for $\alpha\in(-1.5,0)$ and $x\geq 5$, and it follows that

$$f(x,y,\Delta,\alpha)\geq f(x,x,\Delta,\alpha)=$$
$$\left(\frac{2x-2}{x^2}\right)^{\alpha}+2\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(\frac{2}{x}-\frac{1}{2}-\frac{1}{\Delta}\right)-\left(\frac{1}{2}\right)^{\alpha}.$$

And

$$f_x(x,x,\Delta,\alpha)=\frac{2}{x^2}\left[\frac{\alpha(2-x)}{x}\left(\frac{2x-2}{x^2}\right)^{\alpha-1}+2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}\right]$$
$$=\frac{2}{x^2}\left[h(x,\alpha)+2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}\right]$$
$$\geq\frac{2}{x^2}\left[h(5,\alpha)+2\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}\right]$$
$$>\frac{2D_2(\alpha)}{x^2}>0.$$

Then for $3\leq x\leq y\leq\Delta$, we have

$$f(x,y,\Delta,\alpha)\geq f(x,x,\Delta,\alpha)\geq f(5,5,\Delta,\alpha)$$
$$=\left(\frac{8}{25}\right)^{\alpha}+2\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]\left(-\frac{1}{10}-\frac{1}{\Delta}\right)-\left(\frac{1}{2}\right)^{\alpha}$$
$$\geq\left(\frac{8}{25}\right)^{\alpha}-\frac{3}{5}\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\right]-\left(\frac{1}{2}\right)^{\alpha}$$
$$>\left(\frac{8}{25}\right)^{\alpha}+\frac{3}{5}-\frac{8}{5}\left(\frac{1}{2}\right)^{\alpha}>0.\ \text{(by Lemma 2.3)}$$

Thus $f(x,y,\Delta,\alpha)>0$ for $x\geq 5$ and $\alpha\in(-1.5,0)$.

The proof of Lemma 2.7 is now completed. ■

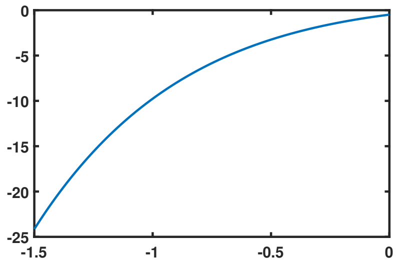

Fig.2. The value of $D_2'(\alpha)$ for $\alpha \in (-1.5, 0)$.

Let G be a connected graph with n $(n \geq 3)$ vertices and maximum degree Δ. Let n_x denote the number of vertices with degree x in G for $1 \leq x \leq \Delta$, and let a_{xy} denote the number of edges of G connecting vertices of degree x and y where $1 \leq x \leq y \leq \Delta$. Then the ABC_α index of G can be rewritten as

$$ABC_\alpha(G) = \sum_{1 \leq x \leq y \leq \Delta} a_{xy} \left(\frac{x+y-2}{xy} \right)^\alpha . \tag{1}$$

For positive integers n, m and Δ with $3 \leq \Delta \leq n-1 \leq m$ and $m \equiv 0 \pmod{\Delta}$, let $\Gamma_{n,m,\Delta}$ be the set of connected graphs with n vertices, m edges and maximum degree Δ such that $a_{xy} = 0$ for all x, y with $x \geq 3$ or $y \neq \Delta$.

Lemma 2.8 ([24]) Let n, m and Δ be positive integers with $3 \leq \Delta \leq n-1 \leq m$,

(i) if $G \in \Gamma_{n,m,\Delta}$, then $a_{1\Delta} = 2n - m - \dfrac{2m}{\Delta}$, $a_{2\Delta} = 2m - 2n + \dfrac{2m}{\Delta}$, $n_\Delta = \dfrac{m}{\Delta}$ and

$$ABC_\alpha(G) = \left(\frac{\Delta - 1}{\Delta} \right)^\alpha \left(2n - m - \frac{2m}{\Delta} \right) + \left(\frac{1}{2} \right)^\alpha \left(2m - 2n + \frac{2m}{\Delta} \right);$$

(ii) $\Gamma_{n,m,\Delta} \neq \emptyset$ if and only if $m \leq 2n - \dfrac{2m}{\Delta}$ and $m \equiv 0 \pmod{\Delta}$.

Now we can establish a sharp lower bound on $ABC_\alpha(G)$ in terms of n, m, Δ and α, where $\alpha < 0$ and G is a connected graph with n vertices, m edges and maximum degree Δ.

Theorem 2.1 Let G be a connected graph of order n, size m and maximum degree Δ, where $2 \leq \Delta \leq n-1$ and $\alpha < 0$. Then

$$ABC_\alpha(G) \geq \left(\frac{\Delta - 1}{\Delta} \right)^\alpha \left(2n - m - \frac{2m}{\Delta} \right) + \left(\frac{1}{2} \right)^\alpha \left(2m - 2n + \frac{2m}{\Delta} \right)$$

with equality if and only if $G \cong P_n$ for $\Delta = 2$, and $G \in \Gamma_{n,m,\Delta}$ for $\Delta \geq 3$.

Proof. If $\Delta = 2$, then $G \cong P_n$ and the result follows. Assume that $3 \leq \Delta \leq n-1$. Let n_x, a_{xy} be defined as in Eq.(1), where $1 \leq x \leq y \leq \Delta$. Then

$$\begin{cases} n_1 + n_2 + ... + n_\Delta = n, \\ n_1 + 2n_2 + ... + \Delta n_\Delta = 2m, \\ \sum\limits_{2\leq x\leq \Delta} a_{1x} = n_1, \\ \sum\limits_{1\leq y\leq \Delta, x\neq y} a_{xy} + 2a_{xx} = xn_x \qquad (x = 2, 3, .., \Delta). \end{cases}$$

Suppose that

$$\begin{cases} b_1 = \sum\limits_{2\leq y\leq \Delta-1} a_{1y}, \\ b_2 = \sum\limits_{1\leq y\leq \Delta-1, y\neq 2} a_{2y} + 2a_{22}, \\ b_x = \sum\limits_{1\leq y\leq \Delta, y\neq x} a_{xy} + 2a_{xx} \qquad (x = 3, 4, .., \Delta - 1), \\ b_\Delta = \sum\limits_{3\leq y\leq \Delta-1} a_{\Delta y} + 2a_{\Delta\Delta}. \end{cases}$$

i.e.,

$$\begin{cases} b_1 = n_1 - a_{1\Delta}, \\ b_2 = 2n_2 - a_{2\Delta}, \\ b_x = xn_x \qquad (x = 3, 4, .., \Delta - 1), \\ b_\Delta = \Delta n_\Delta - a_{1\Delta} - a_{2\Delta}. \end{cases}$$

Then we have

$$\begin{cases} \sum\limits_{1\leq x\leq \Delta} b_x = 2m - 2(a_{1\Delta} + a_{2\Delta}), \\ \sum\limits_{1\leq x\leq \Delta} \frac{b_x}{x} = n - \left(1 + \frac{1}{\Delta}\right) a_{1\Delta} - \left(\frac{1}{2} + \frac{1}{\Delta}\right) a_{2\Delta}. \end{cases}$$

Thus we obtain

$$\begin{aligned} a_{1\Delta} &= 2n - m - \frac{2m}{\Delta} - \sum_{1\leq x\leq \Delta} \left(\frac{2}{x} - \frac{1}{2} - \frac{1}{\Delta}\right) b_x \\ &= 2n - m - \frac{2m}{\Delta} - \sum_{\substack{1 \leq x \leq y \leq \Delta \\ (x,y) \neq (1,\Delta),(2,\Delta)}} \left(\frac{2}{x} + \frac{2}{y} - 1 - \frac{2}{\Delta}\right) a_{xy}, \end{aligned}$$

and

$$a_{2\Delta} = 2m - 2n + \frac{2m}{\Delta} + \sum_{1\leq x\leq \Delta} \left(\frac{2}{x} - 1 - \frac{1}{\Delta}\right) b_x$$

$$= 2m - 2n + \frac{2m}{\Delta} + \sum_{\substack{1 \le x \le y \le \Delta \\ (x,y) \neq (1,\Delta),(2,\Delta)}} \left(\frac{2}{x} + \frac{2}{y} - 2 - \frac{2}{\Delta} \right) a_{xy}.$$

Substituting them back into Eq.(1), we get

$$ABC_\alpha(G) = \left(\frac{\Delta - 1}{\Delta} \right)^\alpha a_{1\Delta} + \left(\frac{1}{2} \right)^\alpha a_{2\Delta} + \sum_{\substack{1 \le x \le y \le \Delta \\ (x,y) \neq (1,\Delta),(2,\Delta)}} \left(\frac{x+y-2}{xy} \right)^\alpha a_{xy}$$

$$= \left(\frac{\Delta - 1}{\Delta} \right)^\alpha \left(2n - m - \frac{2m}{\Delta} \right) + \left(\frac{1}{2} \right)^\alpha \left(2m - 2n + \frac{2m}{\Delta} \right)$$

$$+ \sum_{\substack{1 \le x \le y \le \Delta \\ (x,y) \neq (1,\Delta),(2,\Delta)}} f(x,y,\Delta,\alpha) a_{xy} \tag{2}$$

By Lemma 2.7, we have $f(x,y,\Delta,\alpha) > 0$ for all positive integers $1 \le x \le y \le \Delta$ with $(x,y) \notin \{(1,\Delta),(2,\Delta)\}$ and $\alpha < 0$, then

$$ABC_\alpha(G) \ge \left(\frac{\Delta - 1}{\Delta} \right)^\alpha \left(2n - m - \frac{2m}{\Delta} \right) + \left(\frac{1}{2} \right)^\alpha \left(2m - 2n + \frac{2m}{\Delta} \right)$$

with equality if and only if $a_{xy} = 0$ for all positive integers $1 \le x \le y \le \Delta$ with $(x,y) \notin \{(1,\Delta),(2,\Delta)\}$, implying that

$$\begin{cases} a_{1\Delta} = 2n - m - \dfrac{2m}{\Delta}, \\ a_{2\Delta} = 2m + \dfrac{2m}{\Delta} - 2n, \end{cases}$$

that is, $G \in \Gamma_{n,m,\Delta}$ for $\Delta \ge 3$.

This completes the proof of Theorem 2.1. ■

Remark 1. By Lemma 2.8, if $m > 2n - \frac{2m}{\Delta}$ or $m \not\equiv 0 \pmod{\Delta}$, then $\Gamma_{n,m,\Delta} = \emptyset$. Thus, in these cases the lower bound in Theorem 2.1 cannot be attained.

3 Upper bound of ABC_α indices for $0 < \alpha \le 1$ among connected graphs with fixed maximum degree

In this section, for $\alpha \in (0,1]$, we will consider the upper bound of ABC_α indices among all connected graphs with n ($n \ge 3$) vertices and maximum degree Δ, and characterize the corresponding extremal graphs.

Lemma 3.1 Let $A(x,\alpha) = \left(\frac{x-1}{x} \right)^\alpha \left[\frac{\alpha(x-2)}{2(x-1)} - 1 \right]$, where $\alpha \in (0,1)$ and $x \ge 3$. Then $A(x,\alpha)$ is strictly decreasing in x.

Proof. By direct calculation, we have

$$A_x(x,\alpha) = \left(\frac{x-1}{x}\right)^{\alpha-1} \frac{\alpha}{x^2}\left[\frac{\alpha(x-2)}{2(x-1)} - 1\right] + \left(\frac{x-1}{x}\right)^{\alpha} \frac{\alpha}{2(x-1)^2}$$

$$= \left(\frac{x-1}{x}\right)^{\alpha} \frac{\alpha}{x(x-1)}\left[\frac{\alpha(x-2)-2(x-1)}{2(x-1)}\right] + \left(\frac{x-1}{x}\right)^{\alpha} \frac{\alpha}{2(x-1)^2}$$

$$= \left(\frac{x-1}{x}\right)^{\alpha} \frac{\alpha}{x-1}\frac{(\alpha-1)(x-2)}{2x(x-1)}.$$

Hence, $A_x(x,\alpha) < 0$ for $\alpha \in (0,1)$ and $x \geq 3$. It follows that the result is true. ∎

Lemma 3.2 Let x, y and Δ be positive integers with $3 \leq x \leq y \leq \Delta$. Then $f(x,y,\Delta,\alpha) \leq f(x,x,x,\alpha)$ for $\alpha \in (0,1)$.

Proof. By direct calculation, we have

$$f_\Delta(x,y,\Delta,\alpha) = \frac{2}{\Delta^2}\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha} - \alpha\left(\frac{\Delta-1}{\Delta}\right)^{\alpha-1}\left(\frac{1}{x}+\frac{1}{y}-\frac{1}{2}-\frac{1}{\Delta}\right)\right].$$

Let $T = \frac{1}{2} - \frac{1}{x} - \frac{1}{y}$, then

$$f_\Delta(x,y,\Delta,\alpha) = \frac{2}{\Delta^2}\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha} + \alpha\left(\frac{\Delta-1}{\Delta}\right)^{\alpha-1}\left(T+\frac{1}{\Delta}\right)\right].$$

Because $T = \frac{1}{2} - \frac{1}{x} - \frac{1}{y} \leq \frac{1}{2} - \frac{1}{\Delta} - \frac{1}{\Delta} = \frac{1}{2} - \frac{2}{\Delta}$, we get

$$f_\Delta(x,y,\Delta,\alpha) \leq \frac{2}{\Delta^2}\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{\Delta-1}{\Delta}\right)^{\alpha} + \alpha\left(\frac{\Delta-1}{\Delta}\right)^{\alpha-1}\left(\frac{1}{2}-\frac{1}{\Delta}\right)\right]$$

$$= \frac{2}{\Delta^2}\left\{\left(\frac{1}{2}\right)^{\alpha} + \left(\frac{\Delta-1}{\Delta}\right)^{\alpha}\left[\frac{\alpha(\Delta-2)}{2(\Delta-1)} - 1\right]\right\}$$

$$= \frac{2}{\Delta^2}\left[\left(\frac{1}{2}\right)^{\alpha} + A(\Delta,\alpha)\right]$$

$$\leq \frac{2}{\Delta^2}\left[\left(\frac{1}{2}\right)^{\alpha} + A(3,\alpha)\right] \text{ (By Lemma 3.1)}$$

$$= \frac{2}{\Delta^2}\left[\left(\frac{1}{2}\right)^{\alpha} + \left(\frac{2}{3}\right)^{\alpha}\left(\frac{\alpha}{4}-1\right)\right].$$

Let $Q(\alpha) = \left(\frac{1}{2}\right)^{\alpha} + \left(\frac{2}{3}\right)^{\alpha}\left(\frac{\alpha}{4}-1\right)$, we have $Q(1) = 0$ and $Q(0) = 0$. Moreover, by the value of $Q'(\alpha)$ for $\alpha \in (0,1)$ (shown in Fig.3), we obtain $Q(\alpha) < 0$ for $\alpha \in (0,1)$. It follows that $f_\Delta(x,y,\Delta,\alpha) < 0$ for $3 \leq x \leq y \leq \Delta$ and $\alpha \in (0,1)$. Then

$$f(x,y,\Delta,\alpha) \leq f(x,y,y,\alpha) = \left(\frac{x+y-2}{xy}\right)^{\alpha} + 2\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{y-1}{y}\right)^{\alpha}\right]\left(\frac{1}{x}-\frac{1}{2}\right) - \left(\frac{1}{2}\right)^{\alpha},$$

and

$$f_y(x,y,y,\alpha) = \alpha\left(\frac{x+y-2}{xy}\right)^{\alpha-1}\frac{2-x}{xy^2} - \alpha\left(\frac{y-1}{y}\right)^{\alpha-1}\frac{2}{y^2}\left(\frac{1}{x}-\frac{1}{2}\right)$$

$$= \frac{\alpha(2-x)}{xy^2}\left[\left(\frac{x+y-2}{xy}\right)^{\alpha-1} - \left(\frac{y-1}{y}\right)^{\alpha-1}\right]$$
$$= \frac{\alpha(2-x)}{xy^{\alpha+1}}\left[\left(\frac{x+y-2}{x}\right)^{\alpha-1} - (y-1)^{\alpha-1}\right].$$

Since $\frac{x+y-2}{x} < y-1$, we have $\left(\frac{x+y-2}{x}\right)^{\alpha-1} - (y-1)^{\alpha-1} > 0$. Then $f_y(x,y,y,\alpha) < 0$ for $3 \le x \le y \le \Delta$ and $\alpha \in (0,1)$.

Thus $f(x,y,\Delta,\alpha) \le f(x,y,y,\alpha) \le f(x,x,x,\alpha)$ for $3 \le x \le y \le \Delta$ and $\alpha \in (0,1)$.

This completes the proof of Lemma 3.2. ■

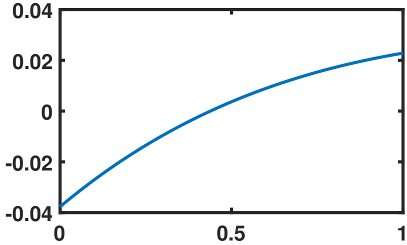

Fig.3. The value of $Q'(\alpha)$ for $\alpha \in (0,1)$.

Lemma 3.3 Let $W(x) = \ln(2x) - \sqrt{2x} + 1$, where $0 < x \le 1$. Then $W\left(\frac{1}{2}\right) = 0$ and $W(x)$ is increasing in x.

Proof. By direct calculation, we have $W\left(\frac{1}{2}\right) = 0$ and $W'(x) = \frac{1}{x} - \frac{1}{\sqrt{2x}} > 0$ for $0 < x \le 1$. Then the result follows. ■

Lemma 3.4 Let $0 < x < 0.5 < y \le 1$, $\alpha \in (0, 0.5]$ and $0 < \beta < 1$. If $\frac{\sqrt{2x}-1}{\sqrt{2y}-1} < -\beta$, then $x^\alpha + \beta y^\alpha - (1+\beta)\left(\frac{1}{2}\right)^\alpha < 0$.

Proof. As in the proof of Lemma 2.3, it suffices to verify that $K(x,y,\alpha,\beta) = \frac{(2x)^\alpha+\beta(2y)^\alpha}{1+\beta}$ < 1 for $0 < x < 0.5 < y \le 1$, $\alpha \in (0, 0.5]$ and $0 < \beta < 1$.

Recall that $K_\alpha(x,y,\alpha,\beta)$ is strictly increasing in α. By Lemma 3.3, we have $\frac{\ln 2x}{\ln 2y} < \frac{\sqrt{2x}-1}{\sqrt{2y}-1}$. Then $K_\alpha(x,y,0,\beta) = \frac{\ln 2x + \beta \ln 2y}{1+\beta} < 0$.

On the other hand, $K_\alpha(x,y,\frac{1}{2},\beta) = \frac{\sqrt{2x}\ln 2x + \beta\sqrt{2y}\ln 2y}{1+\beta}$.

(i) If $\frac{\sqrt{2x}\ln 2x}{\sqrt{2y}\ln 2y} < -\beta$, then $K_\alpha(x,y,\frac{1}{2},\beta) < 0$. We have $K(x,y,\alpha,\beta) < K(x,y,0,\beta) = 1$.

(ii) If $\frac{\sqrt{2x}\ln 2x}{\sqrt{2y}\ln 2y} > -\beta$, then $K_\alpha(x,y,\frac{1}{2},\beta) > 0$. Since $\frac{\sqrt{2x}-1}{\sqrt{2y}-1} < -\beta$, it follows that $K(x,y,\frac{1}{2},\beta) = \frac{\sqrt{2x}+\beta\sqrt{2y}}{1+\beta} < 1$ and $K(x,y,0,\beta) = 1$.

Then $K(x,y,\alpha,\beta)<1$ for $\alpha\in(0,0.5]$. The result follows. ■

Lemma 3.5 For $0.5<\alpha<1$, we have $\left(\frac{4}{9}\right)^{\alpha}+\frac{1}{3}\left(\frac{2}{3}\right)^{\alpha}-\frac{4}{3}\left(\frac{1}{2}\right)^{\alpha}<0$.

Proof. It is sufficient to prove that $\frac{3}{4}\left(\frac{8}{9}\right)^{\alpha}+\frac{1}{4}\left(\frac{4}{3}\right)^{\alpha}<1$.

Let $D_3(\alpha)=\frac{3}{4}\left(\frac{8}{9}\right)^{\alpha}+\frac{1}{4}\left(\frac{4}{3}\right)^{\alpha}$, we have

$D_3''(\alpha)=\frac{3}{4}\left(\frac{8}{9}\right)^{\alpha}\left(\ln\left(\frac{8}{9}\right)\right)^{2}+\frac{1}{4}\left(\frac{4}{3}\right)^{\alpha}\left(\ln\left(\frac{4}{3}\right)\right)^{2}>0.$

Hence $D_3'(x)$ is increasing in x. By direct calculation, $D_3'\left(\frac{1}{2}\right)\approx 0.034>0$. Then $D_3(\alpha)<D_3(1)=1$ for $0.5<\alpha<1$. ■

Lemma 3.6 Let x,y and Δ be positive integers with $3\le x\le y\le\Delta$. Then $f(x,x,x,\alpha)<0$ for $\alpha\in(0,0.5]$.

Proof. Note that

$$f(x,x,x,\alpha)=\left(\frac{2x-2}{x^2}\right)^{\alpha}+2\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{x-1}{x}\right)^{\alpha}\right]\left(\frac{1}{x}-\frac{1}{2}\right)-\left(\frac{1}{2}\right)^{\alpha}.$$

As $x\ge 3$ and $\alpha\in(0,0.5]$, we have $\frac{1}{x}-\frac{1}{2}>-\frac{1}{2}$ and $\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{x-1}{x}\right)^{\alpha}<0$. Then

$$2\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{x-1}{x}\right)^{\alpha}\right]\left(\frac{1}{x}-\frac{1}{2}\right)<-\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{x-1}{x}\right)^{\alpha}\right].$$

Hence

$$f(x,x,x,\alpha)<\left(\frac{2x-2}{x^2}\right)^{\alpha}+\left(\frac{x-1}{x}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}.$$

Note that $\left(\frac{2x-2}{x^2}\right)^{\alpha}$ is strictly decreasing in x for $x\ge 3$. If $x\ge 11$, then

$$f(x,x,x,\alpha)<\left(\frac{2x-2}{x^2}\right)^{\alpha}+\left(\frac{x-1}{x}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}<1+\left(\frac{20}{121}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}.$$

By Lemma 3.4, we have $1+\left(\frac{20}{121}\right)^{\alpha}-2\left(\frac{1}{2}\right)^{\alpha}<0$ for $\alpha\in(0,0.5]$. Thus $f(x,x,x,\alpha)<0$ for $11\le x\le y\le\Delta$ and $\alpha\in(0,0.5]$.

If $7\le x\le 10$ then $\frac{1}{x}\ge\frac{1}{10}$. We have $\frac{1}{x}-\frac{1}{2}\ge-\frac{2}{5}$, and

$$\begin{aligned}f(x,x,x,\alpha)&\le\left(\frac{2x-2}{x^2}\right)^{\alpha}-\frac{4}{5}\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{x-1}{x}\right)^{\alpha}\right]-\left(\frac{1}{2}\right)^{\alpha}\\&=\left(\frac{2x-2}{x^2}\right)^{\alpha}+\frac{4}{5}\left(\frac{x-1}{x}\right)^{\alpha}-\frac{9}{5}\left(\frac{1}{2}\right)^{\alpha}\\&\le\left(\frac{12}{49}\right)^{\alpha}+\frac{4}{5}\left(\frac{9}{10}\right)^{\alpha}-\frac{9}{5}\left(\frac{1}{2}\right)^{\alpha}\\&<0\ \text{(by Lemma 3.4)}.\end{aligned}$$

Then $f(x,x,x,\alpha)<0$ for $7\le x\le 10$ and $\alpha\in(0,0.5]$.

Similarly, for $x=3,4,5,6$ and $\alpha\in(0,0.5]$, by Lemma 3.4, we have

- $f(3,3,3,\alpha) = \left(\frac{4}{9}\right)^{\alpha} + \frac{1}{3}\left(\frac{2}{3}\right)^{\alpha} - \frac{4}{3}\left(\frac{1}{2}\right)^{\alpha} < 0,$
- $f(4,4,4,\alpha) = \left(\frac{3}{8}\right)^{\alpha} + \frac{1}{2}\left(\frac{3}{4}\right)^{\alpha} - \frac{3}{2}\left(\frac{1}{2}\right)^{\alpha} < 0,$
- $f(5,5,5,\alpha) = \left(\frac{8}{25}\right)^{\alpha} + \frac{3}{5}\left(\frac{4}{5}\right)^{\alpha} - \frac{8}{5}\left(\frac{1}{2}\right)^{\alpha} < 0,$
- $f(6,6,6,\alpha) = \left(\frac{5}{18}\right)^{\alpha} + \frac{2}{3}\left(\frac{5}{6}\right)^{\alpha} - \frac{5}{3}\left(\frac{1}{2}\right)^{\alpha} < 0.$

Thus the proof is now complete. ■

Lemma 3.7 Let $h(x,\alpha) = \frac{\alpha(2-x)}{x}\left(\frac{2x-2}{x^2}\right)^{\alpha-1}$, where $\alpha \in (0.5, 1)$ and $x \geq 6$. Then $h_\alpha(x,\alpha)$ is strictly increasing in x.

Proof. Consider the derivative $h(x,\alpha)$ with respect to α.

$$h_\alpha(x,\alpha) = \frac{\alpha(2-x)}{x}\left(\frac{2x-2}{x^2}\right)^{\alpha-1}\ln\frac{2x-2}{x^2} + \frac{2-x}{x}\left(\frac{2x-2}{x^2}\right)^{\alpha-1}$$

$$= \frac{2-x}{x}\left(\frac{2x-2}{x^2}\right)^{\alpha-1}\left(\alpha\ln\frac{2x-2}{x^2}+1\right).$$

Then

$$h_{\alpha x}(x,\alpha) = \frac{-2}{x^2}\left(\frac{2x-2}{x^2}\right)^{\alpha-1}\left(\alpha\ln\frac{2x-2}{x^2}+1\right) + \frac{\alpha(2-x)(4-2x)}{x^2(2x-2)}\left(\frac{2x-2}{x^2}\right)^{\alpha-1}$$

$$+ \frac{(\alpha-1)(2-x)(4-2x)}{x^4}\left(\frac{2x-2}{x^2}\right)^{\alpha-2}\left(\alpha\ln\frac{2x-2}{x^2}+1\right)$$

$$= \left(\frac{2x-2}{x^2}\right)^{\alpha-1}\left(\alpha\ln\frac{2x-2}{x^2}+1\right)\frac{(\alpha-1)(2-x)(4-2x)-2(2x-2)}{x^2(2x-2)}$$

$$+ \left(\frac{2x-2}{x^2}\right)^{\alpha-1}\frac{\alpha(2-x)(4-2x)}{x^2(2x-2)}$$

$$= \left(\frac{2x-2}{x^2}\right)^{\alpha-1}\frac{1}{x^2(2x-2)}\Bigg\{\left(\alpha\ln\frac{2x-2}{x^2}+1\right)$$

$$\left[2(\alpha-1)(x-2)^2-4(x-1)\right]+2\alpha(x-2)^2\Bigg\}.$$

For $x \geq 6$, we have $\alpha\ln\frac{2x-2}{x^2}+1 < 1-\frac{6\alpha}{5}$, and

$$\left[2(\alpha-1)(x-2)^2-4(x-1)\right]\left(\alpha\ln\frac{2x-2}{x^2}+1\right)+2\alpha(x-2)^2$$

$$
\begin{aligned}
&> \left(1-\frac{6\alpha}{5}\right)\left[2(\alpha-1)(x-2)^2-4(x-1)\right]+2\alpha(x-2)^2\\
&= \frac{2(-6\alpha^2+16\alpha-5)}{5}(x-2)^2-\frac{4(5-6\alpha)}{5}(x-1)\\
&> \frac{3}{5}(x-2)^2-\frac{8}{5}(x-1) \quad (\text{for } 0.5<\alpha<1)\\
&= \frac{1}{5}(3x^2-20x+20)>0 \quad (\text{for } x\geq 6).
\end{aligned}
$$

Thus $h_{\alpha x}(x,\alpha)>0$ for $x\geq 6$ and $\alpha\in(0.5,1)$, the result follows. ■

Lemma 3.8 Let $P(x,\alpha)=\left(\frac{x-1}{x}\right)^{\alpha}\left[1+\frac{\alpha(x-2)}{2(x-1)}\right]$, where $x\geq 3$ and $\alpha\in(0.5,1)$. Then $P_{\alpha}(x,\alpha)$ is strictly increasing in x.

Proof. By directed calculation,

$$P_{\alpha}(x,\alpha)=\left(\frac{x-1}{x}\right)^{\alpha}\left\{\ln\frac{x-1}{x}\left[1+\frac{\alpha(x-2)}{2(x-1)}\right]+\frac{x-2}{2(x-1)}\right\}.$$

Then

$$
\begin{aligned}
P_{\alpha x}(x,\alpha) &= \alpha\left(\frac{x-1}{x}\right)^{\alpha-1}\frac{1}{x^2}\left\{\ln\frac{x-1}{x}\left[1+\frac{\alpha(x-2)}{2(x-1)}\right]+\frac{x-2}{2(x-1)}\right\}\\
&\quad +\left(\frac{x-1}{x}\right)^{\alpha}\left\{\frac{1}{x(x-1)}\left[1+\frac{\alpha(x-2)}{2(x-1)}\right]+\frac{\alpha}{2(x-1)^2}\ln\frac{x-1}{x}+\frac{1}{2(x-1)^2}\right\}\\
&= \frac{(x-1)^{\alpha-1}}{x^{\alpha+1}}\left\{\left(\alpha\ln\frac{x-1}{x}+1\right)\left[1+\frac{\alpha(x-2)}{2(x-1)}\right]+\frac{\alpha(x-2)}{2(x-1)}\right\}+\\
&\qquad \frac{(x-1)^{\alpha-2}}{2x^{\alpha}}\left(\alpha\ln\frac{x-1}{x}+1\right).
\end{aligned}
$$

For $\alpha\in(0.5,1)$, $x\geq 3$, we have $-\frac{1}{\alpha}<-1$ and $\frac{x-1}{x}\geq\frac{2}{3}$. It follows that $-\frac{1}{\alpha}<-1<\ln\frac{x-1}{x}$. Thus $\alpha\ln\frac{x-1}{x}+1>0$. Since $\frac{\alpha(x-2)}{2(x-1)}>0$, we have $P_{\alpha x}(x,\alpha)>0$ for $\alpha\in(0.5,1)$ and $x\geq 3$.

The result follows. ■

Lemma 3.9 Let x,y and Δ be positive integers with $3\leq x\leq y\leq\Delta$. Then $f(x,x,x,\alpha)<0$ for $\alpha\in(0.5,1)$.

Proof. Note that

$$f(x,x,x,\alpha)=\left(\frac{2x-2}{x^2}\right)^{\alpha}+2\left[\left(\frac{1}{2}\right)^{\alpha}-\left(\frac{x-1}{x}\right)^{\alpha}\right]\left(\frac{1}{x}-\frac{1}{2}\right)-\left(\frac{1}{2}\right)^{\alpha}.$$

Then

$$f_x(x,x,x,\alpha) = \alpha\left(\frac{2x-2}{x^2}\right)^{\alpha-1}\frac{4-2x}{x^3} - \frac{2\alpha}{x^2}\left(\frac{x-1}{x}\right)^{\alpha-1}\left(\frac{1}{x}-\frac{1}{2}\right)$$
$$-\frac{2}{x^2}\left[\left(\frac{1}{2}\right)^{\alpha} - \left(\frac{x-1}{x}\right)^{\alpha}\right]$$
$$= \frac{2}{x^2}\left\{\left(\frac{2x-2}{x^2}\right)^{\alpha-1}\frac{\alpha(2-x)}{x} + \left(\frac{x-1}{x}\right)^{\alpha}\left[1+\frac{\alpha(x-2)}{2(x-1)}\right] - \left(\frac{1}{2}\right)^{\alpha}\right\}$$
$$= \frac{2}{x^2}\left[h(x,\alpha)+P(x,\alpha)-\left(\frac{1}{2}\right)^{\alpha}\right].$$

Let $J(x,\alpha) = h(x,\alpha)+P(x,\alpha)-\left(\frac{1}{2}\right)^{\alpha}$. For $x=3$, we have

$$J(3,\alpha) = -\frac{\alpha}{3}\left(\frac{4}{9}\right)^{\alpha-1} + \left(\frac{2}{3}\right)^{\alpha}\left(1+\frac{\alpha}{4}\right) - \left(\frac{1}{2}\right)^{\alpha},$$

and

$$J_\alpha(3,\alpha) = -\frac{1}{3}\left(\frac{4}{9}\right)^{\alpha-1}\left(\alpha\ln\frac{4}{9}+1\right) + \left(\frac{2}{3}\right)^{\alpha}\left[\ln\frac{2}{3}\left(1+\frac{\alpha}{4}\right)+\frac{1}{4}\right] - \left(\frac{1}{2}\right)^{\alpha}\ln\frac{1}{2}.$$

By the value of $J_\alpha(3,\alpha)$ for $\alpha\in(0.5,1)$ (shown in Fig.4), we have $J_\alpha(3,\alpha)>0$.

Similarly, for $x=4,5,6$, we get $J_\alpha(x,\alpha)>0$ (shown in Fig.5,6,7).

For $x>6$, by Lemmas 3.7, 3.8, we obtain $J_\alpha(x,\alpha)>J_\alpha(6,\alpha)>0$ for $\alpha\in(0.5,1)$. Then $J_\alpha(x,\alpha)>0$ for $x\geq 3$ and $\alpha\in(0.5,1)$.

Thus $J(x,\alpha)<J(x,1)=0$ for $x\geq 3$ and $\alpha\in(0.5,1)$. Then $f_x(x,x,x,\alpha)<0$, and

$$f(x,x,x,\alpha)\leq f(3,3,3,\alpha) = \left(\frac{4}{9}\right)^{\alpha} + \frac{1}{3}\left(\frac{2}{3}\right)^{\alpha} - \frac{4}{3}\left(\frac{1}{2}\right)^{\alpha}.$$

Using Lemma 3.5, we get $f(x,x,x,\alpha)\leq f(3,3,3,\alpha)<0$ for $\alpha\in(0.5,1)$.

The result follows. ■

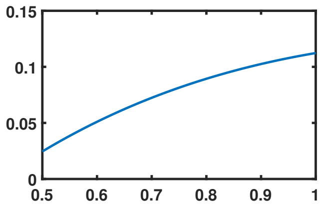

Fig.4. The value of $J_\alpha(3,\alpha)$ for $\alpha\in(0.5,1)$.

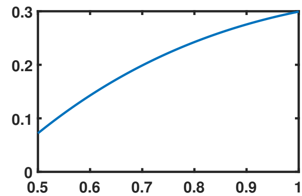

Fig.5. The value of $J_\alpha(4,\alpha)$ for $\alpha\in(0.5,1)$.

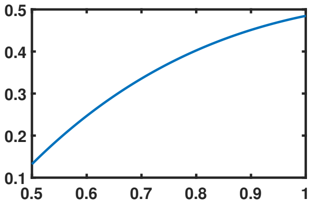

Fig.6. The value of $J_\alpha(5,\alpha)$ for $\alpha \in (0.5, 1)$.

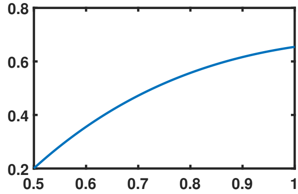

Fig.7. The value of $J_\alpha(6,\alpha)$ for $\alpha \in (0.5, 1)$.

Lemma 3.10 Let x, y and Δ be positive integers with $x \leq y \leq \Delta$ and $\Delta \geq 3$. Then $f(x, y, \Delta, \alpha) < 0$ for $(x, y) \notin \{(1, \Delta), (2, \Delta)\}$ and $\alpha \in (0, 1)$.

Proof. For $x = 1, 2$ and $\alpha \in (0, 1)$, by similar arguments as in the proof of Lemma 2.7, we have

$$f(1, y, \Delta, \alpha) = \left(\frac{y-1}{y}\right)^\alpha - \left(\frac{\Delta-1}{\Delta}\right)^\alpha + \left[\left(\frac{1}{2}\right)^\alpha - \left(\frac{\Delta-1}{\Delta}\right)^\alpha\right]\left(\frac{2}{y} - \frac{2}{\Delta}\right) < 0,$$

and

$$f(2, y, \Delta, \alpha) = 2\left[\left(\frac{1}{2}\right)^\alpha - \left(\frac{\Delta-1}{\Delta}\right)^\alpha\right]\left(\frac{2}{y} - \frac{2}{\Delta}\right) < 0.$$

For $x \geq 3$ and $\alpha \in (0, 0.5]$, one can get the result from Lemmas 3.2, 3.6. And for $\alpha \in (0.5, 1)$, one can obtain the result from Lemmas 3.2, 3.9.

The lemma follows. ■

Now we can establish an upper bound on $ABC_\alpha(G)$ in terms of n, m, Δ and α $(0 < \alpha < 1)$, where G is a connected graph with n $(n \geq 3)$ vertices, m edges and maximum degree Δ. Especially when $m \leq 2n - \dfrac{2m}{\Delta}$ and $m \equiv 0 \pmod{\Delta}$, this upper bound can be obtained if and only if $G \in \Gamma_{n,m,\Delta}$.

Theorem 3.1 Let G be a connected graph of order n, size m and maximum degree Δ, where $2 \leq \Delta \leq n - 1$ and $0 < \alpha < 1$. Then

$$ABC_\alpha(G) \leq \left(\frac{\Delta-1}{\Delta}\right)^\alpha \left(2n - m - \frac{2m}{\Delta}\right) + \left(\frac{1}{2}\right)^\alpha \left(2m - 2n + \frac{2m}{\Delta}\right)$$

with equality if and only if $G \cong P_n$ for $\Delta = 2$, and $G \in \Gamma_{n,m,\Delta}$ for $\Delta \geq 3$.

Proof. If $\Delta = 2$, then $G \cong P_n$ and the result follows.

Assume that $3 \leq \Delta \leq n - 1$. By Lemma 3.10, we have $f(x, y, \Delta, \alpha) < 0$ for all $1 \leq x \leq y \leq \Delta$ with $(x, y) \notin \{(1, \Delta), (2, \Delta)\}$ and $0 < \alpha < 1$. Since G is a connected graph with n vertices, m edges and maximum degrees Δ, by the formula (2) in Theorem 2.1, we have

$$ABC_\alpha(G) \le \left(\frac{\Delta-1}{\Delta}\right)^\alpha \left(2n-m-\frac{2m}{\Delta}\right) + \left(\frac{1}{2}\right)^\alpha \left(2m-2n+\frac{2m}{\Delta}\right)$$

with equality if and only if $a_{xy}=0$ for all $1 \le x \le y \le \Delta$ with $(x,y) \notin \{(1,\Delta),(2,\Delta)\}$, that is, $G \in \Gamma_{n,m,\Delta}$ for $\Delta \ge 3$.

This completes the proof of Theorem 3.1. □

Remark 2. By Lemma 2.8, if $m > 2n - \frac{2m}{\Delta}$ or $m \not\equiv 0 \pmod{\Delta}$, then $\Gamma_{n,m,\Delta} = \emptyset$. Thus the upper bound in Theorem 3.1 for $ABC_\alpha(G)$ cannot be obtained. So, when $m > 2n - \frac{2m}{\Delta}$ or $m \not\equiv 0 \pmod{\Delta}$ the problem of finding an sharp upper bound of ABC_α indices for $0 < \alpha < 1$ among connected graphs with fixed maximum degree remains open.

For positive integers n, m and Δ with $3 \le \Delta \le n-1 \le m$ and $m \equiv 0 \pmod{\Delta}$, let $\Phi_{n,m,\Delta}$ be the set of connected graphs with n vertices, m edges and maximum degree Δ such that $a_{xy}=0$ for all $1 \le x \le y < \Delta$. Then for $\alpha = 1$, we have the following theorem.

Theorem 3.2 Let G be a connected graph of order n, size m and maximum degree Δ, where $2 \le \Delta \le n-1$ and $\alpha = 1$. Then

$$ABC_{\alpha=1}(G) \le \frac{\Delta-1}{\Delta}\left(2n-m-\frac{2m}{\Delta}\right) + \frac{1}{2}\left(2m-2n+\frac{2m}{\Delta}\right)$$

with equality if and only if $G \cong P_n$ for $\Delta = 2$, and $G \in \Phi_{n,m,\Delta}$ for $\Delta \ge 3$.

Proof. If $\Delta = 2$, then $G \cong P_n$ and the result follows.

Assume that $3 \le \Delta \le n-1$. For $\alpha = 1$, we have

$$\begin{aligned} f(x,y,\Delta,1) &= \frac{x+y-2}{xy} + 2\left(\frac{1}{2}-\frac{\Delta-1}{\Delta}\right)\left(\frac{1}{x}+\frac{1}{y}-\frac{1}{2}-\frac{1}{\Delta}\right) - \frac{1}{2} \\ &= \frac{1}{y}+\frac{1}{x}-\frac{2}{xy} + \left(\frac{2}{\Delta}-1\right)\left(\frac{1}{x}+\frac{1}{y}-\frac{1}{2}-\frac{1}{\Delta}\right) - \frac{1}{2} \\ &= \frac{2}{x\Delta}+\frac{2}{y\Delta}-\frac{2}{xy}-\frac{2}{\Delta^2} \\ &= 2\left(\frac{1}{\Delta}-\frac{1}{y}\right)\left(\frac{1}{x}-\frac{1}{\Delta}\right). \end{aligned}$$

Note that $f(x,y,\Delta,1) < 0$ for $1 \le x \le y < \Delta$. Then by the formula (2), we obtain

$$ABC_{\alpha=1}(G) \le \frac{\Delta-1}{\Delta}\left(2n-m-\frac{2m}{\Delta}\right) + \frac{1}{2}\left(2m-2n+\frac{2m}{\Delta}\right)$$

with equality if and only if $a_{xy}=0$ for $1 \le x \le y < \Delta$, that is, $G \in \Phi_{n,m,\Delta}$.

This completes the proof of Theorem 3.2. ■

For $3 \le \Delta \le n-2$ and $n \equiv 1 \pmod{\Delta}$, let $\mathcal{T}_{n,\Delta}$ be the set of trees obtained by subdividing every edge of a tree on $\frac{n-1}{\Delta}$ vertices with maximum degree at most Δ, whose vertices are denoted by $v_1, v_2, \ldots, v_{\frac{n-1}{\Delta}}$, and then attaching some pendent vertices to v_i until the degree of v_i is equal to Δ for $i = 1, 2, ..., \frac{n-1}{\Delta}$. One can readily see that $\mathcal{T}_{n,2} = \{P_n\}$ and $\mathcal{T}_{n,n-1} = \{S_n\}$, where P_n and S_n are the path and the star on n vertices, respectively. Then by Theorems 2.1, 3.1 and 3.2, we have the following corollaries.

Corollary 3.1 Let T be a tree with n vertices and maximum degree Δ, where $2 \leq \Delta \leq n-1$. We have,

(i) if $\alpha < 0$ then

$$ABC_\alpha(T) \geq \left(\frac{\Delta-1}{\Delta}\right)^\alpha \left[n+1-\frac{2(n-1)}{\Delta}\right] + \left(\frac{1}{2}\right)^\alpha \left[\frac{2(n-1)}{\Delta} - 2\right]$$

with equality if and only if $T \cong P_n$ for $\Delta = 2$, and $T \in \mathcal{T}_{n,\Delta}$ for $\Delta \geq 3$;

(ii) if $0 < \alpha < 1$ then

$$ABC_\alpha(T) \leq \left(\frac{\Delta-1}{\Delta}\right)^\alpha \left[n+1-\frac{2(n-1)}{\Delta}\right] + \left(\frac{1}{2}\right)^\alpha \left[\frac{2(n-1)}{\Delta} - 2\right]$$

with equality if and only if $T \cong P_n$ for $\Delta = 2$, and $T \in \mathcal{T}_{n,\Delta}$ for $\Delta \geq 3$;

(iii) if $\alpha = 1$ then

$$ABC_{\alpha=1}(T) \leq \frac{\Delta-1}{\Delta} \left[n+1-\frac{2(n-1)}{\Delta}\right] + \frac{1}{2} \left[\frac{2(n-1)}{\Delta} - 2\right]$$

with equality if and only if $T \cong P_n$ for $\Delta = 2$, and $T \in \Phi_{n,n-1,\Delta}$ for $\Delta \geq 3$.

Recall that chemical trees are trees with $\Delta \leq 4$. If $\Delta = 2$, then $T \cong P_n$ and we have $ABC_\alpha(P_n) = (n-1)\left(\frac{1}{2}\right)^\alpha$. Let

$$t(n,\Delta,\alpha) = \left(\frac{\Delta-1}{\Delta}\right)^\alpha \left[n+1-\frac{2(n-1)}{\Delta}\right] + \left(\frac{1}{2}\right)^\alpha \left[\frac{2(n-1)}{\Delta} - 2\right].$$

For chemical trees, we may assume that $\Delta = 3$ or 4.

If $\alpha < 0$, then

$$\begin{aligned} t(n,\Delta,\alpha) &= -\left(\frac{\Delta-1}{\Delta}\right)^\alpha \left[\frac{2(n-1)}{\Delta} - n - 1\right] + \left(\frac{1}{2}\right)^\alpha \left[\frac{2(n-1)}{\Delta} - 2\right] \\ &= \left[\left(\frac{1}{2}\right)^\alpha - \left(\frac{\Delta-1}{\Delta}\right)^\alpha\right] \left[\frac{2(n-1)}{\Delta} - n - 1\right] + \left(\frac{1}{2}\right)^\alpha (n-1) \\ &\geq \left[\left(\frac{1}{2}\right)^\alpha - \left(\frac{3}{4}\right)^\alpha\right] \left[\frac{n-1}{2} - n - 1\right] + \left(\frac{1}{2}\right)^\alpha (n-1) \\ &= \left(\frac{3}{4}\right)^\alpha \left(\frac{n}{2} + \frac{3}{2}\right) + \left(\frac{1}{2}\right)^\alpha \left(\frac{n}{2} - \frac{5}{2}\right). \end{aligned}$$

In a similar manner, if $0 < \alpha < 1$, then

$$t(n,\Delta,\alpha) \leq \left(\frac{3}{4}\right)^\alpha \left(\frac{n}{2} + \frac{3}{2}\right) + \left(\frac{1}{2}\right)^\alpha \left(\frac{n}{2} - \frac{5}{2}\right).$$

Let $\mathcal{T}_c$ be the set of chemical trees, we have the following corollary.

Corollary 3.2 Let $T \in \mathcal{T}_c$ be a chemical tree with n vertices,

(i) if $\alpha < 0$ then

$$ABC_\alpha(T) \geq \left(\frac{3}{4}\right)^\alpha \left(\frac{n}{2}+\frac{3}{2}\right) + \left(\frac{1}{2}\right)^\alpha \left(\frac{n}{2}-\frac{5}{2}\right)$$

with equality if and only if $T \in \mathcal{T}_{n,4}$;

(ii) if $0 < \alpha < 1$ then

$$ABC_\alpha(T) \leq \left(\frac{3}{4}\right)^\alpha \left(\frac{n}{2}+\frac{3}{2}\right) + \left(\frac{1}{2}\right)^\alpha \left(\frac{n}{2}-\frac{5}{2}\right)$$

with equality if and only if $T \in \mathcal{T}_{n,4}$;

(iii) if $\alpha = 1$ then

$$ABC_{\alpha=1}(T) \leq \frac{5n}{8} - \frac{1}{8}$$

with equality if and only if $T \in \Phi_{n,n-1,4} \cap \mathcal{T}_c$.

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