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Maximum atom-bond connectivity index with given graph parameters[☆]

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ABSTRACT

The atom-bond connectivity (ABC) index is a degree-based topological index. It was introduced due to its applications in modeling the properties of certain molecular structures and has been since extensively studied. In this note, we examine the influence on the extremal values of the ABC index by various graph parameters. More specifically, we consider the maximum ABC index of connected graphs of given order, with fixed independence number, number of pendent vertices, chromatic number and edge-connectivity respectively. We provide characterizations of extremal structures as well as some conjectures. Numerical analysis of the extremal values is also presented.

1. Introduction and preliminaries

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, the degree of u, denoted by $d(u)$, is the number of neighbors of u in G. An independent set is a set of vertices of which no pair is adjacent. The independence number $\beta(G)$ of a graph G is the size of a largest independent set of G. The chromatic number $\chi(G)$ of a graph G is the least number of colors assigned to $V(G)$ such that no adjacent elements receive the same color. The edge connectivity $k(G)$ of a graph G is the minimum number of edges needed to disconnect G.

The atom bond connectivity (ABC) index of G is defined [8] as

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

The ABC index is one of many so called topological indices that are extensively used in theoretical chemistry to correlate physico-chemical properties with the molecular structures of chemical compounds. It appears that the ABC index shows

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a strong correlation with heat of formation of alkanes [8]. Some topological approaches were also developed based on the ABC index to explain the differences in the energy of linear and branched alkanes [7].

In the study of topological indices in general, it is often of interest to consider the extremal values of a certain index among graphs under various constrains. Along this line, the extremal values of the ABC index have been extensively explored [2–6,9–16].

We intend to expand this study by exploring the maximum ABC index of connected graphs of given order, with fixed independence number, number of pendent vertices, edge-connectivity, and chromatic number respectively. First we will introduce some simple but useful facts.

Theorem 1.1 ([1]). *Let G be a graph with n vertices, if $x, y \in V(G)$ and $xy \in E(\overline{G})$, then*

$$ABC(G) \leqslant ABC(G + xy)$$

with equality if and only if x and y are both isolated vertices. Furthermore,

$$ABC(G) \leqslant ABC(K_n)$$

with equality if and only if $G = K_n$.

To simplify notations, we define the following functions:

- $f(x, y) = \sqrt{\frac{x+y-2}{xy}}$;
- $g(x, y) = f(x + 1, y) - f(x, y)$;
- $F(x) = xf(x + m, 1)$,

for $x, y, m \geq 1$.

Lemma 1.2 ([14]). *For the function $f(x, y)$ we have:*

- *$f(x, 1)$ is strictly increasing with respect to x;*
- *$f(x, 2) = \frac{\sqrt{2}}{2}$;*
- *$f(x, y)$ is strictly decreasing with respect to x for any fixed $y \geq 3$.*

Lemma 1.3 ([4,14]). *The function $g(x, y)$ is strictly decreasing with respect to x if $y = 1$, and increasing with respect to x if $y \geq 2$.*

Lemma 1.4. *The function $F(x)$ is convex and strictly increasing for $x \geq 1$. As a result of the convexity we have*

$$F(x_1 + 1) - F(x_1) > F(x_2) - F(x_2 - 1)$$

if $x_1 \geq x_2 \geq 1$.

Proof. Note that $F(x) = xf(x + m, 1) = x\sqrt{\frac{x+m-1}{x+m}}$, then we have

$$\begin{aligned} F'(x) &= \sqrt{\frac{x+m-1}{x+m}} + \frac{x}{2} \cdot \sqrt{\frac{x+m}{x+m-1}} \cdot \frac{1}{(x+m)^2} \\ &= \sqrt{\frac{x+m-1}{x+m}} \left(1 + \frac{1}{2} \cdot \frac{x}{(x+m-1)(x+m)}\right) > 0 \end{aligned}$$

and

$$\begin{aligned} F''(x) &= \frac{1}{2} \cdot \sqrt{\frac{x+m}{x+m-1}} \cdot \frac{1}{(x+m)^2} \left(1 + \frac{1}{2}\left(\frac{m}{x+m} - \frac{m-1}{x+m-1}\right)\right) \\ &\quad + \sqrt{\frac{x+m-1}{x+m}} \left(-\frac{m}{2(x+m)^2} + \frac{m-1}{2(x+m-1)^2}\right) \\ &= \sqrt{\frac{x+m-1}{x+m}} \left(\frac{1 + \frac{1}{2}\left(\frac{m}{x+m} - \frac{m-1}{x+m-1}\right)}{2(x+m-1)(x+m)} - \frac{m}{2(x+m)^2} + \frac{m-1}{2(x+m-1)^2}\right) \\ &= \frac{(4m-1)x + 4m(m-1)}{4(x+m)^{\frac{5}{2}}(x+m-1)^{\frac{3}{2}}} > 0 \end{aligned}$$

when $x, m \geq 1$. □

Lemma 1.5. *Let $G(a, b) = f(a, b - 1) - f(a - 1, b)$ for some $a > b > 0$. Then $G(a, b) > 0$.*

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