Remarks on maximum atom-bond connectivity index with given graph parameters

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Abstract

The atom-bond connectivity (ABC) index is a degree-based molecular structure descriptor that can be used for modelling thermodynamic properties of organic chemical compounds. Motivated by its applicable potential, a series of investigations have been carried out in the past several years. In this note we first consider graphs with given edge-connectivity that attain the maximum ABC index. In particular, we give an affirmative answer to the conjecture about the structure of graphs with edge-connectivity equal to one that maximize the ABC index, which was recently raised by Zhang, Yang, Wang and Zhang \cite{33}. In addition, we provide supporting evidence for another conjecture posed by the same authors which concerns graphs that maximize the ABC index among all graphs with chromatic number equal to some fixed $\chi \geq 3$. Specifically, we confirm this conjecture in the case where the order of the graph is divisible by $\chi$.

1 Introduction

Let $G$ be a simple undirected graph of order $n = |V(G)|$ and size $m = |E(G)|$. For $v \in V(G)$, let $d_G(v)$ denote the degree of $v$, that is, the number of edges incident to $v$. The atom-bond connectivity (ABC) index is defined as

$$\text{ABC}(G) = \sum_{uv \in E(G)} f(d(u), d(v)),$$

where $f(d(u), d(v)) = \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$.

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The ABC index was introduced in 1998 by Estrada, Torres, Rodríguez and Gutman [17], who showed that this index correlates well with the heats of formation of alkanes and can therefore serve the purpose of predicting their thermodynamic properties. Various physico-chemical applications of the ABC index were presented in a few other works, including [16,23]. These results triggered a number of mathematical and computational investigations into the ABC index and its extension [1,3–15,18–22,24,26–32]. For recent advances in chemical graph theory, one may consult the following two surveys [2,25].

Recently, in [33] the maximum ABC index across all connected graphs of a given order, with a fixed independence number, number of pendant vertices, chromatic number or edge-connectivity was considered. There, among other results, an upper bound and a characterization of graphs with a given edge-connectivity \( k \geq 2 \) that attain the maximum ABC index was given. Before we state this result, we need the following definitions:

• Given two disjoint graphs \( G \) and \( H \) with disjoint vertex sets \( V(G) \) and \( V(H) \) and disjoint edge sets \( E(G) \) and \( E(H) \), the disjoint union of \( G \) and \( H \) is the graph \( G + H \) with vertex set \( V(G) \cup V(H) \) and edge set \( E(G) \cup E(H) \).

• The join of two simple undirected graphs \( G \) and \( H \) is the graph \( G \vee H \) with vertex set \( V(G \vee H) = V(G) \cup V(H) \) and edge set \( E(G \vee H) = E(G) \cup E(H) \cup \{uv : u \in V(G), v \in V(H)\} \).

• The chromatic number \( \chi(G) \) of a graph \( G \) is the smallest number of colours needed to colour the vertices of \( G \) in such a way that no two adjacent vertices are coloured the same.

Let \( K_n(k) \) denote the graph \( K_k \vee (K_1 + K_{n-k-1}) \). Observe that the graph \( K_n(k) \) is simply a graph obtained by joining one vertex to \( k \) vertices in \( K_{n-1} \). An illustration of \( K_6(3) \) is depicted in Figure 1.

Let \( T_{n,l} \) denote a complete \( l \)-partite graph of order \( n \) with \( \left| t_i - t_j \right| \leq 1 \), where \( t_i, i = 1, 2, \ldots, l \), is the number of vertices in the \( i \)-th partition set of \( T_{n,l} \).

The following result about graphs with prescribed edge-connectivity that attain the maximum ABC index was obtained by Zhang, Yang, Wang and Zhang in [33].

**Theorem 1.1.** Let \( G \) be a connected graph on \( n \geq 6 \) vertices with edge-connectivity \( k \geq 2 \). Then,

\[
\text{ABC}(G) \leq k \sqrt{\frac{n+k-3}{k(n-1)}} + \frac{k(k-1)}{2(n-1)} \sqrt{2n-4} + \frac{(n-k-1)(n-k-2)}{2(n-2)} \sqrt{2n-6} + \frac{k(n-k-1)}{(n-1)(n-2)} \frac{2n-5}{\sqrt{2n-6}}
\]

with equality if and only if \( G \cong K_n(k) \).

In [33] it was conjectured that Theorem 1.1 also holds for \( k = 1 \). In addition, in the same paper, the following theorem and a conjecture related to it were posed.
Theorem 1.2. For any connected graph $G$ of order $n$ with chromatic number $\chi = 2$:

- if $n$ is even, then $\text{ABC}(G) \leq \frac{n}{2} \sqrt{n - 2}$ with equality if and only if $G \cong T_{n,2}$;
- if $n$ is odd, then $\text{ABC}(G) \leq \frac{1}{2} \sqrt{(n - 2)(n^2 - 1)}$ with equality if and only if $G \cong T_{n,2}$.

Conjecture 1.1. Let $G$ be an $n$-vertex connected graph with chromatic number $\chi \geq 3$. Then,

$$\text{ABC}(G) \leq \text{ABC}(T_{n,\chi}),$$

with equality if and only if $G \cong T_{n,\chi}$.

Before we affirm the conjecture related to Theorem 1.1 and prove a special case of Conjecture 1.1, we state a few auxiliary results. Namely, adding an edge to a graph strictly increases its ABC index [7] or, equivalently, removing an edge from a graph strictly decreases it [4]. This has the following immediate consequence.

Corollary 1.3. Among all connected graphs with $n$ vertices, the maximum value of the ABC index is attained exactly by the complete graph $K_n$.

The subsequent result plays an important role in the next section, where we prove the first of the aforementioned conjectures.

Theorem 1.4. [Karamata’s inequality] Let $U \subseteq \mathbb{R}$ be an open interval and $f : U \to U$ a convex function. Let $a_1 \geq a_2 \geq \cdots \geq a_n$ and $b_1 \geq b_2 \geq \cdots \geq b_n$ be such elements in $U$ that inequalities $a_1 + a_2 + \cdots + a_i \geq b_1 + b_2 + \cdots + b_i$ hold for every $i \in \{1, 2, \ldots, n\}$ and equality holds for $i = n$. Then, $f(a_1) + f(a_2) + \cdots + f(a_n) \geq f(b_1) + f(b_2) + \cdots + f(b_n)$.

2 Graphs with edge-connectivity one that maximize the ABC index

Theorem 2.1. Let $G$ be a graph with the maximum atom-bond connectivity index among all graphs with $n$ vertices and edge-connectivity 1. Then, $G \cong K_n(1)$.

Proof. Let $e = uv$ be an edge of $G$ whose deletion disconnects $G$ into two connected components with $x$ and $y = n - x$ vertices, respectively. Since $G$ maximizes the ABC index, it follows by Corollary 1.3 that these two components must be complete subgraphs $K_x$ and $K_y$. Let $u \in V(K_x)$ and $v \in V(K_y)$. Due to symmetry, we may assume that the possible values of $x$ are $1, 2, \ldots, \lfloor n/2 \rfloor$.

If $x = 1$, then the theorem holds. If $x = 2$, then $K_x$ is comprised of one edge, denoted here by $wu$. Now, we add edges between $u$ and every vertex of $V(K_y) \setminus \{v\}$, thus obtaining a graph $G'$ which is comprised of $K_1$ and $K_{n-1}$ and the edge $wu$ that connects them. Corollary 1.3 implies that $\text{ABC}(G') > \text{ABC}(G)$.

For $x \geq 3$ it holds that

$$\text{ABC}(G) = \left(\frac{x - 1}{2}\right)f(x - 1, x - 1) + (x - 1)f(x - 1, x) + f(x, y)$$

$$+ \left(\frac{y - 1}{2}\right)f(y - 1, y - 1) + (y - 1)f(y - 1, y).$$

Let $w$ be a vertex in $V(K_x)$ different from $u$. Let $G'$ be a graph obtained from $G$ by deleting all edges adjacent to $w$ and adding edges between $w$ and each vertex in $V(K_y)$. It follows that

$$\text{ABC}(G') = \left(\frac{x - 2}{2}\right)f(x - 2, x - 2) + (x - 2)f(x - 2, x - 1) + f(x - 1, y + 1)$$

$$+ \left(\frac{y - 1}{2}\right)f(y - 1, y - 1) + (y - 1)f(y - 1, y).$$
\begin{align*}
  + \left( \frac{y}{2} \right) f(y, y) + yf(y, y + 1).
\end{align*}

For \( z > 1 \), let
\[
  s(z) = \left( \frac{z}{2} \right) f(z, z) + zf(z, z + 1).
\]

Next, we show that the function \( s(z) \) is convex. After simplification, the second derivative of \( s(z) \) reads
\[
  s''(z) = \frac{1}{8} \left( \frac{3\sqrt{2}}{\sqrt{z - 1}} + \frac{24}{(z + 1)^{5/2} \sqrt{z(2z-1)}} - \frac{2(1-2z(z+2))^2}{(z+1)^{5/2}(2z-1)^{3/2}} \right).
\]

The expression \( 24/((z+1)^{5/2}/\sqrt{z(2z-1)}) \) is positive for \( z > 1 \). The remainder is positive as well, which can be shown by comparing the square of the minuend to the square of the subtrahend (notice that both the minuend and the subtrahend are positive). More precisely, after clearing denominators, we need to show that
\[
  18(z+1)^5(2z^2-z)^3 > 4(1-2z^2-4z)^4(z-1)
\]
holds for all \( z > 1 \). Clearly, \( (z+1) > (z-1) \) is satisfied, and the inequality \( (2z^2-z) > (1-2z^2-4z) \) follows immediately from
\[
  2z^2-z-1+2z^2+4z = 4z^2+3z-1 = (4z-1)(z+1) > 0.
\]
It now suffices to show that \((z+1)^2 > (1-2z^2-4z)\) holds. Since
\[
  z^2+2z+1-1+2z^2+4z = 3z^2+6z > 0,
\]
we finally conclude that \( s''(z) \) is positive, and thus that \( s(z) \) is a convex function.

Consider now the difference \( \text{ABC}(G') - \text{ABC}(G) \). It holds that
\[
  \text{ABC}(G') - \text{ABC}(G) = s(x-2) + f(x-1, y+1) + s(y) - s(x-1) - f(x, y) - s(y-1).
\]

Recall that the range of values of \( x \) is \( 1, 2, \ldots, \lfloor n/2 \rfloor \), which implies \( y \geq x \). Under this constraint, a straightforward verification shows that
\[
  f(x-1, y+1) > f(x, y). \tag{1}
\]

Since \( y > y-1 \) and \( y + (x-2) = (y-1) + (x-1) \) and the function \( s \) is convex, it follows by Theorem \([1,3]\) that
\[
  s(y) + s(x-2) \geq s(y-1) + s(x-1). \tag{2}
\]

Inequalities \([1]\) and \([2]\) imply the validity of \( \text{ABC}(G') - \text{ABC}(G) > 0 \), which concludes the proof of the theorem.

As the class of \( k \)-vertex-connected graphs is a subclass of the class of \( k \)-edge-connected graphs where \( k \geq 1 \), and as \( K_n(k) \) is a \( k \)-vertex-connected graph, we may conclude from Theorems \([1,1]\) and \([2,1]\) that a graph that maximizes the ABC index among all \( k \)-edge-connected graphs also maximizes the ABC index among all \( k \)-vertex-connected graphs.

**Corollary 2.2.** Let \( G \) be a graph with the maximum atom-bond connectivity index among all graphs with \( n \) vertices and vertex-connectivity \( k \geq 1 \). Then, \( G \cong K_n(k) \).
3 Graphs with chromatic number $\chi$ that maximize the ABC index

In this section, we prove a special case of Conjecture 1.1. Specifically, we show that this conjecture holds when $\chi$ divides $n$.

**Theorem 3.1.** Let $G$ be an $n$-vertex connected graph with chromatic number $\chi \geq 2$ and suppose that $\chi$ divides $n$. Then,

$$\text{ABC}(G) \leq \text{ABC}(T_{n,\chi}),$$

with equality if and only if $G \cong T_{n,\chi}$.

**Proof.** As the case $\chi = 2$ has already been proven in [33], we may assume from now on that $\chi \geq 3$.

Consider a $\chi$-colouring of $G$ and denote by $t_i$ the size of the $i$-th colour class, that is, the number of vertices that are assigned the $i$-th colour for $i = 1, 2, \ldots, \chi$.

First of all, since adding an edge to a graph strictly increases its ABC index, notice that

$$\text{ABC}(G) \leq \sum_{i<j} t_it_j \frac{2n-t_i-t_j-2}{(n-t_i)(n-t_j)} = \sum_{i<j} \frac{t_it_j}{\sqrt{n-t_i\sqrt{n-t_j}}} \sqrt{2n-(t_i+t_j)-2}. \quad (3)$$

Write $x_{ij}$ and $y_{ij}$ as an abbreviation for the first factor and the second factor on the right-hand side, respectively, i.e.,

$$x_{ij} = \frac{t_it_j}{\sqrt{n-t_i\sqrt{n-t_j}}} \quad \text{and} \quad y_{ij} = \sqrt{2n-(t_i+t_j)-2}.$$

Observe now that the right-hand side of $(3)$ is equivalent to the standard scalar product $\langle x, y \rangle$ of vectors $x := (x_{ij})_{i<j}$ and $y := (y_{ij})_{i<j}$ of length $(\binom{\chi}{2})$. Thus, by the Cauchy-Schwarz inequality,

$$\text{ABC}(G) \leq |\langle x, y \rangle| \leq \|x\|\|y\|. \quad (4)$$

In the following, we show that this upper bound on ABC($G$) is attained exactly whenever $t_i = n/\chi$ for all $i = 1, 2, \ldots, \chi$ and every vertex has degree $n - n/\chi$ (this follows from maximizing the number of edges); that is, by $T_{n,\chi}$, as claimed.

Note that the equality $|\langle x, y \rangle| = \|x\|\|y\|$ in $(4)$ holds if and only if $x$ and $y$ are linearly dependent, that is, if and only if $x = \mu y$ holds for some scalar $\mu \neq 0$. Hence, if and only if

$$\mu = x_{ij}/y_{ij} = \frac{t_it_j}{\sqrt{n-t_i\sqrt{n-t_j}}} \left(\sqrt{2n-(t_i+t_j)-2}\right)^{-1}$$

for each pair of indices $i < j$.

Take indices $i, j, k$ such that $1 \leq i < j < k \leq \chi$. From $\mu = x_{ij}/y_{ij} = x_{ik}/y_{ik}$ it follows that

$$t_j^2(n-t_k)(2n-(t_i+t_k)-2) = t_i^2(n-t_j)(2n-(t_i+t_j)-2).$$

One finds that $t_j = t_k$ must hold. If not, then $t_j > t_k$ (or vice versa), which implies $n-t_k > n-t_j$ and $2n-t_i-t_k - 2 > 2n-t_i-t_j - 2$. Hence, as these terms are all non-zero, the left-hand side is strictly greater than the right-hand side, which leads to a contradiction.

Since $i, j$ and $k$ were chosen arbitrarily, this establishes that $t_1 = t_2 = \cdots = t_\chi$ and thus, since $\sum_{i=1}^\chi t_i = n$, it follows that $t_i = n/\chi$ for all $i = 1, 2, \ldots, \chi$, as desired. \qed

As a consequence of Theorem 3.1, we obtain the following corollary.
Corollary 3.2. Let $G$ be an $n$-vertex connected graph with chromatic number $\chi \geq 2$ and suppose that $\chi$ divides $n$. Then,

$$ABC(G) \leq n\sqrt{\frac{\chi(n-1)-n}{2\chi}},$$

with equality if and only if $G \cong T_{n,\chi}$.

Proof. Let us now compute the upper bound (4) on $ABC(G)$. The calculation of $\|y\|$ is straightforward (and its value is independent of $t_i$):

$$\|y\|^2 = \sum_{i<j}(2n - (t_i + t_j) - 2) = 2n\left(\frac{\chi}{2}\right) - (\chi - 1)n - 2\left(\frac{\chi}{2}\right) = (\chi - 1)(\chi(n - 1) - n).$$

We proceed by evaluating the expression $\|x\|$ at $t_i = n/\chi$:

$$\|x\|^2 = \frac{n^2}{2\chi(\chi - 1)}.$$

Thus, combining these statements and plugging them in (4), we find that

$$ABC^2(G) \leq \frac{(\chi - 1)(\chi(n - 1) - n)n^2}{2\chi(\chi - 1)} = \frac{n^2(\chi(n - 1) - n)}{2\chi}.$$

Notice that this upper bound is attained if and only if $G \cong T_{n,\chi}$, which concludes the proof. \qed

4 Concluding comments

In this note we consider graphs with given edge-connectivity that attain the maximum ABC index. The case where the connectivity is greater or equal to two was solved in [33]. Here we resolve the remaining case where edge-connectivity equals one. The authors of [33] also posed a conjecture about the structure of graphs with chromatic number equal to some fixed $\chi \geq 3$ that maximize the ABC index. Herein we confirm a special case of this conjecture, more specifically, the case where the order of the graph is divisible by $\chi$.

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