Applied Mathematics, Modeling and Computer Simulation
C.-H. Chen et al. (Eds.)

doi:10.3233/ATDE240807

Proof of a Conjecture on the Minimum ABS Index of Bicyclic Graphs

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Abstract. The atom-bond sum-connectivity (ABS) index of a connected graph $G=(V,E)$ is defined as $ABS(G)=\sum_{uv\in E}\sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$, where $d(w)$ is the degree of vertex $w\in V$. It was shown that this recently proposed topological index has comparable predictive applicability in chemistry with some famous indices, such as the Randić index, sum-connectivity index, and atom-bond connectivity index. Recently, the chemical bicyclic graphs with minimum ABS index were characterized. It was conjectured that this result also holds for general bicyclic graphs. We confirm this conjecture in the present paper.

Keywords. Bicyclic graphs, Extremal graphs, Atom-bond sum-connectivity index, Lower bound

1. Introduction

Let G be a connected simple graph with vertex set $V=\{v_1,v_2,\dots,v_n\}$ and edge set E. If $|E|=n-1+c$, then G is called a c-cyclic graph. A 2-cyclic graph is also called a bicyclic graph. Denote by $N(v_i)$ the neighbor set of v_i, and by $d_i=d(v_i)=|N(v_i)|$ the degree of v_i. Let $\Delta(G)$ denote the maximum degree of G. If $\Delta(G)\le 4$, G is called a chemical graph. A pendent vertex of G is a vertex of degree one. The (non-increasing) degree sequence of G is $\pi(G)=(d_1,d_2,\dots,d_n)$ (with $d_1\ge d_2\ge\cdots\ge d_n$). Denote by $\mathcal{C}(\pi)$ the set of connected graphs with degree sequence π.

Let $f(x,y)=\sqrt{(x+y-2)/(x+y)}$, where $x,y\ge 1$. Recently Ali et al. [1] introduced the atom-bond sum-connectivity (ABS) index of G as $ABS(G)=\sum_{v_iv_j\in E} f(d_i,d_j)$. The chemical applicability of this topological index was examined in [2–5] on several data sets. It turns out that the predictive applicability of the ABS index is comparable to those of some famous indices, such as the Randić index [6], sum-connectivity index [7], and atom-bond connectivity index [8]. In the recent two years, the extremal results of the ABS index over a number of classes of graphs have been obtained. Most known results can be found in the survey [9].

For $1\le i\le j\le n-1$, let $m_{i,j}=m_{i,j}(G)=|\{uv\in E|d(u)=i,d(v)=j\}|$. Denote by $\mathcal{B}_n$ the set of bicyclic graphs of order n. Let $\mathcal{B}_n^*(\subseteq\mathcal{B}_n)$ be the set of (chemical) (bicyclic) graphs satisfying $m_{2,2}=n-4$, $m_{2,3}=4$, and $m_{3,3}=1$. Note that $\mathcal{B}_n^*\ne\emptyset$ if $n\ge 4$, and

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$|\mathcal{B}_n^*| \geq 2$ if $n \geq 6$. See the Figure 7 in [9] for examples. The chemical bicyclic graphs with minimum ABS index was characterized recently in [10]. The related result can be restated as follows.

Lemma 1.1 [10]**.** If G is a chemical bicyclic graph of order $n \geq 6$, then

$$ABS(G) \geq f(3,3) + 4f(2,3) + (n-4)f(2,2),$$

with equality iff $G \in \mathcal{B}_n^*$.

Ali et al. conjectured that, Lemma 1.1 also holds for general bicyclic graphs (the Conjecture 1 in [9]). We confirm this conjecture in the present paper. Namely, the following result will be proved.

Theorem 1.2. If G is a (chemical) bicyclic graph of order $n \geq 4$, then

$$ABS(G) \geq f(3,3) + 4f(2,3) + (n-4)f(2,2),$$

with equality iff $G \in \mathcal{B}_n^*$.

In Section 2, we consider the bicyclic graphs with given degree sequence having minimum ABS index, and Theorem 1.2 will be proved in Section 3.

2. Graphs with given degree sequence having minimum ABS index

Regard a connected graph G with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ as a rooted graph with root v_1. Let $h_i = h(v_i)$ denote the distance between v_i and v_1 in G.

Definition 2.1 [11]**.** Let G be a connected graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$. If there is a well ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ which satisfies the following conditions, then this ordering is said to be a breadth-first searching (BFS) ordering, and G is called a BFS graph.

(1) $d_1 \geq d_2 \geq \cdots \geq d_n$ and $h_1 \leq h_2 \leq \cdots \leq h_n$;

(2) Let $v \in N(u) - N(x)$ and $y \in N(x) - N(u)$ with $h(u) = h(x) = h(v) - 1 = h(y) - 1$. If $u \prec x$, then $v \prec y$.

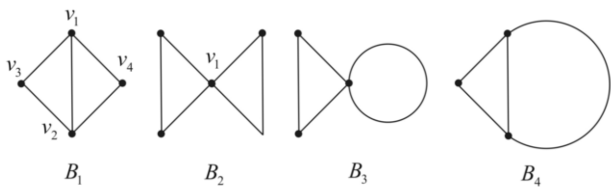

Figure 1. The four bicyclic graphs B_1, B_2, B_3, and B_4.

For a connected graph G with pendent vertices, we can recursively delete the pendent vertices of the remaining graph. The resulted graph without pendent vertices will be denoted by $\mathcal{R}(G)$. Obviously, if $c \geq 1$ and G is a c-cyclic graph, then $\mathcal{R}(G)$ is also a c-cyclic graph. A path $P = u_0u_1 \cdots u_l$ of length $l \geq 1$ of G is called a pendent path, if $d(u_0) \geq 3$, $d(u_l) = 1$, and $d(u_1) = \cdots = d(u_{l-1}) = 2$. We say some pendent paths have almost equal lengths, if their lengths differ at most 1. Let B_i, $i = 1,2,3,4$, be the four bicyclic graphs shown in Figure 1. Suppose $\pi = (d_1, d_2, \ldots, d_n)$ is the non-increasing degree sequence of a bicyclic graph. Since $\sum_{i=1}^{n} d_i = 2n+2$, π should be one of the following four cases. Define a special BFS bicyclic graph $B^*(\pi)$ as follows:

Case 1. $d_1 \geq d_2 \geq 3$ and $d_n = 1$. Let $B^*(\pi)$ be a BFS graph with $\mathcal{R}(B^*(\pi)) = B_1$;

Case 2. $d_1 \geq 5$, $d_2 = 2$, and $d_n = 1$. Let $B^*(\pi)$ be the graph of order n obtained from B_2 by attaching $d_1 - 4$ pendent paths having almost equal lengths at vertex v_1;

Case 3. $d_1 = 4$ and $d_2 = d_3 = \cdots = d_n = 2$. Let $B^*(\pi) = B_3$;

Case 4. $d_1 = d_2 = 3$ and $d_3 = d_4 = \cdots = d_n = 2$. Let $B^*(\pi) = B_4$.

For fixed $t \geq 1$, define $g_t(x,y) = f(x,y) - f(x-t,y)$, $x \geq t+1$ and $y \geq 1$. Write $g_1(x,y)$ as $g(x,y)$.

Lemma 2.2 [4, 12]**.**

(1) $f(x,y)$ strictly increases with x and y;

(2) $g_t(x,y)$ strictly decreases with x and y.

Lemma 2.3. Let $\lambda(y) = 2f(2,y) - f(1,y)$. Then $\lambda(y) \geq \lambda(3) > \lambda(2)$ for $y \geq 3$.

Proof. Since $y \geq 3$, we have $3y^4 + 2y^3 \geq 33y^2$. Hence

$$\begin{aligned}
&\lambda'(y) = \frac{2}{\sqrt{y}(y+2)^{\frac{3}{2}}} - \frac{1}{\sqrt{y-1}(y+1)^{\frac{3}{2}}} > 0 \\
&\Leftrightarrow 3y^4 + 2y^3 - 12y^2 - 16y - 4 > 0 \\
&\Leftarrow 21y^2 - 16y - 4 > 0 \\
&\Leftarrow 20y^2 - 16y - 4 > 0 \\
&\Leftarrow y \geq 3.
\end{aligned}$$

That is, $\lambda(y)$ strictly increases in $[3, +\infty)$. It follows that $\lambda(y) \geq \lambda(3) \approx 0.842087 > \lambda(2) \approx 0.836863$. ■

The ABS index is one of the so-called bond incident degree or vertex-degree based invariants (see [13, 14]). From Lemma 2.2 (2), it is easily seen that

$$g(y+1,x+1) = f(x+1,y+1) - f(x+1,y) < f(x,y+1) - f(x,y) = g(y+1,x)$$

for any positive integers x,y. Hence $f(x,y)$ is a so-called de-escalating function (see [14]). Consequently, the Theorem 2.2 in [14] implies the following result.

Theorem 2.4. If $\pi = (d_1, d_2, \ldots, d_n)$ is the degree sequence of a bicyclic graph, then $B^*(\pi)$ has minimum ABS index in $\mathcal{C}(\pi)$.

3. Proof of Theorem 1.2

Denote by $G(k,l)$ the graph obtained from a non-trivial connected graph G by attaching two pendent paths $uu_1u_2\cdots u_k$ and $uv_1v_2\cdots v_l$ at vertex $u \in V(G)$, $k \geq l \geq 0$. Partial of the following result can be found in [4, 5].

Lemma 3.1. Let $G(k,l)$ be the graph defined above. If $k \geq l \geq 0$ and $k \geq 1$, then

$$ABS(G(k+l,0)) \leq ABS(G(k,l)) \leq ABS(G(k+l-1,1)),$$

with the two equalities iff $l = 0$ and $l = 1$, respectively.

Proof. Let y denote the degree of u in $G(k,l)$. Then $y \geq 3$ if $k \geq l \geq 1$.

Case 1. $k \geq l \geq 2$. From Lemma 2.2 (2) we have

$$\begin{aligned}
&ABS(G(k+l-1,1)) - ABS(G(k,l)) \\
&= f(1,y) + f(2,2) - f(2,y) - f(1,2) \\
&= g(2,2) - g(2,y) \\
&> 0,
\end{aligned}$$

and from Lemma 2.2 (1) and Lemma 2.3 it holds that

$$\begin{aligned}
&ABS(G(k,l)) - ABS(G(k+l,0)) \\
&> 2f(2,y) + f(1,2) - f(2,y-1) - 2f(2,2) \\
&= 2f(2,y) - f(1,y) - [2f(2,2) - f(1,2)] \\
&= \lambda(y) - \lambda(2) \\
&> 0.
\end{aligned}$$

Case 2. $k > l = 1$. From Lemma 2.2 (1) it holds that

$$\begin{aligned}
&ABS(G(k,1)) - ABS(G(k+1,0)) \\
&> f(1,y) + f(2,y) - f(2,y-1) - f(2,2) \\
&= f(2,y) - f(2,2) \\
&> 0.
\end{aligned}$$

Case 3. $k = l = 1$. From Lemma 2.2 (1) it holds that

$$\begin{aligned}
&ABS(G(1,1)) - ABS(G(2,0)) \\
&> 2f(1,y) - f(2,y-1) - f(1,2) \\
&= f(1,y) - f(1,2) \\
&> 0.
\end{aligned}$$

Case 4. $k > l = 0$. If $k = 1$, the result holds because $G(1,0) \cong G(0,1)$. Otherwise, if $k \geq 2$, the result follows from Cases 2 and 3.

The proof is completed by the above four cases. ■

Let $\Phi(n) = f(3,3) + 4f(2,3) + (n-4)f(2,2) \approx \frac{n}{\sqrt{2}} + 1.08646$. Now, we are in the position to prove Theorem 1.2.

Proof of Theorem 1.2. For $n = 4,5$, the conclusion can be easily confirmed, because $|\mathcal{B}_4| = 1$ and $|\mathcal{B}_5| = 3$.

Suppose G is a bicyclic graph of order $n \geq 6$ with minimum ABS index, and $\pi = (d_1, d_2, \ldots, d_n)$ its non-increasing degree sequence. From Theorem 2.4, $ABS(G) = ABS(B^*(\pi))$. Recall that π should be one of the four cases below.

Case 1. $d_1 \geq d_2 \geq 3$ and $d_n = 1$. Then $B^*(\pi)$ is obtained from B_1 by attaching a tree T_i at vertex v_i, $i = 1,2,3,4$. From Lemma 3.1, each T_i should be a pendent path, say of length $l_i \geq 0$. Denote $B^*(\pi)$ by $B(l_1,l_2;l_3,l_4)$. By symmetry, assume $l_1 \geq l_2$ and $l_3 \geq l_4$.

(1) If $l_1 \geq l_2 \geq 2$, from Lemma 2.2 (1) we have

$$\begin{aligned} &ABS(B(l_1,l_2;l_3,l_4)) - ABS(B(l_1+l_2,0;l_3,l_4)) \\ &> f(1,2)+f(2,4)-2f(2,2)+g(4,4) \\ &\approx 0.000504437 > 0. \end{aligned}$$

(2) If $l_1 > l_2 = 1$, from Lemma 2.2 (1) we have

$$\begin{aligned} &ABS(B(l_1,1;l_3,l_4)) - ABS(B(l_1+1,0;l_3,l_4)) \\ &> f(1,4)-f(2,2) > 0. \end{aligned}$$

(3) If $l_1 = l_2 = 1$, from Lemma 2.2 (1) we have

$$\begin{aligned} &ABS(B(1,1;l_3,l_4)) - ABS(B(2,0;l_3,l_4)) \\ &> 2f(1,4)-f(1,2)-f(2,4) \\ &\approx 0.155346 > 0. \end{aligned}$$

From (1)–(3), we deduce $l_2 = 0$, and so $d_1 \leq 4$ and $d_2 = 3$. Similarly, we further have $l_4 = 0$, and then $l_1 = 0$. That is $B^*(\pi) = B(0,0;l_3,0)$, where $l_3 = n-4 \geq 2$. Hence

$$\begin{aligned} ABS(G) &= f(1,2)+3f(2,3)+3f(3,3)+(n-6)f(2,2) \\ &\approx \frac{n}{\sqrt{2}} + 1.10799 > \Phi(n). \end{aligned}$$

Case 2. $d_1 \geq 5$, $d_2 = 2$, and $d_n = 1$. From Lemma 3.1, $B^*(\pi)$ is the graph obtained from B_2 by attaching a pendent path of length $n-5$ at v_1. If $n = 6$, then

$$ABS(G) = f(1,5)+2f(2,2)+4f(2,5) \approx 5.61133 > \Phi(6) \approx 5.3291.$$

Otherwise, if $n \geq 7$, then

$$ABS(G) = f(1,2)+5f(2,5)+(n-5)f(2,2) \approx \frac{n}{\sqrt{2}} + 1.26759 > \Phi(n).$$

Case 3. $d_1 = 4$ and $d_2 = d_3 = \cdots = d_n = 2$. Then $B^*(\pi) = B_3$, and

$$ABS(G) = 4f(2,4)+(n-3)f(2,2) \approx \frac{n}{\sqrt{2}} + 1.14467 > \Phi(n).$$

Case 4. $d_1 = d_2 = 3$ and $d_3 = d_4 = \cdots = d_n = 2$. By counting the edges of G that are incident to vertices of degree $i = 2,3$, we have $2m_{2,2}+m_{2,3} = 2n-4$ and $m_{2,3}+2m_{3,3} = 6$. Moreover, $m_{3,3} = 0,1$, because either $v_1v_2 \notin E$ or $v_1v_2 \in E$.

If $m_{3,3} = 0$, then $m_{2,2} = n-5$, $m_{2,3} = 6$, and

$$ABS(G) = (n-5)f(2,2) + 6f(2,3) \approx \frac{n}{\sqrt{2}} + 1.11205 > \Phi(n).$$

Otherwise, if $m_{3,3} = 1$, then we have $m_{2,2} = n-4$ and $m_{2,3} = 4$, hence $G \in \mathcal{B}^*(n)$ and $ABS(G) = \Phi(n)$.

Combining Cases 1–4, it holds that $ABS(G) \geq \Phi(n)$, with equality iff $G \in \mathcal{B}^*(n)$. ■

Acknowledgments

The research is supported by the NSFC of China (No. 12271182).

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