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Research Article

Atom-bond sum-connectivity index of line graphs

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Abstract

The recently introduced atom-bond sum-connectivity (ABS) index is receiving nowadays significant attention in chemical graph theory. In this paper, an inequality between the ABS index of a graph and its line graph is established. As a consequence of the obtained inequality, the unique graph with the minimum ABS index among all line graphs of unicyclic graphs of fixed order is determined.

Keywords: atom-bond sum-connectivity index; line graph; extremal graph.

2020 Mathematics Subject Classification: 05C05, 05C07, 05C09, 05C35.

1. Introduction

Let $G = (V(G), E(G))$ be a simple finite undirected graph of order n and of size m, where $n = |V(G)|$ and $m = |E(G)|$. For $x \in V(G)$, we use $d_G(x)$ and $N_G(x)$ to denote the degree and the set of neighbors of x in G, respectively. The minimum degree of G is denoted by $\delta(G)$. Let $I_G(x) = \{xx_i : xx_i \in E(G) \text{ and } x_i \in N_G(x)\}$. If there is no confusion, we simply denote the above notation as $d(x)$, $N(x)$, $I(x)$, and δ. A vertex x is said to be pendant vertex if $d(x) = 1$. As usual, P_n, C_n, S_n, T_n, and K_n denote the path, cycle, star, tree, and complete graph of order n, respectively.

For a graph G, the line graph of G, denoted by $L(G)$, is a graph with $V(L(G)) = E(G)$, in which two vertices are adjacent if and only if they (being edges) are adjacent in G. A connected graph G is said to be a unicyclic graph if $|V(G)| = |E(G)|$. Let U_n denote the unicyclic graph of order n.

In mathematical chemistry, the connectivity index [13] (also known as the Randić index) is a famous degree-based topological index, which is commonly used to predict the physicochemical properties and biological activity of chemical compounds. For a graph G, the connectivity index is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

The harmonic index [8], the sum-connectivity index [14], and the atom-bond-connectivity index [7] are among the successful variants of the connectivity index, and they are defined, respectively, as

$$\begin{aligned} H(G) &= \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}, \\ SCI(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}, \quad \text{and} \\ ABC(G) &= \sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}. \end{aligned}$$

Inspired by these indices, Ali et al. [3] introduced a new connectivity index, namely the atom-bond sum-connectivity index (ABS index, for short), which is defined as

$$ABS(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}} = \sum_{uv \in E(G)} \sqrt{1 - \frac{2}{d(u)+d(v)}}.$$

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This new index has attracted the attention of scholars, which yield various results on this index, see for example [1, 2, 4, 5, 9, 10]. In particular, extremal problems related to the ABS index form an interesting research topic, and such problems for trees, unicyclic graphs, chemical graphs, and general graphs were studied in [3, 4, 6, 11, 12, 15].

In the present paper, an inequality between $ABS(L(G))$ and $ABS(G)$ is given, and the unique graph with the minimum ABS index among all line graphs of unicyclic graphs of fixed order is determined.

2. Preliminaries

A path $P = x_0x_1 \cdots x_k$ of a graph G with length $k \geq 1$ is said to be a 2-extremal path if $d(x_1) = \cdots = d(x_{k-1}) = 2$ for $k \geq 2$, $d(x_0) \neq 2$, and $d(x_k) \neq 2$. In particular, P is called pendant if $d(x_0) = 1$ or $d(x_k) = 1$. Let $End_3(P)$ be the set of end vertices of a 2-extremal path P with degree at least 3 in G. Clearly, $1 \leq |End_3(P)| \leq 2$. Moreover, we use $\mathcal{P}$ to denote the set of all 2-extremal paths in G.

Lemma 2.1 (see [4]). *Among all unicyclic graphs of order $n \geq 3$, the cycle C_n uniquely attains the minimum value of the ABS index.*

Lemma 2.2 (see [3]). *Among all connected graphs of order $n \geq 4$, the path P_n uniquely attains the minimum value of the ABS index, and the complete graph K_n uniquely attains the maximum value of the ABS index.*

It is easy to see that $L(P_n) = P_{n-1}$ and $L(S_n) = K_{n-1}$ for $n \geq 3$. By Lemma 2.2, we obtain the following result.

Proposition 2.1. *If T_n is a tree of order n, then*

$$ABS(L(P_n)) \leq ABS(L(T_n)) \leq ABS(L(S_n)),$$

with the left equality if and only if $T_n \cong P_n$, whereas the right equality holds if and only if $T_n \cong S_n$.

3. Main results

Lemma 3.1. *For a vertex x of a connected graph G of order n with $d(x) \geq 3$,*

$$\sum_{y \in N(x)} \sqrt{1 - \frac{2}{d(x) + d(y)}} \leq \sum_{e,f \in I(x)} \sqrt{1 - \frac{2}{d_L(e) + d_L(f)}},$$

with equality if and only if $G \cong S_4$, and x is the center of S_4.

Proof. Let $N(x) = \{x_1, x_2, \ldots, x_t\}$ and $t = d(x)$. For convenience, we take $e_j = xx_j$ for j satisfying $1 \leq j \leq t$ and we write $d_L(e)$ instead of $d_{L(G)}(e)$ for every $e \in E(G)$. Without loss of generality, we assume that $d(x_1) \leq d(x_2) \leq \ldots \leq d(x_t)$. Since $t \geq 3$, we have

$$\sqrt{1 - \frac{2}{d_L(e_1) + d_L(e_j)}} = \sqrt{1 - \frac{2}{2d(x) + d(x_1) + d(x_j) - 4}} \geq \sqrt{1 - \frac{2}{d(x) + d(x_j)}}$$

for every $j \in \{2, \ldots, t\}$. Also, we have

$$\sqrt{1 - \frac{2}{d_L(e_{t-1}) + d_L(e_t)}} = \sqrt{1 - \frac{2}{2d(x) + d(x_{t-1}) + d(x_t) - 4}} \geq \sqrt{1 - \frac{2}{d(x) + d(x_1)}}.$$

Now, the desired result follows from the last two inequalities. □

Lemma 3.2. *Let G be a connected graph not isomorphic to the path graph. If $P \in \mathcal{P}$, then*

$$\sum_{xy \in E(P);\ x,y \notin End_3(P)} \sqrt{1 - \frac{2}{d(x) + d(y)}} \leq \sum_{\substack{ef \in E(L(G)) \\ e,f \in E(P)}} \sqrt{1 - \frac{2}{d_L(e) + d_L(f)}}. \tag{1}$$

Proof. If the length of P is less than 2 then the result trivially holds. Thus, we assume that P has a length of at least 2. Since G is not a path, P can be labeled as $x_0x_1 \ldots x_k$, where $d(x_0) \geq 3$. Let $e_i = x_{i-1}x_i$ for $i \in \{1, \ldots, k\}$. Hence, to prove (1), it is sufficient to prove

$$\sum_{i=1}^{k-1} \sqrt{1 - \frac{2}{d(x_i) + d(x_{i+1})}} \leq \sum_{i=1}^{k-1} \sqrt{1 - \frac{2}{d_L(e_i) + d_L(e_{i+1})}} \quad \text{if } d(x_k) = 1,$$

$$\sum_{i=1}^{k-2}\sqrt{1-\frac{2}{d(x_i)+d(x_{i+1})}} \leq \sum_{i=1}^{k-1}\sqrt{1-\frac{2}{d_L(e_i)+d_L(e_{i+1})}} \quad \text{if } d(x_k) \geq 3.$$

First, we consider the case when $d(x_k)=1$. Since $d(x_1)=d(x_2)=\ldots=d(x_{k-1})=2$, we have

$$\sum_{i=1}^{k-1}\sqrt{1-\frac{2}{d(x_i)+d(x_{i+1})}} = \frac{\sqrt{2}(k-2)}{2}+\frac{\sqrt{3}}{3} \tag{2}$$

and

$$\sum_{i=1}^{k-1}\sqrt{1-\frac{2}{d_L(e_i)+d_L(e_{i+1})}} = \begin{cases} \sqrt{1-\frac{2}{d(x_0)+2}}+\frac{\sqrt{2}(k-3)}{2}+\frac{\sqrt{3}}{3} & \text{if } k\geq 3, \\ \sqrt{1-\frac{2}{d(x_0)+1}} & \text{if } k=2. \end{cases} \tag{3}$$

Subtracting (2) from (3) yields an equation whose right-hand side is given as follows:

$$\begin{cases} \sqrt{1-\frac{2}{d(x_0)+2}}-\frac{\sqrt{2}}{2} & \text{if } k\geq 3, \\ \sqrt{1-\frac{2}{d(x_0)+1}}-\frac{\sqrt{3}}{3} & \text{if } k=2. \end{cases} \tag{4}$$

Since $d(x_0)\geq 3$, by (4), we have

$$\sum_{i=1}^{k-1}\sqrt{1-\frac{2}{d_L(e_i)+d_L(e_{i+1})}} - \sum_{i=1}^{k-1}\sqrt{1-\frac{2}{d(x_i)+d(x_{i+1})}} \geq 0.$$

Next, we consider the case when $d(x_k)\geq 3$. Since $d(x_1)=d(x_2)=\cdots=d(x_{k-1})=2$, we have

$$\sum_{i=1}^{k-2}\sqrt{1-\frac{2}{d(x_i)+d(x_{i+1})}} = \frac{\sqrt{2}(k-2)}{2} \tag{5}$$

and

$$\sum_{i=1}^{k-1}\sqrt{1-\frac{2}{d_L(e_i)+d_L(e_{i+1})}} = \begin{cases} \sqrt{1-\frac{2}{d(x_0)+2}}+\sqrt{1-\frac{2}{d(x_k)+2}}+\frac{\sqrt{2}(k-3)}{2} & \text{if } k\geq 3, \\ \sqrt{1-\frac{2}{d(x_0)+d(x_k)}} & \text{if } k=2. \end{cases} \tag{6}$$

Subtracting (5) from (6) gives an equation whose right-hand side is given as follows:

$$\begin{cases} \sqrt{1-\frac{2}{d(x_0)+2}}+\sqrt{1-\frac{2}{d(x_k)+2}}-\frac{\sqrt{2}}{2} & \text{if } k\geq 3, \\ \sqrt{1-\frac{2}{d(x_0)+d(x_k)}} & \text{if } k=2. \end{cases}$$

Since $d(x_0)\geq 3$, we have

$$\sum_{i=1}^{k-1}\sqrt{1-\frac{2}{d_L(e_i)+d_L(e_{i+1})}} - \sum_{i=1}^{k-2}\sqrt{1-\frac{2}{d(x_i)+d(x_{i+1})}} \geq 0.$$

This completes the proof. □

Theorem 3.1. *Let G be a connected graph not isomorphic to the path graph. If $P\in\mathcal{P}$, then*

$$ABS(L(G)) \geq \begin{cases} ABS(G) & \text{if } \delta\leq 2, \\ 2ABS(G) & \text{if } \delta\geq 3. \end{cases}$$

Proof. Observe that

$$ABS(G) = \sum_{xy\in E(G)} \sqrt{1 - \frac{2}{d(x)+d(y)}} = \frac{1}{2}\sum_{x\in V(G)}\sum_{y\in N(x)} \sqrt{1 - \frac{2}{d(x)+d(y)}},$$

and

$$ABS(L(G)) = \sum_{x\in V(G)}\sum_{e,f\in I(x)} \sqrt{1 - \frac{2}{d_L(e)+d_L(f)}}.$$

By Lemma 3.1, we have

$$\sum_{y\in N(x)} \sqrt{1 - \frac{2}{d(x)+d(y)}} \le \sum_{e,f\in I(x)} \sqrt{1 - \frac{2}{d_L(e)+d_L(f)}}$$

for each $x \in V(G)$ with $d(x) \ge 3$. Summing up the above facts, we conclude that $ABS(L(G)) \ge 2ABS(G)$ if $\delta \ge 3$. Next, we consider the case when $\delta \le 2$. If $G \cong C_n$, then $L(G) \cong C_n$ and thus $ABS(L(G)) = ABS(G)$. Also, note that

$$ABS(G) = \sum_{\substack{x\in V(G)\\ d(x)\ge 3}} \left(\sum_{y\in N(x)} \sqrt{1 - \frac{2}{d(x)+d(y)}}\right) + \sum_{P\in\mathcal{P}} \left(\sum_{xy\in E(P\setminus End_3(P))} \sqrt{1 - \frac{2}{d(x)+d(y)}}\right)$$

and

$$ABS(L(G)) = \sum_{\substack{x\in V(G)\\ d(x)\ge 3}} \left(\sum_{e,f\in I(x)} \sqrt{1 - \frac{2}{d_L(e)+d_L(f)}}\right) + \sum_{P\in\mathcal{P}} \left(\sum_{\substack{ef\in E(L(G))\\ e,f\in E(P)}} \sqrt{1 - \frac{2}{d_L(e)+d_L(f)}}\right).$$

For each $x \in V(G)$ with $d(x) \ge 3$, by Lemma 3.1, we have

$$\sum_{y\in N(x)} \sqrt{1 - \frac{2}{d(x)+d(y)}} \le \sum_{e,f\in I(x)} \sqrt{1 - \frac{2}{d_L(e)+d_L(f)}}.$$

For $P \in \mathcal{P}$, by Lemma 3.2, we have

$$\sum_{xy\in E(P\setminus End_3(P))} \sqrt{1 - \frac{2}{d(x)+d(y)}} \le \sum_{\substack{ef\in E(L(G))\\ e,f\in E(p)}} \sqrt{1 - \frac{2}{d_L(e)+d_L(f)}}.$$

Combining the above-mentioned facts, we conclude that $ABS(L(G)) \ge ABS(G)$ if $\delta \le 2$. □

Corollary 3.1. *Let U_n be a unicyclic graph of order n. Then*

$$ABS(L(U_n)) \ge ABS(L(C_n))$$

with equality if and only if $U_n \cong C_n$.

Proof. Since $\delta(U_n) \le 2$, by Lemma 2.1 and Theorem 3.1, we have

$$ABS(L(U_n)) \ge ABS(U_n) \ge ABS(C_n) = ABS(L(C_n)),$$

where the equation $ABS(L(U_n)) = ABS(L(C_n))$ holds if and only if $U_n \cong C_n$. □

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