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Research Article

Maximum atom-bond sum-connectivity index of n-order trees with fixed number of leaves

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Abstract

Let G be a graph. For an edge e of G, denote by d_e the number of edges adjacent to e. The atom-bond sum-connectivity (ABS) index of G is defined as $ABS(G) = \sum_{e \in E(G)} \sqrt{1 - 2(d_e + 2)^{-1}}$. A graph of order n is known as an n-order graph. The problem of determining trees possessing the minimum ABS index among all n-order trees with fixed number of leaves has recently been attacked in two preprints independently. This article provides a complete solution to the maximal version of the aforementioned problem.

Keywords: topological index; atom-bond sum-connectivity index; tree; leaf; pendent vertex.

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

1. Introduction and statement of the result

Those graph-theoretical terms that are used in the present article, without providing their definitions here, can be found in the books [7, 8, 12].

A graph invariant is a property of a graph that is preserved by isomorphism [12]. The degree sequence and the size of a graph are examples of graph invariants. In chemical graph theory, those graph invariants that take a single number are called topological indices [20]. According to Ivan Gutman [13], among all topological indices the connectivity index "is the most studied, most often applied, and most popular". The connectivity index was introduced by Milan Randić in [18], where he referred to it as the branching index; this index is nowadays known as the Randić index. The readers interested in getting details about the connectivity index may consult the books [14, 15], review articles [16, 19], and related papers cited therein.

Because of the success of the connectivity index, many modified versions of this index have been introduced and investigated. The sum-connectivity (SC) index [21] and the atom-bond connectivity (ABC) index [9, 10] are among the renowned and well-investigated variants of the connectivity index. Most of the mathematical aspects of the ABC and SC indices can be found in the review articles [1] and [4], respectively.

The present paper is concerned with a recently proposed variant of the ABC index, namely the atom-bond sum-connectivity (ABS) index [2]. The ABS index was defined by utilizing the main concept of the SC and ABC indices. For a graph G, its ABS index is defined by the equation

$$ABS(G) = \sum_{yz \in E(G)} \sqrt{1 - \frac{2}{d_y + d_z}},$$

where $E(G)$ denotes the set of edges of G and d_y indicates the degree of the vertex y in G (similarly, d_z is defined).

Certainly, the ABS index is a vertex-degree-based topological index; however, it can also be considered as an edge-degree-based topological index because the number "$d_y + d_z - 2$" is called the degree of the edge $yz \in E(G)$.

The mathematical study of the ABS index was initiated in the article [2], where some extremal results about the ABS index for (general) graphs and (molecular) trees were reported. Chemical applicability of the ABS index was investigated in [3], where the maximum and minimum values of the ABS index of unicyclic graphs were also found (a connected graph with the same number of edges and vertices is known as a unicyclic graph). Gowtham and Gutman [11] established several inequalities involving the difference between SC and ABS indices. The maximum value of the ABS index of graphs with several fixed parameters was investigated in [6].

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A graph of order n is known as an n-order graph. A leaf of a graph is a vertex of degree one; a leaf is also known as a pendent vertex or an end vertex. The problem of determining trees possessing the minimum ABS index among all n-order trees with fixed number of leaves has recently been attacked in [5, 17] independently; the present article provides a complete solution to the maximal version of this problem (for the case of general graphs, see [6]). Now, we state the main result of this article.

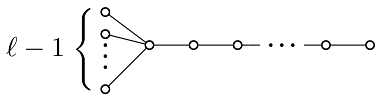

Figure 1: The graph $S_{n,\ell}$ mentioned in Theorem 1.1.

Theorem 1.1. *In the class of all n-order trees with ℓ leaves, $S_{n,\ell}$ is the unique graph having the maximum ABS index, where $2 \le \ell \le n-2$ and $S_{n,\ell}$ is the tree obtained from the path graph $P_{n-\ell+1}$ of order $n-\ell+1$ by attaching $\ell-1$ leaves to exactly one leaf of $P_{n-\ell+1}$ (see Figure 1). The mentioned maximum value is*

$$\frac{1}{\sqrt{2}}(n-\ell-2)+(\ell-1)\sqrt{\frac{\ell-1}{\ell+1}}+\sqrt{\frac{\ell}{\ell+2}}+\frac{1}{\sqrt{3}}.$$

2. Proof of Theorem 1.1

We prove the theorem by induction on n. For $n=4$ one has $\ell=2$ and for $n=5$ one has $\ell \in \{2,3\}$; in any case, the result trivially holds because there is only one tree in each case (and that tree is $S_{n,\ell}$). Assume that $n \ge 6$ and that the result is true for every tree of order $n-1$ with ℓ leaves, where $2 \le \ell \le n-3$. Suppose that T is an n-order tree with ℓ leaves with the constraint $2 \le \ell \le n-2$. It is enough to show that

$$ABS(T) \le \frac{1}{\sqrt{2}}(n-\ell-2)+(\ell-1)\sqrt{\frac{\ell-1}{\ell+1}}+\sqrt{\frac{\ell}{\ell+2}}+\frac{1}{\sqrt{3}}, \tag{1}$$

with equality if and only if T isomorphic to the graph $S_{n,\ell}$.

Take $uv \in E(T)$ such that $d_v = 1$ and $d_u \ge 2$. Let $T-v$ be the tree obtained from T by removing the vertex v. Note that the degree of every vertex, except u, of $T-v$ is the same in both T and $T-v$. In what follows, d_u represents the degree of u in T.

Case 1. $d_u > 2$.
Let $u_1, \cdots, u_{d_u-1}$ be all the neighbors of u different from v. Then

$$ABS(T)-ABS(T-v)=\sqrt{1-\frac{2}{d_u+1}}+\sum_{i=1}^{d_u-1}\left(\sqrt{1-\frac{2}{d_u+d_{u_i}}}-\sqrt{1-\frac{2}{d_u+d_{u_i}-1}}\right). \tag{2}$$

Since $\ell \le n-2$, at least one of the vertices $u_1, \cdots, u_{d_u-1}$ is non-leaf. Also, the function ϕ defined by

$$\phi(x,y)=\sqrt{1-\frac{2}{x+y}}-\sqrt{1-\frac{2}{x+y-1}}, \quad x>2,\ y \ge 1,$$

is strictly decreasing in y. Thus, Equation (2) yields

$$ABS(T)-ABS(T-v) \le \sqrt{\frac{d_u}{d_u+2}}+(d_u-2)\left(\sqrt{\frac{d_u-1}{d_u+1}}-\sqrt{\frac{d_u-2}{d_u}}\right), \tag{3}$$

with equality if and only if exactly one of the vertices $u_1, \cdots, u_{d_u-1}$ is non-leaf provided that this unique non-leaf has the degree 2. Since $d_u \le \ell$ and the function ψ defined by

$$\psi(z)=\sqrt{\frac{z}{z+2}}+(z-2)\left(\sqrt{\frac{z-1}{z+1}}-\sqrt{\frac{z-2}{z}}\right)$$

is strictly increasing for $z>2$, from Equation (3) it follows that

$$ABS(T)-ABS(T-v) \le \sqrt{\frac{\ell}{\ell+2}}+(\ell-2)\left(\sqrt{\frac{\ell-1}{\ell+1}}-\sqrt{\frac{\ell-2}{\ell}}\right). \tag{4}$$

Observe that the equality in (4) holds if and only if $d_u = \ell$ and exactly one of the vertices $u_1, \cdots, u_{d_u-1}$ is non-leaf, which has the degree 2. Note that, in the present case, the inequality $\ell \geq 3$ holds and the tree $T - v$ has exactly $\ell - 1$ leaves. Since $2 \leq \ell - 1 \leq n - 3$, by the inductive hypothesis, we have

$$ABS(T-v) \leq \frac{1}{\sqrt{2}}(n-\ell-2) + (\ell-2)\sqrt{\frac{\ell-2}{\ell}} + \sqrt{\frac{\ell-1}{\ell+1}} + \frac{1}{\sqrt{3}}, \tag{5}$$

with equality if and only if $T - v$ isomorphic to the graph $S_{n-1,\ell-1}$. Thus, from (4) and (5) the desired inequality (that is, (1)) follows.

Case 2. $d_u = 2$.
If $\ell = n - 2$, then T is isomorphic to the graph $S_{n,n-2}$ and hence we are done. Thus, in the following, we assume that $\ell \leq n - 3$. Let $u' \in V(T)$ be the unique neighbor of u different from v. Certainly, $d_{u'} \geq 2$ because $n \geq 6$. It holds that

$$ABS(T) - ABS(T-v) = \frac{1}{\sqrt{3}} + \sqrt{1 - \frac{2}{d_{u'}+2}} - \sqrt{1 - \frac{2}{d_{u'}+1}} \leq \frac{1}{\sqrt{2}}$$

where the right equality holds if and only if $d_{u'} = 2$. Observe that, in the present case, the tree $T - v$ has exactly ℓ leaves. Since $2 \leq \ell \leq n - 3$, by the inductive hypothesis, it holds that

$$\begin{aligned} ABS(T) &\leq ABS(T-v) + \frac{1}{\sqrt{2}} \\ &\leq \frac{1}{\sqrt{2}}(n-\ell-3) + (\ell-1)\sqrt{\frac{\ell-1}{\ell+1}} + \sqrt{\frac{\ell}{\ell+2}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{2}} \\ &= \frac{1}{\sqrt{2}}(n-\ell-2) + (\ell-1)\sqrt{\frac{\ell-1}{\ell+1}} + \sqrt{\frac{\ell}{\ell+2}} + \frac{1}{\sqrt{3}}. \end{aligned}$$

Note that the equation

$$ABS(T) = \frac{1}{\sqrt{2}}(n-\ell-2) + (\ell-1)\sqrt{\frac{\ell-1}{\ell+1}} + \sqrt{\frac{\ell}{\ell+2}} + \frac{1}{\sqrt{3}}$$

holds if and only if $T - v$ is isomorphic to the graph $S_{n-1,\ell}$ and $d_{u'} = 2$, which is equivalent to say that T is isomorphic to the graph $S_{n,\ell}$.

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