On Second Atom–Bond Connectivity Index

M. ROSTAMI¹, M. SOHRABI–HAGHIGHAT² AND M. GORBANI*³

¹Department of Mathematics, Mahallat Branch, Islamic Azad University, Mahallat, Iran
²Department of Mathematics, Arak University, Arak, Iran
³Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785-136, I. R. Iran

ABSTRACT

The atom–bond connectivity index of graph is a topological index proposed by Estrada et al. as $ABC(G) = \sum_{uv \in E(G)} \sqrt{(d_u + d_v - 2)} / d_u d_v$, where the summation goes over all edges of $G$, $d_u$ and $d_v$ are the degrees of the terminal vertices $u$ and $v$ of edge $uv$. In the present paper, some upper bounds for the second type of atom–bond connectivity index are computed.

Keywords: atom–bond connectivity index, topological index, star–like graph.

1. INTRODUCTION

All graphs considered in this paper are simple graph and connected. The vertex and edge sets of a graph $G$ are denoted by $V(G)$ and $E(G)$, respectively. A topological index of $G$ is a numeric quantity related to it. In other word, let $\Lambda$ be the class of connected graphs, then a topological index is a function $f: \Lambda \rightarrow \mathbb{R}^+$, with this property that if $G$ and $H$ are isomorphic, then $f(G) = f(H)$. Topological indices are important tools in prediction of chemical phenomena, that’s why several types of topological indices have been defined. One of them is the atom–bond connectivity index (or $ABC$ index for short). This topological index was proposed by Estrada et al. [1] as follows:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{d_u + d_v - 2} / d_u d_v,$$

where the summation goes over all edges $e = uv$ of $G$ and $d_u$ and $d_v$ are degrees of vertices $u$ and $v$, respectively. For more details about this topological index see references [1–4]. Some upper bounds of $ABC$ index with different parameters have been given in [5]. The properties of $ABC$ index of trees have also been studied in [5–7]. Recently, Graovač and

*Author to whom correspondence should be addressed.(e-mail: m.ghorbani@srttu.edu).
Ghorbani, defined a new version of the atom-bond connectivity index namely the second atom–bond connectivity index [8]:

$$ABC_2(G) = \sum_{uv \in E(G)} \sqrt[2]{\frac{n_u + n_v - 2}{n_u n_v}},$$

where $n_u$ is the number of vertices closer to vertex $u$ than vertex $v$ and $n_v$ defines similarly. Some upper and lower bounds of $ABC_2$ index have been studied in [8]. Throughout this paper, our notations are standard and mainly taken from [9]. In this paper, in the next section, we give the necessary definitions and some preliminary results and in Section 3 we introduce some upper and lower bounds of $ABC_2$ index with given number of pendent vertices.

2. Definitions and Preliminaries

Let $K_n$, $S_n$, and $P_n$ be the complete graph, star and path on $n$ vertices, respectively. Let also $K_{n,m}$ be the complete bipartite graph on $n + m$ vertices. A tree is said to be star–like if exactly one of its vertices has degree greater than two. By $S(2r,s)$, $r, s \geq 1$, we denote a star–like tree with diameter less than or equal to 4, which has a vertex $v_1$ of degree $r + s$ and

$$S(2r,s) \setminus \{v_1\} = p_2 \cup \ldots \cup p_2 \cup p_1 \cup \ldots \cup p_1.$$

One can prove that, this tree has $2r + s + 1 = n$ vertices. We say that the star–like tree $S(2r,s)$ has $r + s$ branches, where the lengths of them are $2, \ldots, 2, 1, \ldots, 1$ respectively. For $n, m \geq 2$, denoted by $S_{n,m}$ means a tree with $n + m$ vertices formed by adding a new edge connecting the centers of the stars $S_n$ and $S_m$. Finally, the complement $\overline{G}$ of a simple graph $G$ is a simple graph with vertex set $V$ and two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in $G$.

3. Bounds of $ABC_2$ Index

In this section some basic mathematical features of second atom–bond connectivity index are given. A pendent vertex is a vertex of degree one and an edge of a graph is said to be pendant if one of its vertices is a pendent vertex.

**Theorem 1.** Let $G$ be a connected graph of order $n$ with $m$ edges and $p$ pendent vertices, then
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\[ ABC_2(G) < p \sqrt{\frac{n-2}{n-1}} + (m - p). \]

**Proof.** Assume \( n \geq 3 \). For a pendant edge \( uv \) of graph \( G \) we have \( n_u = 1 \), and \( n_v = n - 1 \). On the other hand, for a non-pendant edge \( uv \) \( \frac{n_u + n_v - 2}{n_u n_v} < 1 \) and so,

\[ ABC_2(G) = \sum_{uv \in E} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} = \sum_{uv \in E, d_u = 1} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} + \sum_{uv \in E, d_u, d_v \neq 1} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} < p \sqrt{\frac{n-2}{n-1}} + m - p. \]

An easy calculation shows that the Diophantine equation \( x + y - 2 = xy \) does not have positive solution and so this bound is not sharp.

**Theorem 2.** Let \( T \) a tree of order \( n > 2 \) with \( p \) pendent vertices. Then

\[ ABC_2(T) \leq p \sqrt{\frac{n-2}{n-1}} + \frac{\sqrt{2}}{2} (n - p - 1) \tag{1} \]

with equality if and only if \( T \cong K_{1,n-1} \) or \( T \cong S(2r,s) \), \( n = 2r + s + 1 \).

**Proof.** Let \( T \) be an arbitrary tree with \( n \geq 3 \) vertices, for any edge \( e = uv, n_u + n_v = n \). This implies that

\[ ABC_2(T) = \sqrt{n-2} \sum_{uv \in E(T)} \frac{1}{\sqrt{n_u n_v}}. \]

Now we assume that the tree \( T \) have \( p \) pendent vertices. One can easily prove that for pendant edge \( e = uv, n_u = 1, n_v = n - 1 \) and for other edges \( 2 \leq n_u, n_v \leq n - 2 \). Hence

\[ ABC_2(T) = \sqrt{n-2} \left( \sum_{uv \in E(T), d_u = 1} \frac{1}{\sqrt{n_u n_v}} + \sum_{uv \in E(T), d_u, d_v \neq 1} \frac{1}{\sqrt{n_u n_v}} \right) \leq \sqrt{n-2} \left( \sum_{uv \in E(T), d_u = 1} \frac{p}{\sqrt{n-1}} + \frac{n-p-1}{\sqrt{2(n-2)}} \right) = p \sqrt{\frac{n-2}{n-1}} + \frac{\sqrt{2}}{2} (n - p - 1). \tag{2} \]

Suppose now equality holds in equation (1), hence we should consider two following cases:

**Case (a)** \( p = n - 1 \), in this case for all edges \( e = uv, n_u = n - 1, n_v = 1 \) and so \( T \cong K_{1,n-1} \).

**Case (b)** \( p < n - 1 \), in this case the diameter of \( T \) is strictly greater than 2. Let \( a \) be a pendent vertex. One can easily prove that there is a vertex in \( N_G(a) \) such as \( w \) adjacent to some non-pendent vertices. Since for all edges \( e = wx \) incidence with \( w, n_x = n - 2 \) and
\( n_w = 2 \), we conclude that \( T \cong S(2r,s) \). Conversely, one can prove that in (1) for two graphs \( K_{1,n-1} \) and \( S(2r,s) \) \((n=2r+s)\) equality holds.

**Theorem 3.** Let \( G \) be a graph on \( n > 2 \) vertices, \( m \) edges and \( p \) pendent vertices. Then

\[
ABC_2(G) \geq p \sqrt{\frac{n-2}{n-1}}
\]

with equality if and only if \( G \cong K_{1,n-1} \) or \( G \cong K_n \).

**Proof.** For each pendant edge \( uv \), \( n_u = 1 \), \( n_v = n - 1 \) and for the others \( n_u, n_v \geq 1 \). This implies that

\[
ABC_2(G) = \sum_{uv \in E} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} = \sum_{uv \in E, d_u = 1} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} + \sum_{uv \in E, d_u, d_v \neq 1} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}
\]

\[
= p \sqrt{\frac{n-2}{n-1}} + \sum_{uv \in E, d_u, d_v \neq 1} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} \geq p \sqrt{\frac{n-2}{n-1}}.
\]

For equality we should consider two cases:

**Case(a)** \( p = 0 \), in this case for all edges \( e = uv \), \( n_u = n_v = 1 \) and this implies \( G \cong K_n \).

**Case(b)** \( p = m \), in this case all edges are pendant and so \( G \cong K_{1,n-1} \).

**Theorem 4.** Let \( T \) be a tree of order \( n > 2 \) with \( p \) pendent vertices. Then

\[
ABC_2(T) \geq p \sqrt{\frac{n-2}{n-1}} + 2 \sqrt{\frac{n-2}{n}} (n-p-1)
\]

with equality if and only if \( T \cong K_{1,n-1} \) or \( T \cong S_{n/2,n/2} \).

**Proof.** It is clear that in a tree for every edge \( uv \), \( n_u + n_v = n \) and hence

\[
ABC_2(T) = \sqrt{n-2} \sum_{uv \in E(T)} \frac{1}{\sqrt{n_u n_v}}.
\]

Now we assume that \( T \) have \( p \) pendent vertices, then there exist \( p \) edges such as \( e = uv \) where \( n_u = 1 \) and \( n_v = n - 1 \). Also, for each non-pendant edge \( uv \), \( n_u n_v \leq n^2 / 4 \) and so
\[
ABC_2(T) = \sqrt{n-2} \left( \sum_{uv \in E(T), d_u \neq 1} \frac{1}{\sqrt{n_u n_v}} + \sum_{uv \in E(T), d_u, d_v \neq 1} \frac{1}{\sqrt{n_u n_v}} \right)
\]

\[
= \sqrt{n-2} \left( \frac{p}{\sqrt{n-1}} + \sum_{uv \in E(T), d_u, d_v \neq 1} \frac{1}{\sqrt{n_u n_v}} \right)
\]

\[
\geq \sqrt{n-2} \left( \frac{p}{\sqrt{n-1}} + \frac{2}{n} (n-p-1) \right) = p \sqrt{\frac{n-2}{n-1}} + 2 \sqrt{\frac{n-2}{n}} (n-p-1).
\]

Let in above formula equality holds, we can consider two following cases:

**Case (a)** \( p = n-1 \), in this case all edges are pendant. Therefore \( T \cong K_{1,n-1} \) and so

\[
ABC_2(T) = \sqrt{(n-1)(n-2)}.
\]

**Case (b)** \( p < n-1 \), in this case equality holds if and only if for all non–pendant edges, \( n_u = n_v = n/2 \) and this completes the proof.

**Theorem 5.** Let \( G \) and \( \overline{G} \) are connected graphs on \( n \) vertices with \( p \) and \( \overline{p} \) pendent vertices, respectively. Then

\[
ABC_2(G) + ABC_2(\overline{G}) < (p + \overline{p}) \left( \frac{n-2}{\sqrt{n-1}} - 1 \right) + \left( \frac{n}{2} \right).
\]

**Proof.** Since \( m + \overline{m} = n(n-1)/2 \) by using Theorem 1, we get

\[
ABC_2(G) + ABC_2(\overline{G}) < \frac{n-2}{\sqrt{n-1}} + \overline{p} \sqrt{\frac{n-2}{n-1}} + m - p + \overline{m} - \overline{p}
\]

\[
= (p + \overline{p}) \left( \frac{n-2}{\sqrt{n-1}} - 1 \right) + \left( \frac{n}{2} \right).
\]

**Corollary 6.** We have

\[
ABC_2(G) + ABC_2(\overline{G}) \geq (p + \overline{p}) \sqrt{\frac{n-2}{n-1}}.
\]

**REFERENCES**


