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Further Results on New Version of Atom–Bond Connectivity Index

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Abstract

Recently a new version of Atom–Bond Connectivity Index defined by Graovac and Ghorbani (ABC_2), which is closely related to the vertex Szeged and second geometric-arithmetic indices. In this paper we give lower and upper bounds for the ABC_2 index of graphs. We also determine the n-vertex trees with the minimum, well as the first and second maximum ABC_2 indices.

1. Introduction

Molecular descriptors play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations. Among them, special place is reserved for so-called topological indices [2]. Nowadays, there exists a legion of topological indices that found some applications in chemistry [15]. Let G is a simple undirected graph, with the vertex and edge-sets of which are represented by $V(G)$ and $E(G)$, respectively. Also let $|V(G)| = n$ and $|E(G)| = m$. The topological index of the graph G is a numeric quantity related to G. The atom–bond connectivity (ABC) index of G, proposed by Estrada et al. in [4], and is defined as

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

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. It found applications in chemical research [4,5]. Upper bounds for the ABC index of general graphs using some other graph parameters have been given in [22]. The properties of ABC index for trees have been studied in [6, 19,22]. More properties for the ABC index may be found in [2, 18].

The vertex PI index is another topological index and their definition is as follows [10, 11, 12 ,13].

$$PI_u(G) = \sum_{uv \in E(G)} [n_u + n_v]$$

where n_u is the number of vertices of graph G lying closer to u and n_v is the number of vertices of graph G lying closer to v. Notice that vertices equidistance from u and v are not taken into account.

The vertex Szeged index is another topological index introduced by Gutman [9, 14, 15]. The vertex Szeged index of the graph G is defined as

$$Sz_u(G) = \sum_{uv \in E(G)} [n_u n_v] \ .$$

Recently, a new class of topological descriptors, based on some properties of vertices of graph is presented. These indices are named as geometric-arithmetic indices $(GA_{general})$. The second member of this class is defined as [7, 21],

$$GA_2(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_u n_v}}{n_u + n_v} \ .$$

It found applications of geometric-arithmetic indices in chemical research [7, 17]. Upper and lower bounds for the geometric-arithmetic indices of general graphs, molecular graphs and molecular trees have been given in [7,17,21,20].

Recently, Graovac and Ghorbani, defined a new version of the atom–bond connectivity index [8], and we called second atom–bond connectivity index.

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

Upper and lower bounds for the ABC_2 index of general graphs have been given in [8]. In this paper, we establish further bounds on the ABC_2 index using other graph invariant, and determine the trees with the minimum and maximum ABC_2 index.

2. Preliminaries

Let K_n, C_n, S_n and P_n be the complete graph, cycle, star and path on n vertices, respectively. Let $K_{n,m}$ be the complete bipartite graph on n and m vertices in its two partition sets, respectively. The hypercube Q_n is the graph whose vertices are the ordered $n-$tuples of $0'$s and $1'$s, two vertices being joined if and only if they differ in exactly one coordinate [1].

3. Lower and upper bounds for the ABC_2 index

In this section are given some basic mathematical features of second atom–bond connectivity index(ABC_2).

Example 1: *Consider the cycle C_n. Using a simple calculation, one can show that,*

$$ABC_2(C_n) = \begin{cases} 2\sqrt{n-2}\ , & \text{if n is even,} \\ \dfrac{2n\sqrt{n-3}}{n-1}\ , & \text{if n is odd .} \end{cases}$$

Now consider complete bipartite graph $K_{n,m}$. A simple calculation shows that $n_u = n$, $n_v = m$ for each uv of $K_{n,m}$. Then

$$ABC_2(K_{n,m}) = \sqrt{nm(n+m-2)}\ .$$

As another example, consider hypercube graph. For each edge uv of hypercube graph (Q_n), it is obtained $n_u = n_v = 2^{n-1}$. Then the value of ABC_2 index for hypercube graph (Q_n) is

$$ABC_2(Q_n) = n\sqrt{2^n - 2}\ .$$

Theorem 1: *Let G be a simple graph on n vertices and m edges, then*

$$0 \le ABC_2(G) < m\ .$$

Lower bound is achieved if and only if G is a complete graph and upper bound does not happen.

Proof: We know that $n_u \ge 1$ and $n_v \ge 1$ then $\dfrac{n_u + n_v - 2}{n_u n_v} \ge 0$. Therefore,

$$ABC_2(G) \ge 0\ .$$

Above, equality occurs if and only if $n_u = n_v = 1$ holds for all $e = uv$, which implies $G \cong K_n$.

For any $e = uv$ of graph G, we have $n_u + n_v - 2 < n_u n_v$. Therefore,

$$\frac{n_u + n_v - 2}{n_u n_v} < 1$$

Which implies, $ABC_2(G) < m$. Simple calculation shows that the Diophantine equation $x + y - 2 = xy$ does not have any solution in natural numbers set. So no graph exists with $ABC_2(G) = m$.

Theorem 2: *Let G be a simple graph on n vertices and m edges, then*

$$ABC_2(G) \le \sqrt{m\left(PI_u(G) - 2m\right)}.$$

with equality if and only if graph G is a complete graph.

Proof: For all edges $e = uv \in E(G)$, $n_u n_v \ge 1$ then $\frac{1}{\sqrt{n_u n_v}} \le 1$. Therefore,

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

Applying the Cauchy-Schwarz inequality,

$$\sum_{uv \in E(G)} \sqrt{n_u + n_v - 2} = \sum_{uv \in E(G)} 1.\sqrt{n_u + n_v - 2} \le \sqrt{\left(\sum_{uv \in E(G)} 1\right)\left(\sum_{uv \in E(G)} n_u + n_v - 2\right)}$$
$$= \sqrt{m\left(PI_u(G) - 2m\right)} \quad .$$

Above, equality occurs if and only if $n_u = n_v = 1$ holds for all $e = uv$, which implies $G \cong K_n$.

Theorem 3: *Let G be a simple graph on n vertices and m edges, then*

$$ABC_2(G) \le \sqrt{Sz_u(G)\left(PI_u(G) - 2m\right)}.$$

with equality if and only if G is a complete graph.

Proof: For all edges $e = uv \in E(G)$, $n_u n_v \ge 1$ then $\frac{1}{\sqrt{n_u n_v}} \le \sqrt{n_u n_v}$. Therefore,

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

Applying the Cauchy-Schwarz inequality, we conclude

$$\sum_{uv\in E(G)} \sqrt{(n_u n_v)(n_u+n_v-2)} = \sum_{uv\in E(G)} \sqrt{n_u n_v}.\sqrt{n_u+n_v-2} \le \sqrt{\left(\sum_{uv\in E(G)} n_u n_v\right)\left(\sum_{uv\in E(G)} n_u+n_v-2\right)}$$

$$= \sqrt{Sz_u(G)\left(PI_u(G)-2m\right)} .$$

So,

$$ABC_2(G) \le \sqrt{Sz_u(G)\left(PI_u(G)-2m\right)} .$$

Above, equality occurs if and only if $n_u = n_v = 1$ holds for all $e = uv$, which implies $G \cong K_n$.

Theorem 4: *Let G be a simple graph on n vertices and $m \ge 2$ edges, then*

$$ABC_2(G) < \sqrt{PI_u(G)+m(m-3)} .$$

upper bound does not happen.

Proof:

$$\left(ABC_2(G)\right)^2 = \sum_{uv\in E(G)} \frac{n_u+n_v-2}{n_u n_v} + 2\sum_{uv\ne u'v'} \sqrt{\frac{n_u+n_v-2}{n_u n_v}}\sqrt{\frac{n_{u'}+n_{v'}-2}{n_{u'} n_{v'}}} .$$

For all edges $e = uv \in E(G)$ we know that $\frac{1}{n_u n_v} \le 1$ and $n_u + n_v - 2 < n_u n_v$ then $\frac{n_u + n_v - 2}{n_u n_v} < 1$.

So

$$\left[ABC_2(G)\right]^2 < \sum_{uv\in E(G)} [n_u+n_v-2] + 2\sum_{uv\ne u'v'} (1).(1)$$

$$= PI_u(G) - 2m + 2.\frac{m(m-1)}{2} = PI_u(G) + m(m-3) .$$

So,

$$ABC_2(G) < \sqrt{PI_u(G)+m(m-3)} .$$

Simple calculation shows that the Diophantine equation $x + y - 2 = xy$ dose not have solution in natural numbers set. So upper bound does not happen.

Theorem 5: *Let G be a simple graph on n vertices and m edges, then*

$$ABC_2(G) > \frac{2}{n}\sqrt{PI_u(G)-2m} .$$

lower bound does not happen.

Proof: Note that $n_u + n_v \le n$ implies $n_u n_v \le \frac{n^2}{4}$. So $\frac{1}{\sqrt{n_u n_v}} \ge \frac{2}{n}$ and therefore

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

Using a simple calculation, one can show that $\sum_{i=1}^{n} \sqrt{a_i} > \sqrt{\sum_{i=1}^{n} a_i}$, for positive real number. Then,

$$\frac{2}{n} \sum_{uv\in E(G)} \sqrt{n_u + n_v - 2} > \frac{2}{n} \sqrt{\sum_{uv\in E(G)} n_u + n_v - 2} = \frac{2}{n} \sqrt{PI_u(G) - 2m} .$$

Theorem 6: *Let G be a connected bipartite graph with $n \ge 2$ vertices and m edges, then*

$$ABC_2(G) \ge \sqrt{\frac{m^3(n-2)}{Sz_u(G)}}$$

with equality if and only if $n_u.n_v$ is a constant for any $uv \in E(G)$.

Proof: If G is a connected bipartite graph with $n \ge 2$ vertices then for any edge uv, $n_u + n_v = n$. So,

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

Applying the Cauchy-Schwarz inequality, we know that $\sum_{i=1}^{n} \frac{1}{a_i} \ge \frac{n^2}{\sum_{i=1}^{n} a_i}$, and

$$\sum_{uv\in E(G)} \sqrt{n_u n_v} \le \sqrt{\left(\sum_{uv\in E(G)} 1\right)\left(\sum_{uv\in E(G)} n_u n_v\right)} = \sqrt{m.Sz_u(G)} .$$

Therefore,

$$ABC_2(G) = \sqrt{n-2} \sum_{uv\in E(G)} \frac{1}{\sqrt{n_u n_v}} \ge \frac{m^2\sqrt{n-2}}{\sum_{uv\in E(G)} \sqrt{n_u n_v}} \ge \frac{m^2\sqrt{n-2}}{\sqrt{m.Sz_u(G)}} .$$

So,

$$ABC_2(G) \geq \sqrt{\frac{m^3(n-2)}{Sz_u(G)}} .$$

With equality if and only if $n_u.n_v$ is a constant for all edges $e = uv \in E(G)$.

Theorem 7: *Let* G *be a complete bipartite graph with* $n \geq 4$ *vertices, then*

$$ABC_2(S_{1,n-1}) \leq ABC_2(G) \leq ABC_2\left(K_{\left\lfloor \frac{n}{2} \right\rfloor, \left\lceil \frac{n}{2} \right\rceil}\right) .$$

Proof: If G is a connected complete bipartite graph with $n \geq 4$ vertices, then for any edge uv of graph G we have $n_u + n_v = n$. So,

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

Suppose the vertices set of graph G partitioned into two sets V_1 and V_2. We assume $|V_1| = n_1$ then $|V_2| = n - n_1$ and $|V_1| + |V_2| = n$. The number of edges in graph G is $n_1(n-n_1)$, and for any edge uv we have $n_u = n_1$ and $n_v = n - n_1$ where $1 \leq n_1 \leq n-1$. Then the second atom band connectivity index of complete bipartite graph with $n \geq 4$ vertices as follows,

$$ABC_2(G) = \sqrt{n_1(n-n_1)(n-2)} = f(n_1) .$$

The variable n_1 takes values between 1 and $n-1$. By simple calculation in function $f(n_1)$ we can show that the maximum and minimum value of $f(n_1)$ happened in $n_1 = \frac{n}{2}$ and $n_1 = 1$ respectively. Then,

$$ABC_2(S_{1,n-1}) \leq ABC_2(G) \leq ABC_2\left(K_{\left\lfloor \frac{n}{2} \right\rfloor, \left\lceil \frac{n}{2} \right\rceil}\right) .$$

4. Trees with extremal ABC_2 index

Let T be a tree on n vertices. For any edge uv of trees we have $n_u + n_v = n$, then ABC_2 is simplified as

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

Note that the summation on the right-hand side of the above formula goes over $n-1$ terms.

Theorem 8: *The star S_n is the $n-$vertex tree with the maximum second atom–bond connectivity index.*

Proof: The equality $n_u + n_v = n$ implies that the minimum value of $n_u n_v$ is $1\times(n-1) = n-1$ therefore,

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

The right hand side of the above inequality is the second atom–bond connectivity index of S_n. Note that equality occurs if and only if $n_u = 1$ and $n_v = n-1$ holds for all $uv \in E(T)$, which implies the only such tree is star.

In order to determine the tree with the minimum ABC_2-value, we need an auxiliary result. Consider the trees T_1 and T_2 depicted in Fig.1. These two trees differ only in the position of a terminal vertex. In tree T_2 the terminal vertex is moved from the b-branch to the a-branch. In what follows we assume that $a \ge b$. In the difference of the ABC_2-values of T_1 and T_2, namely in

$$ABC_2(T_1) - ABC_2(T_2) = \sqrt{n-2}\left[\sum_{uv\in E(T_1)}\frac{1}{\sqrt{n_u n_v}} - \sum_{u'v'\in E(T_2)}\frac{1}{\sqrt{n_{u'} n_{v'}}}\right].$$

All terms cancel out except the terms pertaining to the edges indicated by arrows in Fig.1, in which, for edge $e = uv$ of tree T_1 we have $n_u.n_v = b(n-b)$, and for edge $e = u'v'$ of tree T_2 we have $n_{u'}.n_{v'} = (a+1)(n-a-1)$.

From

$$(a+1)(n-a-1) - b(n-b) = (a-b+1)(n-a-b-1)$$

we conclude that

$$\frac{1}{b(n-b)} - \frac{1}{(a+1)(n-a-1)} = \frac{(a-b+1)(n-a-b-1)}{b(n-b)(a+1)(n-a-1)}\ .$$

Therefore,

$$\sqrt{n-2}\left[\frac{1}{\sqrt{b(n-b)}}-\frac{1}{\sqrt{(a+1)(n-a-1)}}\right]\geq 0\ .$$

For $a \geq b$, implies that

$$ABC_2(T_1) > ABC_2(T_2)\ .$$

In other words, the transformation $T_1 \rightarrow T_2$, in which a vertex from a shorter branch is moved to a longer branch decreases the second atom–bond connectivity index. We are now ready to state and prove the following theorem.

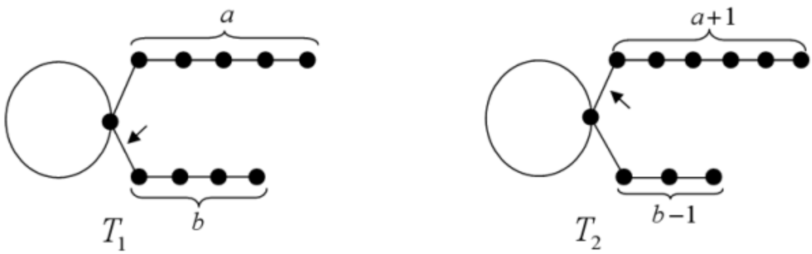

Fig. 1: The transformation $T_1 \rightarrow T_2$ decreases the ABC_2 index provided $a \geq b$

Theorem 9: *The path P_n is the n-vertex tree with the minimum second atom–bond connectivity index.*

Proof: By continuing the above described transformation $T_1 \rightarrow T_2$ we can move all vertices from the shorter branch to the longer branch, always decreasing the ABC_2- value. Repeating the transformation sufficiently many times, we necessarily arrive to the path P_n. The value of the second atom–bond connectivity index for path P_n equals to:

$$ABC_2(P_n) = \sqrt{n-2}\sum_{i=1}^{n-1}\frac{1}{\sqrt{i(n-i)}}\ .$$

Corollary 1: *Among all n-vertex trees with $n \geq 5$, the tree formed by attaching two pendent vertices to a terminal vertex of the path P_{n-2}, is the unique tree with the second maximum ABC_2-value.*

5. Numerical examples

Here is shown that the second atom–bond connectivity index is an appropriate and functional index in comparison to the geometric-arithmetic and vertex Szeged indices.

In Table 1, are given the second geometric-arithmetic (GA_2), vertex Szeged (Sz_u) and second atom–bond connectivity (ABC_2) indices of the octane isomers. The correlation between Sz_u and ABC_2 also GA_2 and ABC_2 are shown in Fig.2.

#	Octanes	Sz_v	GA_2	ABC_2
1	n-Octane	84	5.9914	5.1431
2	2-Metherl heptane	79	5.7868	5.3619
3	3-Metherl heptane	76	5.6846	5.4365
4	4-Metherl heptane	75	5.6546	5.4566
5	3-Ethyl-hexane	72	5.5506	5.5312
6	2,2-dimethyl-hexane	71	5.4800	5.6552
7	2,3-dimethyl-hexane	70	5.4483	5.6753
8	2,4-dimethyl-hexane	71	5.4800	5.6552
9	2,5-dimethyl-hexane	74	5.5822	5.5806
10	3,3-dimethyl-hexane	67	5.3460	5.7499
11	3,4-dimethyl-hexane	68	5.3778	5.7299
12	2-methyl-3-ethyl-pentane	67	5.3460	5.7499
13	3-methyl-3-ethyl-pentane	64	4.2438	5.8246
14	2,2,3-trimethyl-pentane	63	5.1732	5.9486
15	2,2,4-trimethyl-pentane	66	5.2754	5.8739
16	2,3,3-trimethyl-pentane	62	5.1415	5.9687
17	2,3,4-trimethyl-pentane	65	5.2437	5.8940
18	2,2,3,3-tetramethyl-butane	58	4.9686	6.1673

Table 1: The ABC_2, GA_2 and Sz_v indices of the octane isomers.

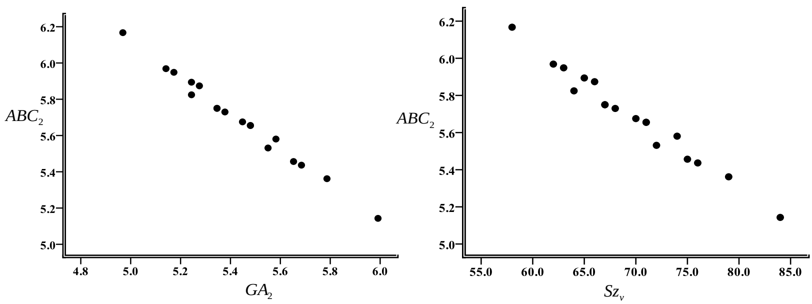

Fig.2: Graphs showing correlation between (ABC_2, GA_2) and (ABC_2, Sz_v) indices respectively.

The linear correlations between ABC_2 and both GA_2 and Sz_u are given below.

$$ABC_2(G) = -0.038(\pm 0.102)Sz_v(G) + 8.315(\pm 0.001), \qquad R = 0.9882,$$

and

$$ABC_2(G) = -0.980(\pm 0.240)GA_2(G) + 11.013(\pm 0.131), \qquad R = 0.9952 \quad .$$

6. Conclusion

It has been demonstrated that the Szeged and general geometrical-arithmetic indices have many applications in QSPR and QSAR research. The appropriate correlations between second atom–bond connectivity, Szeged and second geometrical-arithmetic indices mentioned in section 5 shows that second atom–bond connectivity index can be used in QSPR and QSAR research.

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