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On ABC Index of Graphs

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Abstract

The atom–bond connectivity index (ABC) of a graph G is defined as the sum over all pairs of adjacent vertices v_i, v_j of the terms $\sqrt{(d_i + d_j - 2)/(d_i\, d_j)}$, where d_i is the degree of the vertex v_i. Recently, in the paper M. Hemmasi, A. Iranmanesh, Some inequalities for the atom–bond connectivity index of graph, *J. Comput. Theor. Nanosci.* **12** (2015) 2172–2179, lower and upper bounds on ABC in terms of Randić index, first Zagreb index, second Zagreb index, and modified second Zagreb index were reported. Several of these bounds were erroneous. We now correct these results.*

1 Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let d_i be the degree of the vertex v_i for $i = 1, 2, \ldots, n$. The maximum and minimum vertex degrees are denoted by Δ and δ, respectively. A vertex of a graph is said to be pendent if its neighborhood contains exactly

*It would be usual and reasonable to communicate these corrections in the same journal in which the erroneous results were published. Unfortunately, the *Journal of Computational and Theoretical Nanoscience* charges a "*manuscript–processing fee*" of 980 US \$ per article from all countries. The present authors were not in position, and were not willing, to cover this exorbitant publication cost.

one vertex. The number of pendent vertices will be denoted by ρ. The complement of a graph G is denoted by $\overline{G}$.

The atom–bond connectivity index ABC is one of the popular degree–based topological indices in chemical graph theory [26], and is defined as

$$ABC = ABC(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i\, d_j}} . \tag{1}$$

The ABC index has proven to be a valuable predictive index in the study of the heat of formation in alkanes [20, 21, 33]. The mathematical properties of this index were reported in numerous papers, e.g., in [1, 2, 6, 9, 10, 13, 16–19, 22–25, 29, 30, 36, 39–41, 43].

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined as follows:

$$M_1(G) = \sum_{i=1}^{n} d_i^2 \qquad \text{and} \qquad M_2(G) = \sum_{v_i\, v_j \in E(G)} d_i\, d_j \, .$$

Some results on the Zagreb indices can be found the papers in [4, 5, 7, 8, 11, 12, 14, 15, 27, 32] and in the recent surveys [3, 26, 31].

The modified second Zagreb index $M_2^*(G)$ is equal to the sum of the reciprocal products of degrees of pairs of adjacent vertices [42], that is,

$$M_2^*(G) = \sum_{v_i v_j \in E(G)} \frac{1}{d_i\, d_j} \, .$$

In 1975, Randić proposed topological index based on the degree of the vertices of an edge which defined as:

$$R(G) = \sum_{v_i v_j \in E(G)} \frac{1}{\sqrt{d_i\, d_j}} \, .$$

We refer to the monographs [28, 37] and the survey article [38] for the various results on the Randić index.

Let $G = (V, E)$. If $V(G)$ is the disjoint union of two nonempty sets $V_1(G)$ and $V_2(G)$ such that every vertex in $V_1(G)$ has degree r and every vertex in $V_2(G)$ has degree s $(r \geq s)$, then G is an (r, s)-semiregular graph. When $r = s$, then G is a regular graph.

In [34], Hemmasi and Iranmanesh gave some lower and upper bounds on the ABC index in terms of Randić index, first Zagreb index, second Zagreb index, and modified second Zagreb index. Several of these bounds were erroneous. In this paper we offer corrected versions of these results.

2 Main Results

First we correct a typo in Theorem 3.1 of [34]. The correct statement is the following.

Theorem 1. *Let G be a connected graph with m edges, maximum degree Δ, and minimum degree δ. Then*

$$\frac{m\sqrt{2\,\delta-2}}{\Delta} \le ABC(G) \le \frac{m\sqrt{2\,\Delta-2}}{\delta}$$

with equality holding if and only if G is regular.

Theorem 3.2 in [34] is not true. The correct statement is as follows. We omit the proof because it is similar to the proof of Theorem 3.2 in [34].

Theorem 2. *Let G be a connected graph with m edges, maximum degree Δ, and minimum degree δ. Then*

$$R(G)\sqrt{2\,\delta-2} \le ABC(G) \le R(G)\sqrt{2\,\Delta-2}$$

with equality holding if and only if G is regular.

Theorem 3.3 in [34] is not correct because the authors used the wrong Lemma 2.1 (Chebyshev's inequality). First we state Chebyshev's inequality:

Lemma 1. (Chebyshev's inequality) *Let $a_1 \ge a_2 \ge \cdots \ge a_n$ and $b_1 \ge b_2 \ge \cdots \ge b_n$ be real numbers. Then*

$$n\sum_{i=1}^{n} a_i\,b_i \ge \left(\sum_{i=1}^{n} a_i\right)\left(\sum_{i=1}^{n} b_i\right)$$

with equality holding if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$.

So Lemma 2.1 in [34] is not correct. In general, we cannot use this lemma for finding the result stated in [34] as Theorem 3.3. Moreover, another mistake in this theorem is that n should be replaced by m.

In [34], in connection with Theorem 3.4 the Diaz–Metcalf inequality is mentioned.

Lemma 2. (Diaz–Metcalf inequality). *If a_i and b_i are real numbers such that $ha_i \le b_i \le Ha_i$ for $i = 1, 2, \ldots, m$, then*

$$\sum_{i=1}^{m} b_i^2 + hH\sum_{i=1}^{m} a_i^2 \le (h+H)\sum_{i=1}^{m} a_i\,b_i$$

with equality holding if and only if $b_i = ha_i$ or $b_i = Ha_i$ for $i = 1, 2, \ldots, m$.

Theorem 3.4 in [34] is not correct. For example, if G is an r-regular graph ($r > n/2$), then

$$\frac{M_1(G) - 2m + 2\,\Delta\,\delta\,\sqrt{(\Delta-1)\,(\delta-1)}}{\Delta\sqrt{2(\Delta-1)} + \delta\sqrt{2(\delta-1)}} \;=\; (n+2r)\sqrt{\frac{r-1}{8}}$$

$$> \sqrt{\frac{2(r-1)}{r^2}} \cdot \frac{nr}{2} = ABC(G)\,.$$

Using the same technique in the proof of Theorem 3.4 in [34], we now give its correct statement:

Theorem 3. *Let G be a simple connected graph with n vertices and m edges. Then*

$$\frac{M_1(G) - 2m + 2\,\Delta\,\delta\,M_2^*(G)\,\sqrt{(\Delta-1)\,(\delta-1)}}{\Delta\sqrt{2(\Delta-1)} + \delta\sqrt{2(\delta-1)}} \le ABC(G) \tag{2}$$

with equality holding if and only if G is regular.

Proof. Setting that in Lemma 2, each i corresponds to an edge $v_jv_k \in E(G)$ and

$$b_{jk} = \sqrt{d_j + d_k - 2}\;\;,\;\; a_{jk} = \frac{1}{\sqrt{d_j\,d_k}}\;\;,\;\; h = \delta\sqrt{2\,(\delta-1)}\;\;,\;\; H = \Delta\sqrt{2\,(\Delta-1)}$$

we get

$$\sum_{v_jv_k\in E(G)} (d_j + d_k - 2) + 2\,\Delta\,\delta\,\sqrt{(\Delta-1)\,(\delta-1)} \sum_{v_jv_k\in E(G)} \frac{1}{d_j\,d_k}$$

$$\le \left[\delta\sqrt{2\,(\delta-1)} + \Delta\sqrt{2\,(\Delta-1)}\right] \sum_{v_jv_k\in E(G)} \sqrt{\frac{d_j+d_k-2}{d_j\,d_k}}\,. \tag{3}$$

From the above, we arrive at the required result (2). The first part of the proof is done.

Suppose that equality holds in (2). Then the inequality in (3) must be equality. By Lemma 2, for each edge $v_jv_k \in E(G)$, we have

$$d_j\,d_k\,(d_j + d_k - 2) = 2\,\delta^2\,(\delta-1) \qquad \text{or} \qquad d_j\,d_k\,(d_j + d_k - 2) = 2\,\Delta^2\,(\Delta-1)$$

that is,

$$d_j = d_k = \delta \qquad \text{or} \qquad d_j = d_k = \Delta\,.$$

Since G is connected, it must be $d_i = \Delta = \delta$ for $v_i \in V(G)$. Hence G is a regular graphs.

Conversely, one can see easily that the equality holds in (2) for regular graph. $\square$

Corollary 3. *Let G be a simple connected graph with n vertices and m edges. Then*

$$\frac{M_1(G) - 2m + n\,\delta\,\sqrt{(\Delta-1)\,(\delta-1)}}{\Delta\sqrt{2(\Delta-1)} + \delta\sqrt{2(\delta-1)}} \leq ABC(G) \tag{4}$$

with equality holding if and only if G is regular.

Proof. Since

$$\sum_{i=1}^{m} \frac{1}{d_{u_i}\,d_{v_i}} = \frac{1}{2}\sum_{i=1}^{n}\sum_{v_j:\,v_iv_j\in E(G)} \frac{1}{d_i\,d_j} \geq \frac{1}{2}\sum_{i=1}^{n}\frac{1}{\Delta} = \frac{n}{2\,\Delta}$$

from (2), we get the required result (4). Moreover, equality holds in (4) if and only if G is regular. □

In [34], the following inequality is mentioned:

Lemma 4. (Pólya–Szegő inequality, according to [34]) *Suppose a_i and b_i are positive real numbers for $i = 1, 2, \ldots, m$, such that $a \leq a_i \leq A$ and $b \leq b_i \leq B$, then*

$$\frac{\sum\limits_{i=1}^{n} a_i^2 \sum\limits_{i=1}^{n} b_i^2}{\left(\sum\limits_{i=1}^{n} a_i\,b_i\right)^2} \leq \frac{1}{4}\left(\sqrt{\frac{AB}{ab}} + \sqrt{\frac{ab}{AB}}\right)^2. \tag{5}$$

The inequality becomes an equality if and only if

$$\rho = \frac{A/a}{A/a + B/b}\,n \qquad \textit{and} \qquad \sigma = \frac{B/b}{A/a + B/b}\,n$$

are integers, $a_1 = a_2 = \cdots = a_\rho = a$, $a_{\rho+1} = a_{\rho=2} = \cdots = a_n = A$, $b_1 = b_2 = \cdots = b_\sigma = B$, and $b_{\sigma+1} = b_{\sigma+2} = \cdots = b_n = b$.

This lemma is wrongly written. The inequality is correct, but the characterization of the equality case is not. For odd n with $a = a_1 = \cdots = a_n = A$ and $b = b_1 = \cdots = b_n = B$, the equality holds in (5), but the characterization in the lemma is not correct (ρ and σ are not integers). Moreover, Theorem 3.5 in [34] is wrong. Using Lemma 4, we obtain the following result (this is the corrected statement of Theorem 3.5 in [34]):

Theorem 4. *Let G be a simple connected graph with n vertices and m edges. Then*

$$ABC(G) \geq \frac{\sqrt{8\Delta\,\delta}\sqrt{(M_1(G)-2m)\,M_2^*(G)\sqrt{(\Delta-1)\,(\delta-1)}}}{\Delta\sqrt{2(\Delta-1)} + \delta\sqrt{2(\delta-1)}}. \tag{6}$$

In [34], in Theorem 3.6, Hemmasi and Iranmanesh gave an upper bound on $ABC(G)$, but did not characterize the extremal graphs. Here we characterize the extremal graphs. For completeness we also include the upper bound.

Theorem 5. *Let G be a connected graph with n vertices and m edges. Then*

$$\big[M_1(G) - 2m\big]\, M_2^*(G) \geq ABC(G)^2 \tag{7}$$

with equality holding if and only if G is a regular graph or G is a bipartite semiregular graph.

Proof. By the Cauchy–Schwarz inequality, we have

$$\left(\sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i\, d_j}}\right)^2 \leq \sum_{v_iv_j \in E(G)} (d_i + d_j - 2) \sum_{v_iv_j \in E(G)} \frac{1}{d_i\, d_j}$$

from which inequality (7) straightforwardly follows.

Suppose that equality holds in (7). Then by the Cauchy–Schwarz inequality,

$$(d_i + d_j - 2)\, d_i\, d_j = (d_i + d_k - 2)\, d_i\, d_k$$

for any edges v_iv_j , $v_iv_k \in E(G)$, that is,

$$(d_j - d_k)\,(d_i + d_j + d_k - 2) = 0$$

that is, $d_j = d_k$ for any edges v_iv_j , $v_iv_k \in E(G)$. Hence we conclude that G is a regular graph or a bipartite semiregular graph.

Conversely, one can see easily that the equality holds in (7) for regular graph or bipartite semiregular graph. □

In [34], the equality in Theorem 3.9 is not correct. From the proof, we can get the correct statement as follows:

Theorem 6. *Let G be a connected graph with m edges, maximum degree Δ, and minimum degree δ. Then*

$$ABC(G) < \frac{m\,(\Delta + \delta)}{\sqrt{\Delta\, \delta}}\,.$$

In [34], the inequality in Theorem 3.10 is correct, but the equality case is not. The proof is same as the proof of Theorem 3.10 of [34], but the inequality is strict because this proof depends on the inequality in Theorem 6. The correct statement is the following:

Theorem 7. *Let G and $\overline{G}$ be a connected graphs of order n. Then*

$$ABC(G) + ABC(\overline{G}) < \binom{n}{2} \frac{k^2 + 1}{k}$$

where

$$k = \max\left\{\sqrt{\frac{\Delta}{\delta}}, \sqrt{\frac{n-1-\delta}{n-1-\Delta}}\right\}.$$

In [34], in Theorem 3.12 the following upper bound for ABC is claimed to hold:

$$ABC(G) \leq \rho\sqrt{\frac{\delta-1}{\Delta}} \tag{8}$$

where ρ, Δ, and δ are the number of pendent vertices, the maximum degree, and the minimum degree of the graph G, respectively.

The right–hand side of (8) is always equal to zero, implying the impossible inequality $ABC(G) \leq 0$.

Indeed, if the minimum degree δ is greater than 1, then $\rho = 0$ and thus the right–hand side of (8) is equal to zero. Otherwise, $\delta = 1$, and thus $\sqrt{(\delta-1)/\Delta} = 0$.

Besides, the proof of Theorem 3.12 in [34] is totally wrong.

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