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On atom–bond connectivity index

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Abstract. The atom–bond connectivity index (ABC) is a vertex–degree based graph invariant, put forward in the 1990s, having applications in chemistry. Let $G = (V, E)$ be a graph, d_i the degree of its vertex i, and ij the edge connecting the vertices i and j. Then $ABC = \sum_{ij \in E} \sqrt{(d_i + d_j - 2)/(d_i\, d_j)}$. Upper bounds and Nordhaus–Gaddum type results for ABC are established.

1. Introduction

Several graph invariants found applications and are currently used in chemistry, pharmacology, environmental sciences, etc. [10, 15, 16]. One of these is the so-called "*atom–bond connectivity index*" (ABC). It is defined as follows [6].

Let $G = (V(G), E(G))$ be a graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. The degree (= number of first neighbors) of a vertex $i \in V(G)$ is denoted by d_i. The edge connecting the vertices i and j is denoted by ij. Then

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

In [6] it was shown that ABC can be used for modeling thermodynamic properties of organic chemical compounds. However, this paper did not receive much attention. In 2008, Estrada published another paper, applying ABC as tool for explaining the stability of branched alkanes [5]. Contrary to [6], this work attracted the attention of mathematically oriented scholars, resulting in a remarkable number of researches on the mathematical properties of the ABC index [1–4, 7–9, 12, 17–19]. In the present paper we report a few more, hitherto unpublished, results on ABC.

We first define the graph theoretic notions that will be used in the subsequent parts of the paper.

The maximal and minimal vertex degree of the graph $G = (V(G), E(G))$ is denoted by Δ and δ, respectively. A vertex i is said to be pendent if $d_i = 1$. The minimal degree of a non-pendent vertex is δ_1. An edge of a graph is said to be pendent if one of its end-vertices is pendent.

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The set of first neighbors of the vertex i is denoted by N_i. Evidently, $|N_i| = d_i$.

The Zagreb indices are well-known graph invariants, introduced almost 40 years ago [15, 16], defined as:

$$M_1 = M_1(G) = \sum_{i \in V(G)} d_i^2 \qquad \text{and} \qquad M_2 = M_2(G) = \sum_{ij \in E(G)} d_i\, d_j\,.$$

A recently proposed variant of the second Zagreb index, denoted by M_2^* and defined as [13]:

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

is known under the name "modified second Zagreb index".

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 $(r \leq s)$, then G is (r, s)–semiregular. If $r = s$, then G is said to be regular. As usual [11], the complete graph, complete bipartite graph, the star, and the path are denoted as K_n, $K_{p,q}$ $(p + q = n)$, $K_{1,n-1}$, and P_n, respectively.

2. Upper bound on ABC index

Upper bounds for the *ABC* index were earlier obtained in [2, 3]. In particular, inequality (2) was reported in [3], but without the characterization of the equality cases (which seems to be its most difficult aspect).

Our starting point is the well– known Cauchy–Schwarz inequality:

Lemma 2.1. *If $\bar{a} = (a_1, a_2, \ldots, a_n)$ and $\bar{b} = (b_1, b_2, \ldots, b_n)$ are sequences of real numbers, then*

$$\left(\sum_{i=1}^{n} a_i\, b_i \right)^2 \leq \sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2$$

with equality if and only if the sequences $\bar{a}$ and $\bar{b}$ are proportional, i. e., there is a $\lambda \in \mathbb{R}$ such that $a_k = \lambda\, b_k$ for each $k \in \{1, 2, \ldots, n\}$.

Theorem 2.2. *Let G be a connected graph with n vertices, p pendent vertices, m edges, maximal degree Δ, and minimal non-pendent vertex degree δ_1. Let M_1 and M_2^* be the first and modified second Zagreb indices of G. Then*

$$ABC(G) \leq p \sqrt{1 - \frac{1}{\Delta}} + \sqrt{[M_1 - 2m - p(\delta_1 - 1)] \left(M_2^* - \frac{p}{\Delta} \right)}\,. \tag{2}$$

Equality in (2) holds if and only if G is regular or $(1, \Delta)$-semiregular or bipartite semiregular.

Recall that for $r \neq s$, a graph G is said to be (r, s)-semiregular if its vertex degrees assume only the values r and s, and if there is at least one vertex of degree r and at least one of degree s. If every vertex of degree r is adjacent to vertices of degree s and vice versa, then G is bipartite (r, s)-semiregular. In Theorem 2.2, under "bipartite semiregular" is meant bipartite (r, s)-semiregular with arbitrary r and s.

Proof. Using $a_{ij} = \sqrt{d_i + d_j - 2}$ and $b_{ij} = 1/\sqrt{d_i\, d_j}$, for each edge $ij \in E(G)$, such that both vertex degrees d_i

and d_j are greater than unity, in Lemma 2.1, we get

$$\begin{aligned}
\left(\sum_{\substack{ij\in E(G)\\ d_i,d_j\neq 1}} \sqrt{\frac{d_i+d_j-2}{d_i\,d_j}}\right)^2 &= \left(\sum_{\substack{ij\in E(G)\\ d_i,d_j\neq 1}} \frac{\sqrt{d_i+d_j-2}}{\sqrt{d_i\,d_j}}\right)^2 \\
&\leq \sum_{\substack{ij\in E(G)\\ d_i,d_j\neq 1}} (d_i+d_j-2) \sum_{\substack{ij\in E(G)\\ d_i,d_j\neq 1}} \frac{1}{d_i\,d_j} \qquad (3)\\
&= \left(\sum_{ij\in E(G)} (d_i+d_j-2) - \sum_{\substack{ij\in E(G)\\ d_i=1}} (d_j-1)\right)\left(\sum_{ij\in E(G)} \frac{1}{d_i\,d_j} - \sum_{\substack{ij\in E(G)\\ d_i=1}} \frac{1}{d_j}\right)\\
&\leq [M_1-2m-p(\delta_1-1)]\left(M_2^*-\frac{p}{\Delta}\right) \qquad (4)
\end{aligned}$$

since $\sum_{ij\in E(G)} (d_i+d_j)=M_1$ and $\delta_1\leq d_i\leq\Delta$. Therefrom inequality (2) follows directly from the definition (1).

The examination of the equality case in (2) is somewhat lengthy.

Suppose that equality holds in (2). Then all inequalities in the above argument must be equalities. We have to consider two cases (i) $p>0$, (ii) $p=0$.

Case (i): From $1-1/d_j=1-1/\Delta$, we get $d_j=\Delta$ for $v_iv_j\in E(G)$, $d_i=1$.

From equality in (4), we get $d_j=\delta_1$ for $v_iv_j\in E(G)$, $d_i=1$.

From these results follows $\Delta=\delta_1$. Hence G is isomorphic to a $(\Delta,1)$–semiregular graph.

Case (ii): In this case $\delta=\delta_1\geq 2$. From equality in (3), for any two adjacent edges $v_iv_j\in E(G)$, $v_iv_k\in E(G)$,

$$\sqrt{d_i\,d_j}\,\sqrt{d_i+d_j-2}=\sqrt{d_i\,d_k}\,\sqrt{d_i+d_k-2}$$

i. e., $\quad d_i\,d_j+d_j^2-2d_j=d_i\,d_k+d_k^2-2d_k$ as $d_i\neq 0$

i. e., $\quad (d_j-d_k)(d_i+d_j+d_k-2)=0$

i. e., $\quad d_j=d_k$ since $d_i+d_j+d_k>2$. (5)

Suppose that $d_i=r$. Then by (5), all vertices adjacent to the vertex v_i are of the same degree (say, s), and all vertices adjacent to the vertex v_j, $v_iv_j\in E(G)$, are of degree r. Using (5) and the fact that G is connected, it follows that each vertex of degree r is adjacent to vertices of degree s, and each vertex of degree s is adjacent to vertices of degree r. Thus G is a bipartite semiregular graph or G is a regular graph.

Conversely, let G be a $(\Delta,1)$–semiregular graph. Then, $M_1(G)=(n-p)\Delta^2+p$, $M_2^*(G)=p/\Delta+(m-p)/\Delta^2$, and $(n-p)\Delta=2(m-p)+p$. Using these relations, we get

$$[M_1(G)-2m-p(\delta_1-1)]\left[M_2^*(G)-\frac{p}{\Delta}\right] = \left[(n-p)\Delta^2+2p-2m-p\Delta\right]\frac{(m-p)}{\Delta^2}=\frac{2(\Delta-1)}{\Delta^2}(m-p)^2\,.$$

Hence equality holds in (2).

Let G be an r-regular graph. Then

$$\sqrt{(M_1(G)-2m)M_2^*(G)}=\sqrt{(nr^2-nr)\frac{m}{r^2}}=m\sqrt{\frac{2}{r}-\frac{2}{r^2}}=ABC(G)$$

since $2m = nr$.

Let G be a bipartite (r,s)–semiregular graph. Also, let k be the number of vertices of degree r, and ℓ be the number of vertices of degree s. Then $kr = \ell s = m$ and we have

$$\sqrt{(M_1(G)-2m)M_2^*(G)} = \sqrt{(kr^2+\ell s^2-2m)\frac{m}{rs}} = m\sqrt{\frac{1}{r}+\frac{1}{s}-\frac{2}{rs}} = ABC(G)$$

which completes the proof of Theorem 2.2. □

By setting $p = 0$ in Theorem 2.2, we get:

Corollary 2.3. *With the same notation as in Theorem 2.2,*

$$ABC(G) \leq \sqrt{(M_1-2m)\,M_2^*}\,. \tag{6}$$

Equality in (6) holds if and only if G is regular or bipartite semiregular.

Corollary 2.4. [2] *With the same notation as in Theorem 2.2,*

$$ABC(G) \leq p\,\sqrt{1-\frac{1}{\Delta}} + \frac{m-p}{\delta_1}\,\sqrt{2(\delta_1-1)}\,. \tag{7}$$

The case of equality in (7) is complicated and has been determined in [2].

3. Nordhaus–Gaddum–type results for ABC index

Motivated by the seminar work of Noradhaus and Gaddum [14], we report here analogous results for the *ABC* index. For this we need:

Lemma 3.1. [2] *Let G be a simple connected graph with m edges and maximal vertex degree Δ. Then*

$$ABC(G) \geq \frac{2^{7/4}\,m\,\sqrt{\Delta-1}}{\Delta^{3/4}\left(\sqrt{\Delta}+\sqrt{2}\right)} \tag{8}$$

where equality is attained if and only if $G \cong P_n$.

Theorem 3.2. *Let G be a simple connected graph of order n with connected complement $\overline{G}$. Then*

$$ABC(G) + ABC(\overline{G}) \geq \frac{2^{3/4}\,n(n-1)\,\sqrt{k-1}}{k^{3/4}\left(\sqrt{k}+\sqrt{2}\right)} \tag{9}$$

where $k = \max\{\Delta, n-\delta-1\}$, and where Δ and δ are the maximal and minimal vertex degrees of G. Moreover, equality in (9) holds if and only if $G \cong P_4$.

Proof. We start by inequality (8). Let $\overline{m}$ and $\overline{\Delta}$ be the number of edges and maximal vertex degree in $\overline{G}$. Then

$$\begin{aligned} ABC(G) + ABC(\overline{G}) &\geq \frac{2^{7/4}\,m\,\sqrt{\Delta-1}}{\Delta^{3/4}\left(\sqrt{\Delta}+\sqrt{2}\right)} + \frac{2^{7/4}\,\overline{m}\,\sqrt{\overline{\Delta}-1}}{\overline{\Delta}^{3/4}\left(\sqrt{\overline{\Delta}}+\sqrt{2}\right)} \\ &= \frac{2^{3/4}\,2m\,\sqrt{\Delta-1}}{\Delta^{3/4}\left(\sqrt{\Delta}+\sqrt{2}\right)} + \frac{2^{3/4}\,(n(n-1)-2m)\,\sqrt{n-\delta-2}}{(n-\delta-1)^{3/4}\left(\sqrt{n-\delta-1}+\sqrt{2}\right)}\,. \end{aligned} \tag{10}$$

Consider the function

$$f(x)=\frac{\sqrt{x-1}}{x^{3/4}\left(\sqrt{x}+\sqrt{2}\right)}$$

for which one can easily show that it monotonically decreases in the interval $[2,\infty]$. Thus

$$\frac{\sqrt{\Delta-1}}{\Delta^{3/4}\,(\sqrt{\Delta}+\sqrt{2})}\geq\frac{\sqrt{k-1}}{k^{3/4}\,(\sqrt{k}+\sqrt{2})}\leq\frac{\sqrt{n-\delta-2}}{(n-\delta-1)^{3/4}\,(\sqrt{n-\delta-1}+\sqrt{2})}\tag{11}$$

since $k\geq\Delta$ and $k\geq n-\delta-1$. Since $2\overline{m}=n(n-1)-2m$, combining the above results with (10), we arrive at (9).

It remains to examine the equality case. It is easy to check that equality in (9) holds if $G\cong P_4$. Suppose now that equality holds in (9). Then all inequalities in (11) must be equalities, and we get $k=\Delta=n-1-\delta$. Equality in (10) implies $G\cong P_n$ and $\overline{G}\cong P_n$. Hence $G\cong P_4$. By this the proof of Theorem 3.2 has been completed. □

Theorem 3.3. *Let G be a simple connected graph of order n with connected complement $\overline{G}$. Then*

$$ABC(G)+ABC(\overline{G})\leq(p+\overline{p})\,\sqrt{\frac{n-3}{n-2}}\left(1-\sqrt{\frac{2}{n-2}}\right)+\binom{n}{2}\sqrt{\frac{2}{k}-\frac{2}{k^2}}\tag{12}$$

where p, $\overline{p}$ and δ_1, $\overline{\delta}_1$ are the number of pendent vertices and minimal non–pendent vertex degrees in G and $\overline{G}$, respectively, and $k=\min\{\delta_1,\overline{\delta}_1\}$. Equality holds in (12) if and only if $G\cong P_4$ or G is an r-regular graph of order $2r+1$.

Proof. We have $\Delta\leq n-2$, as G and $\overline{G}$ are connected, and hence

$$1-\frac{1}{\Delta}\leq\frac{n-3}{n-2}\qquad\text{and}\qquad\frac{2}{\delta_1}-\frac{2}{\delta_1^2}\geq\frac{2(n-3)}{(n-2)^2}\,.$$

Bearing in mind (7), we get

$$\begin{aligned}ABC(G)\ &\leq\ p\,\sqrt{\frac{n-3}{n-2}}-p\,\sqrt{\frac{2(n-3)}{(n-2)^2}}+m\,\sqrt{\frac{2}{\delta_1}-\frac{2}{\delta_1^2}}\\ &=\ p\,\sqrt{\frac{n-3}{n-2}}\left(1-\sqrt{\frac{2}{n-2}}\right)+m\,\sqrt{\frac{2}{\delta_1}-\frac{2}{\delta_1^2}}\end{aligned}\tag{13}$$

from which there holds

$$ABC(G)+ABC(\overline{G})\ \leq\ (p+\overline{p})\,\sqrt{\frac{n-3}{n-2}}\left(1-\sqrt{\frac{2}{n-2}}\right)+m\,\sqrt{\frac{2}{\delta_1}-\frac{2}{\delta_1^2}}+\overline{m}\,\sqrt{\frac{2}{\overline{\delta}_1}-\frac{2}{\overline{\delta}_1^2}}\tag{14}$$

$$\leq\ (p+\overline{p})\,\sqrt{\frac{n-3}{n-2}}\left(1-\sqrt{\frac{2}{n-2}}\right)+(m+\overline{m})\,\sqrt{\frac{2}{k}-\frac{2}{k^2}}\tag{15}$$

as $k\leq\delta_1,\overline{\delta}_1$.

Since $m+\overline{m}=\binom{n}{2}$, from (15), we get the required result (12).

We now examine the equality case.

Suppose that equality holds in (12). Then all inequalities in the above argument must be equalities. From equality in (13) we get $\Delta = \delta_1 = n-2$, $p \neq 0$, that is, $G \cong P_4$ or G is isomorphic to a regular graph, by Lemma 2.4.

Equality in (14) implies that (*i*) $G \cong P_4$ or G is isomorphic to a regular graph and (*ii*) $\overline{G} \cong P_4$ or $\overline{G}$ is isomorphic to a regular graph.

From equality in (15), we get $\delta_1 = \overline{\delta}_1$.

Using the above results, and recalling that $\overline{P_4} \cong P_4$, we conclude that $G \cong P_4$ or G is isomorphic to an r-regular graph with $n = 2r+1$.

Conversely, one can easily see that equality in (12) holds for the path P_4 and for an r-regular graph of order $2r+1$. $\square$

References

[1] J. Chen, X. Guo, Extreme atom–bond connectivity index of graphs, MATCH Commun. Math. Comput. Chem. 65 (2011) 713–722.
[2] K. C. Das, Atom–bond connectivity index of graphs, Discr. Appl. Math. 158 (2010) 1181–1188.
[3] K. C. Das, I. Gutman, B. Furtula, On atom–bond connectivity index, Chem. Phys. Lett. 511 (2011) 452–454.
[4] K. C. Das, N. Trinajstić, Comparison between first geometric–arithmetic index and atom–bond connectivity index, Chem. Phys. Lett. 497 (2010) 149–151.
[5] E. Estrada, Atom–bond connectivity and the energetic of branched alkanes, Chem. Phys. Lett. 463 (2008) 422–425.
[6] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom–bond connectivity index: Modelling the enthalpy of formation of alkanes, Indian J. Chem. 37A (1998) 849–855.
[7] G. A. Fath–Tabar, B. Vaez–Zadah, A. R. Ashrafi, A. Graovac, Some inequalities for the atom–bond connectivity index of graph operations, Discr. Appl. Math. 159 (2011) 1323–1330.
[8] B. Furtula, A. Graovac, D. Vukičević, Atom–bond connectivity index of trees, Discr. Appl. Math. 157 (2009) 2828–2835.
[9] L. Gan, H. Hou, B. Liu, Some results on atom–bond connectivity index of graphs, MATCH Commun. Math. Comput. Chem. 66 (2011) 669–680.
[10] I. Gutman, B. Furtula (Eds.) Novel Molecular Structure Descriptors – Theory and Applications, Vols. I & II, Univ. Kragujevac, Kragujevac, 2010.
[11] F. Harary, Graph Theory, Addison–Wesley, Reading, 1969.
[12] B. Horoldagva, I. Gutman, On some vertex–degree–based graph invariants, MATCH Commun. Math. Comput. Chem. 65 (2011) 723–730.
[13] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, Croat. Chem. Acta 76 (2003) 113–124.
[14] E. A. Nordhaus, J. W. Gaddum, On complementary graphs, Amer. Math. Monthly 63 (1956) 175–177.
[15] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley–VCH, Weinheim, 2000.
[16] R. Todeschini, V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley–VCH, Weinheim, 2009.
[17] R. Xing, B. Zhou, F. Dong, On atom–bond connectivity index of connected graphs, Discr. Appl. Math., in press.
[18] R. Xing, B. Zhou, Z. Du, Further results on atom–bond connectivity index of trees, Discr. Appl. Math. 157 (2010) 1536–1545.
[19] B. Zhou, R. Xing, On atom–bond connectivity index, Z. Naturforsch. 66a (2011) 61–66.