MATEMATIKA, 2016, Volume 32, Number 2, 81–86

Atom-bond connectivity index of graph with two edges added

[1]Mohamad Nazri Husin and [2]Roslan Hasni
School of Informatics and Applied Mathematics
University Malaysia Terengganu
21030 UMT Kuala Nerus, Terengganu, Malaysia
e-mail: [1]naz_reyhusin@yahoo.com, [2]hroslan@umt.edu.my

Abstract The atom-bond connectivity index of a graph G, denoted as $ABC(G)$, is defined as the sum of the weight

$$\sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

of all edges uv of G, where d_u (or d_v) denotes the degree of vertex u (or v) in G. The ABC index provides a good model for the stability of linear and branches alkanes as well as the strain energy of cycloalkanes. In this note, we prove that ABC index of a graph increases when two new edges are added.

Keywords Atom-bond connectivity index; Graph

2010 Mathematics Subject Classification 05C07, 05C90

1 Introduction

All graphs considered here are finite, simple and undirected. The vertex and edge set of G are denoted by $V(G)$ and $E(G)$, respectively. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. For terminologies and notations that are not defined here, please refer West [1].

A graphical invariance is a number related to a graph which is structurally invariant, that is to say it is fixed under graph automorphisms. In chemistry and for chemical graphs, these invariant numbers are known as the topological indices. One of the most important topological indices is the Randic index [2]. But a great variety of physico-chemical properties rest on factors rather than branching. Accordingly, Estrada *et al.* [3] proposed a new index, known as the atom-bond connectivity index of graph G, denoted as $ABC(G)$, is defined as the sum of the weight

$$\sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \tag{1}$$

of all edges uv of G, where d_u (or d_v) denotes the degree of vertex u (or v) in G. The ABC index keeps the spirit of Randic index, and it provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [3, 4]. Some properties of ABC index for trees have been studied in [5, 6]. More mathematical properties for the ABC index may be found in [7–9]. Chen and Guo [10] proved that the ABC index of graph decreases when any edge is deleted. Das *et al.* [11] studied the change of the ABC index when a new edge is inserted into the underlying graph. In this paper, we shall investigate the behaviour of the ABC index when two edges are inserted into the underlying graph. This result was obtained by using the same approach in [11].

2 Main result

We first give some examples of the ABC index for simple graphs. Let P_n, C_n, K_n denote the path, cycle and complete graphs with n vertices, respectively.

Example 1 For $n \geq 3$,

1. $ABC(P_n) = \frac{\sqrt{2}}{2}(n-1)$,
2. $ABC(C_n) = \frac{\sqrt{2}}{2}n$,
3. $ABC(K_n) = \frac{\sqrt{2}}{2}n\sqrt{n-2}$.

Assume that the vertices i and j of graph G are not adjacent. Let $G + \{ij\}$ denotes the graph formed from G by adding the new edge ij into G.

Theorem 1 [11] *Let G be a simple graph with non-adjacent vertices i and j. Then*

$$ABC(G + \{ij\}) > ABC(G).$$

Let $G - uv$ denotes the graph obtained by deleting the edge uv from graph G.

Theorem 2 [10] *Let x_1x_2 be an edge of a graph G and x_1x_2 is not an isolate edge, then*

$$ABC(G - x_1x_2) < ABC(G).$$

Let G be a graph with n vertices. Suppose that the vertices i, j, p, q of G are not adjacent, and insert two new edges $\{ij, pq\}$ to obtain the new graph $G + \{ij, pq\}$.

Now we give our main result.

Theorem 3 *Let G be a simple graph with non-adjacent vertices i, j, p, q. Then*

$$ABC(G + \{ij, pq\}) > ABC(G).$$

Proof Note first that

$$\sqrt{d_i+1} = \sqrt{d_i}\sqrt{1+\frac{1}{d_i}} < \sqrt{d_i}\Big(1+\frac{1}{2d_i}\Big) = \sqrt{d_i} + \frac{1}{2\sqrt{d_i}}, \tag{2}$$

$$\begin{aligned}\sqrt{d_i+d_k-2} &= \sqrt{d_i+d_k-1}\Big(1-\frac{1}{d_i+d_k-1}\Big)^{1/2} \\ &< \sqrt{d_i+d_k-1}\Big(1-\frac{1}{2(d_i+d_k-1)}\Big),\end{aligned} \tag{3}$$

$$\sqrt{d_p+1} = \sqrt{d_p}\sqrt{1+\frac{1}{d_p}} < \sqrt{d_p}\Big(1+\frac{1}{2d_p}\Big) = \sqrt{d_p} + \frac{1}{2\sqrt{d_p}}, \tag{4}$$

$$\begin{aligned}\sqrt{d_p+d_r-2} &= \sqrt{d_p+d_r-1}\Big(1-\frac{1}{d_p+d_r-1}\Big)^{1/2}\\ &< \sqrt{d_p+d_r-1}\Big(1-\frac{1}{2(d_p+d_r-1)}\Big),\end{aligned} \tag{5}$$

and consider the difference between the ABC indices of $G+\{ij,pq\}$ with G:

$$\begin{aligned}&ABC(G+\{ij,pq\})-ABC(G)=\\ &\quad\sum_{k\in N_i}\Big[\sqrt{\frac{1}{d_i+1}+\frac{1}{d_k}-\frac{2}{(d_i+1)d_k}}-\sqrt{\frac{1}{d_i}+\frac{1}{d_k}-\frac{2}{d_id_k}}\Big]+\\ &\quad\sum_{k\in N_j}\Big[\sqrt{\frac{1}{d_j+1}+\frac{1}{d_k}-\frac{2}{(d_j+1)d_k}}-\sqrt{\frac{1}{d_j}+\frac{1}{d_k}-\frac{2}{d_jd_k}}\Big]+\\ &\quad\sqrt{\frac{1}{d_i+1}+\frac{1}{d_j+1}-\frac{2}{(d_i+1)(d_j+1)}}+\\ &\quad\sum_{r\in N_p}\Big[\sqrt{\frac{1}{d_p+1}+\frac{1}{d_r}-\frac{2}{(d_p+1)d_r}}-\sqrt{\frac{1}{d_p}+\frac{1}{d_r}-\frac{2}{d_pd_r}}\Big]+\\ &\quad\sum_{r\in N_q}\Big[\sqrt{\frac{1}{d_q+1}+\frac{1}{d_r}-\frac{2}{(d_q+1)d_r}}-\sqrt{\frac{1}{d_q}+\frac{1}{d_r}-\frac{2}{d_qd_r}}\Big]+\\ &\quad\sqrt{\frac{1}{d_p+1}+\frac{1}{d_q+1}-\frac{2}{(d_p+1)(d_q+1)}}.\end{aligned} \tag{6}$$

Bearing in mind inequalities (2) and (3), we get

$$\begin{aligned}&\sqrt{\frac{1}{d_i}+\frac{1}{d_k}-\frac{2}{d_id_k}}-\sqrt{\frac{1}{d_i+1}+\frac{1}{d_k}-\frac{2}{(d_i+1)d_k}}\\ &\quad=\frac{\sqrt{d_i+1}\sqrt{d_i+d_k-2}-\sqrt{d_i}\sqrt{d_i+d_k-1}}{\sqrt{d_kd_i(d_i+1)}}\\ &\quad<\frac{\sqrt{d_i+d_k-1}}{\sqrt{d_k(d_i+1)}}\Big[\Big(1+\frac{1}{2d_i}\Big)\Big(1-\frac{1}{2(d_i+d_k-1)}\Big)-1\Big]\\ &\quad=\frac{2d_k-3}{4d_i\sqrt{d_k(d_i+1)(d_i+d_k-1)}}<\frac{1}{2d_i\sqrt{d_i+1}}\end{aligned}$$

from which follows

$$\sum_{k\in N_i}\Big[\sqrt{\frac{1}{d_i}+\frac{1}{d_k}-\frac{2}{d_id_k}}-\sqrt{\frac{1}{d_i+1}+\frac{1}{d_k}-\frac{2}{(d_i+1)d_k}}\Big]<\frac{1}{2\sqrt{d_i+1}} \tag{7}$$

and

$$\sum_{k\in N_j}\Big[\sqrt{\frac{1}{d_j}+\frac{1}{d_k}-\frac{2}{d_jd_k}}-\sqrt{\frac{1}{d_j+1}+\frac{1}{d_k}-\frac{2}{(d_j+1)d_k}}\Big]<\frac{1}{2\sqrt{d_j+1}} \tag{8}$$

Similarly, from inequalities (4) and (5), we obtain

$$\sqrt{\frac{1}{d_p}+\frac{1}{d_r}-\frac{2}{d_pd_r}}-\sqrt{\frac{1}{d_p+1}+\frac{1}{d_r}-\frac{2}{(d_p+1)d_r}}<\frac{1}{2d_p\sqrt{d_p+1}}$$

from which follows

$$\sum_{r\in N_p}\Big[\sqrt{\frac{1}{d_p}+\frac{1}{d_r}-\frac{2}{d_pd_r}}-\sqrt{\frac{1}{d_p+1}+\frac{1}{d_r}-\frac{2}{(d_p+1)d_r}}\Big]<\frac{1}{2\sqrt{d_p+1}} \tag{9}$$

and

$$\sum_{r\in N_q}\Big[\sqrt{\frac{1}{d_q}+\frac{1}{d_r}-\frac{2}{d_qd_r}}-\sqrt{\frac{1}{d_q+1}+\frac{1}{d_r}-\frac{2}{(d_q+1)d_r}}\Big]<\frac{1}{2\sqrt{d_q+1}} \tag{10}$$

Without loss of generality, assume that $d_j \le d_i$ and $d_q \le d_p$, and then by simple calculation, we have

$$\frac{1}{2\sqrt{d_i+1}}+\frac{1}{2\sqrt{d_j+1}}<\frac{1}{\sqrt{d_j+1}}\le\frac{\sqrt{d_i+d_j}}{\sqrt{(d_i+1)(d_j+1)}} \tag{11}$$

and

$$\frac{1}{2\sqrt{d_p+1}}+\frac{1}{2\sqrt{d_q+1}}<\frac{1}{\sqrt{d_q+1}}\le\frac{\sqrt{d_p+d_q}}{\sqrt{(d_p+1)(d_q+1)}} \tag{12}$$

Using the formulas (7)–(12), we get

$$\begin{aligned}&\sum_{k\in N_i}\Big[\sqrt{\frac{1}{d_i}+\frac{1}{d_k}-\frac{2}{d_id_k}}-\sqrt{\frac{1}{d_i+1}+\frac{1}{d_k}-\frac{2}{(d_i+1)d_k}}\Big]\\&\quad+\sum_{k\in N_j}\Big[\sqrt{\frac{1}{d_j}+\frac{1}{d_k}-\frac{2}{d_jd_k}}-\sqrt{\frac{1}{d_j+1}+\frac{1}{d_k}-\frac{2}{(d_j+1)d_k}}\Big]\\&\quad<\frac{\sqrt{d_i+d_j}}{\sqrt{(d_i+1)(d_j+1)}}\end{aligned}$$

and

$$\begin{aligned}
&\sum_{r\in N_p}\Big[\sqrt{\frac{1}{d_p}+\frac{1}{d_r}-\frac{2}{d_pd_r}}-\sqrt{\frac{1}{d_p+1}+\frac{1}{d_r}-\frac{2}{(d_p+1)d_r}}\Big]\\
&\quad+\sum_{r\in N_q}\Big[\sqrt{\frac{1}{d_q}+\frac{1}{d_r}-\frac{2}{d_qd_r}}-\sqrt{\frac{1}{d_q+1}+\frac{1}{d_r}-\frac{2}{(d_q+1)d_r}}\Big]\\
&\quad<\frac{\sqrt{d_p+d_q}}{\sqrt{(d_p+1)(d_q+1)}}.
\end{aligned}$$

Combining this with (6), we obtain the result as desired. This completes the proof. □

3 Conclusion

In general, we do not know how the *ABC* index changes when some edges are added or deleted. Das *et al.* [11] studied the change of the *ABC* index when a new edge is inserted into the underlying graph. In this paper, we investigated the behaviour of the *ABC* index when two edges are inserted into the underlying graph. We proved that the *ABC* index of a graph increases when two edges are added. It seems to be very challenging problem to determine the behavior of the *ABC* index when many edges are added (or deleted).

Acknowledgement

The authors are grateful to the anonymous referee for the comments and suggestions that improved this paper.

References

[1] West, D. B. *Introduction to Graph Theory.* 2nd Edition. New Jersey: Prentice-Hall. 2003.

[2] Randic, M. On characterization on molecular branching. *J. Am. Chem. Soc.* 1975. 97: 6609-6615.

[3] Estrada, E., Torres, L., Rodrguez, L. and Gutman, I. An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes. *Indian J. Chem.* 1998. 37A: 849-855.

[4] Estrada, E. Atom-bond connectivity and the energetic of branched alkanes. *Chem. Phys. Lett.* 2008. 463: 422-425.

[5] Furtula, B., Graovac, A. and Vukicevic, D. Atom-bond connectivity index of trees. *Discrete Appl. Math.* 2009. 157: 2828-2835.

[6] Xing, R., Zhou, B. and Du, Z. Further results on atom-bond connectivity index of trees. *Discrete Appl. Math.* 2010. 158: 1536-1545.

[7] Das, K.C. Atom-bond connectivity index of graphs. *Discrete Appl. Math.* 2010. 158: 1181-1188.

[8] Das, K.C. and Trinajstic, N. Comparison between first geometric arithmetic index and atom-bond connectivity index. *Chem. Phys. Lett.* 2010. 497: 149–151

[9] Das, K.C., Gutman, I. and Furtula, B. On atom-bond connectivity index. *Filomat.* 2012. 26(4): 733-738.

[10] Chen, J. and Guo, X. Extreme atom-bond connectivity index of graphs. *MATCH Commun. Chem. Comput. Chem.* 2011. 65: 713-722.

[11] Das, K.C., Gutman, I. and Furtula, B. On atom-bond connectivity index. *Chem. Phys. Lett.* 2011. 511: 452-454.