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On the atom-bond connectivity index and radius of connected graphs

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Abstract

Let G be a connected graph with edge set $E(G)$. The atom-bond connectivity index (ABC index for short) is defined as $ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$, where $d_G(u)$ denotes the degree of vertex u in G. The research of ABC index of graphs is active these years, and it has found a lot of applications in a variety of fields. In this paper, we will focus on the relationship between ABC index and radius of connected graphs. In particular, we determine the upper and lower bounds of the difference between ABC index and radius of connected graphs.

MSC: 05C12; 05C35; 92E10

Keywords: atom-bond connectivity index; degree of vertices; radius

1 Introduction

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $v \in V(G)$, let $d_G(v)$ denote the degree of vertex v in G.

In chemical graph theory, we usually use a graph to represent a molecule graph. One of the most useful tools to study and predict various properties of molecule graphs is the topological indices, which are used directly as simple numerical descriptors in quantitative structure property relationships (QSPR) and quantitative structure activity relationships (QSAR) [1].

In 1998, Estrada *et al.* [2] proposed a topological index based on the degrees of vertices of graphs, which is called the atom-bond connectivity index (ABC index for short). The ABC index of a graph G is defined as [2]

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}}.$$

Initially, in the light of the close relationship between the ABC index and the heats of formation of alkanes, the ABC index became an efficient tool to model the thermodynamic properties of organic chemical compounds [2]. In 2008, Estrada [3] elaborated a novel quantum-theory-like justification for the ABC index and explained the stability of branched alkanes.

Since then, the research on the ABC index of graphs becomes rather active. Xing *et al.* [4] presented an upper bound for the ABC index of connected graphs with fixed number of vertices, number of edges and maximum degree. Das [5] established the lower and upper bounds on ABC index of graphs and trees and showed that these bounds are best possible. Fath-Tabar *et al.* [6] considered the effect on the ABC index of graphs under some graph operations. More results on ABC index of graphs can be found in [7–9], especially for trees [10–12].

In a connected graph G, for $v \in V(G)$, the eccentricity of v in G is defined as the maximum distance from v to another vertex of G. The radius of G, denoted by $r(G)$, is the minimum eccentricity among the vertices in G.

In this paper, we will study the relationship between the ABC index and radius of connected graphs. In particular, we determine the upper and lower bounds of $ABC(G) - r(G)$ for connected graphs G.

2 Preliminaries

For an edge subset M of the graph G, let $G - M$ denote the graph obtained from G by deleting the edges in M, and for an edge subset M^* of the complement of G, let $G + M^*$ denote the graph obtained from G by adding the edges in M^*. In particular, if $M = \{uv\}$, then we write $G - uv$ for $G - \{uv\}$, and if $M^* = \{uv\}$, then we write $G + uv$ for $G + \{uv\}$.

The following result reveals that the deletion of an edge from a graph would decrease the ABC index.

Lemma 1 ([7], Theorem 2) *Let G be a connected graph on $n \geq 3$ vertices. For $uv \in E(G)$, we have*

$$ABC(G) > ABC(G - uv).$$

As an immediate application of Lemma 1, we know that the complete graph is the unique graph with maximum ABC index among connected graphs. Furthermore, we can deduce that the upper bound of $ABC(G) - r(G)$ would be uniquely attained by the complete graph.

Proposition 1 *Let G be a connected graph on $n \geq 2$ vertices. Then*

$$ABC(G) \leq r(G) + \frac{n\sqrt{n-2}}{\sqrt{2}} - 1$$

with equality if and only if G is the complete graph on n vertices.

In the following, we will consider the lower bound of $ABC(G) - r(G)$ for connected graphs G and show that this lower bound would be uniquely attained by the path.

3 Lemmas

First we give several additional lemmas which will be used in our proof later.

Lemma 2 ([7], Lemma 2) *For integers $x \geq 2$ and $y \geq 1$, we have*

$$\sqrt{\frac{x+y-2}{xy}} - \sqrt{\frac{x+y-3}{(x-1)y}} \geq \sqrt{\frac{1}{x}} - \sqrt{\frac{1}{x-1}}.$$

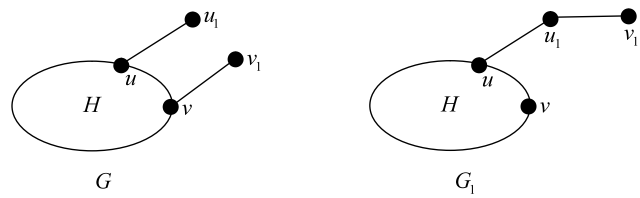

Figure 1 The trees G and G_1 in Lemma 3 when $u \neq v$.

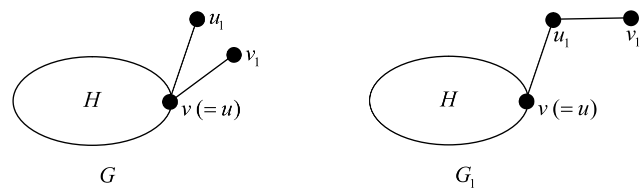

Figure 2 The trees G and G_1 in Lemma 3 when $u = v$.

A vertex of degree 1 is said to be a pendent vertex, while a vertex of degree at least 2 is said to be a non-pendent vertex.

Lemma 3 *Let H be a nontrivial tree, where $u, v \in V(H)$ (possibly $u = v$). Let G be the tree obtained from H by attaching a pendent vertex u_1 to u, and attaching a pendent vertex v_1 to v; see Figure 1. In particular, if $u = v$, then two pendent vertices u_1, v_1 are both attached to vertex $v = u$ in H, see Figure 2. Consider $G_1 = G - vv_1 + u_1v_1$; see Figures 1 and 2. If there are at most two non-pendent neighbors of v in G, then*

$$ABC(G) - ABC(G_1) > -0.5.$$

Proof Denote by a the number of non-pendent neighbors of v in G. According to the hypothesis, $a = 0, 1, 2$.

Clearly, $d_G(v) \geq 2$. For $vx \in E(H)$, if $d_G(x) = 1$, then

$$\begin{aligned} &\sqrt{\frac{d_G(v) + d_G(x) - 2}{d_G(v)d_G(x)}} - \sqrt{\frac{d_G(v) + d_G(x) - 3}{(d_G(v) - 1)d_G(x)}} \\ &\quad = \sqrt{1 - \frac{1}{d_G(v)}} - \sqrt{1 - \frac{1}{d_G(v) - 1}} \\ &\quad > 0, \end{aligned}$$

while if $d_G(x) \geq 2$, then by Lemma 2, we have

$$\begin{aligned} &\sqrt{\frac{d_G(v) + d_G(x) - 2}{d_G(v)d_G(x)}} - \sqrt{\frac{d_G(v) + d_G(x) - 3}{(d_G(v) - 1)d_G(x)}} \\ &\quad \geq \sqrt{\frac{1}{d_G(v)}} - \sqrt{\frac{1}{d_G(v) - 1}}. \end{aligned}$$

So it follows that

$$\sum_{vx\in E(H)}\left(\sqrt{\frac{d_G(v)+d_G(x)-2}{d_G(v)d_G(x)}}-\sqrt{\frac{d_G(v)+d_G(x)-3}{(d_G(v)-1)d_G(x)}}\right)$$
$$\geq a\left(\sqrt{\frac{1}{d_G(v)}}-\sqrt{\frac{1}{d_G(v)-1}}\right). \tag{1}$$

In the following we will split the proof into two cases.

Case 1. $u \neq v$.

In this case, $a = 1, 2$ (if $a = 0$, then G is a star, which is impossible). Moreover, note that $d_G(v) \geq a + 1 \geq 2$. Now by (1), we have

$$\begin{aligned}
&ABC(G)-ABC(G_1)\\
&=\sqrt{\frac{d_G(u)-1}{d_G(u)}}+\sqrt{\frac{d_G(v)-1}{d_G(v)}}+\sum_{vx\in E(H)}\sqrt{\frac{d_G(v)+d_G(x)-2}{d_G(v)d_G(x)}}\\
&\quad-\left(\sqrt{2}+\sum_{vx\in E(H)}\sqrt{\frac{d_G(v)+d_G(x)-3}{(d_G(v)-1)d_G(x)}}\right)\\
&=\left(\sqrt{\frac{d_G(u)-1}{d_G(u)}}+\sqrt{\frac{d_G(v)-1}{d_G(v)}}-\sqrt{2}\right)\\
&\quad+\sum_{vx\in E(H)}\left(\sqrt{\frac{d_G(v)+d_G(x)-2}{d_G(v)d_G(x)}}-\sqrt{\frac{d_G(v)+d_G(x)-3}{(d_G(v)-1)d_G(x)}}\right)\\
&\geq\left(\sqrt{\frac{d_G(u)-1}{d_G(u)}}+\sqrt{\frac{d_G(v)-1}{d_G(v)}}-\sqrt{2}\right)+a\left(\sqrt{\frac{1}{d_G(v)}}-\sqrt{\frac{1}{d_G(v)-1}}\right).
\end{aligned}$$

On one hand, notice that $\sqrt{\frac{d_G(u)-1}{d_G(u)}}=\sqrt{1-\frac{1}{d_G(u)}}$ is increasing on $d_G(u)\geq 2$. On the other hand, $\sqrt{\frac{d_G(v)-1}{d_G(v)}}=\sqrt{1-\frac{1}{d_G(v)}}$ and $\sqrt{\frac{1}{d_G(v)}}-\sqrt{\frac{1}{d_G(v)-1}}$ are both increasing on $d_G(v)\geq a+1$. So we have

$$\begin{aligned}
&ABC(G)-ABC(G_1)\\
&\geq\left(\sqrt{\frac{d_G(u)-1}{d_G(u)}}+\sqrt{\frac{d_G(v)-1}{d_G(v)}}-\sqrt{2}\right)+a\left(\sqrt{\frac{1}{d_G(v)}}-\sqrt{\frac{1}{d_G(v)-1}}\right)\\
&\geq\left(\sqrt{\frac{2-1}{2}}+\sqrt{\frac{(a+1)-1}{a+1}}-\sqrt{2}\right)+a\left(\sqrt{\frac{1}{a+1}}-\sqrt{\frac{1}{(a+1)-1}}\right)\\
&=\begin{cases}\frac{1}{\sqrt{2}}-1 & \text{if } a=1,\\ \sqrt{\frac{2}{3}}+\frac{2}{\sqrt{3}}-\frac{3}{\sqrt{2}} & \text{if } a=2\end{cases}\\
&>-0.5,
\end{aligned}$$

i.e., $ABC(G)-ABC(G_1)>-0.5$.

Case 2. $u = v$.

In this case, $a = 0, 1, 2$. Moreover, note that $d_G(v) \geq a + 2 \geq 2$.

Similar to the arguments in Case 1, we have

$$
\begin{aligned}
&ABC(G) - ABC(G_1) \\
&= \left(2\sqrt{\frac{d_G(v)-1}{d_G(v)}} + \sum_{vx\in E(H)} \sqrt{\frac{d_G(v)+d_G(x)-2}{d_G(v)d_G(x)}}\right) \\
&\quad - \left(\sqrt{2} + \sum_{vx\in E(H)} \sqrt{\frac{d_G(v)+d_G(x)-3}{(d_G(v)-1)d_G(x)}}\right) \\
&= \left(2\sqrt{\frac{d_G(v)-1}{d_G(v)}} - \sqrt{2}\right) + \sum_{vx\in E(H)} \left(\sqrt{\frac{d_G(v)+d_G(x)-2}{d_G(v)d_G(x)}} - \sqrt{\frac{d_G(v)+d_G(x)-3}{(d_G(v)-1)d_G(x)}}\right) \\
&\geq \left(2\sqrt{\frac{d_G(v)-1}{d_G(v)}} - \sqrt{2}\right) + a\left(\sqrt{\frac{1}{d_G(v)}} - \sqrt{\frac{1}{d_G(v)-1}}\right) \\
&\geq \left(2\sqrt{\frac{(a+2)-1}{a+2}} - \sqrt{2}\right) + a\left(\sqrt{\frac{1}{a+2}} - \sqrt{\frac{1}{(a+2)-1}}\right) \\
&= \begin{cases} 0 & \text{if } a = 0, \\ 2\sqrt{\frac{2}{3}} + \frac{1}{\sqrt{3}} - \frac{3}{\sqrt{2}} & \text{if } a = 1, \\ \frac{1}{\sqrt{3}} - \sqrt{2} + 1 & \text{if } a = 2 \end{cases} \\
&> -0.5,
\end{aligned}
$$

i.e., $ABC(G) - ABC(G_1) > -0.5$.

Combining Cases 1 and 2, the result follows. □

The following lemma on the radius of a tree is clear.

Lemma 4 *Let G be a tree. If the diameter of G is d, then* $r(G) = \lfloor \frac{d+1}{2} \rfloor$.

In the following two lemmas, we will show that the path would attain the minimum value $ABC(G) - r(G)$ among trees.

Lemma 5 *Let G be a tree with a diametrical path P. If* $ABC(G) - r(G)$ *is minimum among trees, then there is at most one vertex outside P in G.*

Proof Suppose to the contrary that there are at least two vertices outside P in G.

Assume that $P = v_0v_1\cdots v_d$. Denote by T_i the component of $G - E(P)$ containing v_i, where $0 \leq i \leq d$. Let x_i be a vertex in T_i such that

$$d_G(x_i, v_i) = \max\{d_G(x, v_i) : x \in V(T_i)\},$$

where $0 \leq i \leq d$. Clearly, x_i is a pendent vertex if $|V(T_i)| \geq 2$, and denote by x_i^* the unique neighbor of x_i in G.

Since there are some vertices outside P in G, thus there exists some index, say k, such that $|V(T_k)| \geq 2$, where $1 \leq k \leq d-1$. By the choice of x_k, it is easily seen that there are at most two non-pendent neighbors of x_k^* in G.

Consider $G_1 = G - x_k^* x_k + v_0 x_k$. By Lemma 3, we have

$$ABC(G) - ABC(G_1) > -0.5. \tag{2}$$

Clearly, $x_k \cup P = x_k v_0 v_1 \cdots v_d$ is a diametrical path of G_1, thus the diameter of G_1 is $d+1$.

Observe that there are at least two vertices outside P in G, which implies that there are some vertices outside (diametrical path) $x_k \cup P$ in G_1. Similar to the transformation from G to G_1, we can construct another tree G_2 based on G_1, such that

$$ABC(G_1) - ABC(G_2) > -0.5, \tag{3}$$

and the diameter of G_2 is $d+2$.

Now by (2) and (3), it follows that

$$\begin{aligned} ABC(G) - ABC(G_2) &= \bigl[ABC(G) - ABC(G_1)\bigr] + \bigl[ABC(G_1) - ABC(G_2)\bigr] \\ &> (-0.5) + (-0.5) = -1. \end{aligned} \tag{4}$$

On the other hand, by Lemma 4, we have

$$r(G) - r(G_2) = \left\lfloor \frac{d+1}{2} \right\rfloor - \left\lfloor \frac{d+3}{2} \right\rfloor = -1. \tag{5}$$

Finally, by (4) and (5), we get

$$\begin{aligned} &\bigl[ABC(G) - r(G)\bigr] - \bigl[ABC(G_2) - r(G_2)\bigr] \\ &\quad = \bigl[ABC(G) - ABC(G_2)\bigr] - \bigl[r(G) - r(G_2)\bigr] \\ &\quad > (-1) - (-1) = 0, \end{aligned}$$

i.e., $ABC(G) - r(G) > ABC(G_2) - r(G_2)$, which is a contradiction to the minimality of $ABC(G) - r(G)$.

Then the result follows easily. □

Let P_n be the path on n vertices.

Lemma 6 *Let G be a tree on $n \geq 4$ vertices with a diametrical path P. If there is at most one vertex outside P in G, then*

$$ABC(G) - r(G) \geq \frac{n-1}{\sqrt{2}} - \left\lfloor \frac{n}{2} \right\rfloor$$

with equality if and only if $G \cong P_n$.

Proof From the hypothesis that there are at most one vertex outside P in G, we know that either G is the path P_n, or G is a tree obtained from $P_{n-1} = v_1 v_2 \cdots v_{n-1}$ by attaching a pendent vertex to v_i, where $2 \leq i \leq n-2$.

If G is a tree obtained from $P_{n-1} = v_1 v_2 \cdots v_{n-1}$ by attaching a pendent vertex to v_2 or v_{n-2}, then $ABC(G) \geq \frac{n-3}{\sqrt{2}} + 2\sqrt{\frac{2}{3}}$ with equality when $n \geq 5$ and $r(G) = \lfloor \frac{n-1}{2} \rfloor$, and thus

$$ABC(G) - r(G) \geq \frac{n-3}{\sqrt{2}} + 2\sqrt{\frac{2}{3}} - \left\lfloor \frac{n-1}{2} \right\rfloor.$$

If G is a tree obtained from $P_{n-1} = v_1 v_2 \cdots v_{n-1}$ by attaching a pendent vertex to v_i, where $3 \leq i \leq n-3$, then $ABC(G) = \frac{n-2}{\sqrt{2}} + \sqrt{\frac{2}{3}}$ and $r(G) = \lfloor \frac{n-1}{2} \rfloor$, and thus

$$ABC(G) - r(G) = \frac{n-2}{\sqrt{2}} + \sqrt{\frac{2}{3}} - \left\lfloor \frac{n-1}{2} \right\rfloor.$$

If $G \cong P_n$, then $ABC(P_n) = \frac{n-1}{\sqrt{2}}$ and $r(P_n) = \lfloor \frac{n}{2} \rfloor$, and thus

$$ABC(G) - r(G) = \frac{n-1}{\sqrt{2}} - \left\lfloor \frac{n}{2} \right\rfloor.$$

It is easily verified that

$$\begin{aligned} \frac{n-3}{\sqrt{2}} + 2\sqrt{\frac{2}{3}} - \left\lfloor \frac{n-1}{2} \right\rfloor &> \frac{n-2}{\sqrt{2}} + \sqrt{\frac{2}{3}} - \left\lfloor \frac{n-1}{2} \right\rfloor \\ &> \frac{n-1}{\sqrt{2}} - \left\lfloor \frac{n}{2} \right\rfloor. \end{aligned}$$

Then the result follows easily. □

4 The main result

Now we give the main result of this paper.

Theorem 1 *Let G be a connected graph on $n \geq 2$ vertices. Then*

$$ABC(G) - r(G) \geq \frac{n-1}{\sqrt{2}} - \left\lfloor \frac{n}{2} \right\rfloor$$

with equality if and only if $G \cong P_n$.

Proof Let G be a connected graph on $n \geq 2$ vertices.

If $n = 2$, then $G \cong P_2$, and thus the result holds trivially. If $n = 3$, then either G is the path P_3 or the triangle, and thus the result follows from a simple calculation.

Suppose in the following that $n \geq 4$.

Case 1. G is a tree.

Suppose that G is a tree with minimum value $ABC(G) - r(G)$.

Let P be a diametrical path of G. By Lemma 5, there is at most one vertex outside P in G. Furthermore, by Lemma 6, we have

$$ABC(G) - r(G) \geq \frac{n-1}{\sqrt{2}} - \left\lfloor \frac{n}{2} \right\rfloor$$

with equality if and only if $G \cong P_n$.

Case 2. G is not a tree.

Let T be a spanning tree of G. By Lemma 1, we have $ABC(G) > ABC(T)$. On the other hand, since the removal of edges potentially increases the eccentricities of some vertices, thus $r(G) \leq r(T)$ follows clearly. So we have

$$ABC(G) - r(G) > ABC(T) - r(T).$$

Now together with the arguments in Case 1, we get

$$ABC(G) - r(G) > ABC(T) - r(T) \geq \frac{n-1}{\sqrt{2}} - \left\lfloor \frac{n}{2} \right\rfloor.$$

Combining Cases 1 and 2, the result follows. □

Competing interests
The author declares that they have no competing interests.

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