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Note

On a relation between the atom-bond connectivity and the first geometric–arithmetic indices

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ABSTRACT

The atom-bond connectivity index (ABC) and the first geometric–arithmetic index (GA) are two well-known molecular descriptors, which are found to be useful tools in QSPR/QSAR investigations. In this work, we obtain a relation between these two indices for simple connected graphs on $n \geq 3$ vertices with minimum degree at least s and maximum degree at most t, where $1 \leq s \leq t \leq n-1$ and $t \geq 2$. Using this relation, we prove that if $t \leq 4s^2 - 3s + 1$, then the ABC index is always less than the GA index and this bound is best possible for $s \geq 2$.

1. Introduction

Molecular descriptors are playing a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place. Topological indices are numbers associated with chemical structures derived from their hydrogen-depleted graphs as a tool for compact and effective description of structural formulas which are used to study and predict the structure–property correlations of organic compounds. There are lots of topological indices which have found some applications in theoretical chemistry, especially in QSPR/QSAR studies [20].

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For any vertex $v \in V(G)$, we use d_v to denote the degree of v in G. The minimum degree and maximum degree of G are denoted by δ and Δ, respectively. Let K_n, $K_{s,t}$ $(s+t=n)$ and S_n be the complete graph, the complete bipartite graph and the star with n vertices, respectively. A molecular graph is a connected graph with maximum degree at most 4. Its graphical representation may resemble a structural formula of some (usually organic) molecule. That was a primary reason for employing graph theory in chemistry.

The atom-bond connectivity index (ABC) was introduced by Estrada et al. [12] in 1998. This index is defined as

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

In [12] it was demonstrated that there exists an excellent (linear) correlation between the ABC index and the experimental heats of formation of alkanes. The mathematical properties of this index have been studied extensively (see [1–3,5,14–18,22,23,25]).

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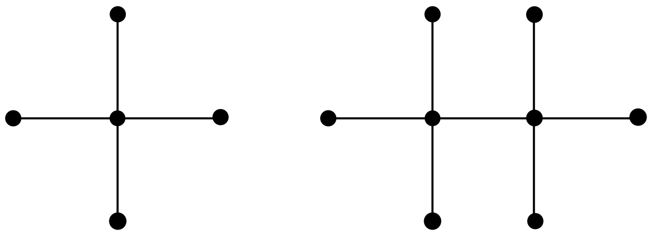

Fig. 1. The two exceptions.

The first geometric–arithmetic index (*GA*) was proposed by Vukičević and Furtula [21] in 2009. This index is defined as

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

In fact, this index belongs to a wider class of so-called geometric–arithmetic indices ($GA_{general}$) proposed by Fath-Tabar et al. [13]. In [21] it was demonstrated, on the example of octane isomers, that the *GA* index is well correlated with a variety of physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation and acentric factor. Moreover, the quality of these correlations was found to be better than for other often employed molecular descriptors [20]. The mathematical properties of the *GA* index were reported in [4,6–11,19,24].

Das and Trinajstić [8] compared the *ABC* and the *GA* indices for molecular graphs and general graphs. It was proved that the *ABC* index is less than the *GA* index for almost all molecular graphs and all simple graphs with $\Delta - \delta \le 3$ except two graphs which are shown in Fig. 1. However, comparison between these two indices, in the case of trees and general graphs, remains an open problem.

In this work, we present a relation between these two indices for simple connected graphs on $n \ge 3$ vertices with minimum degree $\delta \ge s$ and maximum degree $\Delta \le t$, where $1 \le s \le t \le n-1$ and $t \ge 2$. Using this relation, we prove that if $t \le 4s^2 - 3s + 1$, then the *ABC* index is always less than the *GA* index. The complete bipartite graph $K_{s,4s^2-3s+2}$ shows that this bound is best possible for $s \ge 2$. This improves the result of Das and Trinajstić in [8], and partially solve the above-mentioned problem for general graphs.

2. A relation between the *ABC* and the *GA* indices

In this section, we obtain a relation between the *ABC* and the *GA* indices for simple connected graphs on $n \ge 3$ vertices.

Theorem 2.1. *Let G be a simple connected graph on $n \ge 3$ vertices with minimum degree $\delta \ge s$ and maximum degree $\Delta \le t$, where $1 \le s \le t \le n-1$ and $t \ge 2$. Then*

(i) $\frac{\sqrt{2t-2}}{t} GA(G) \le ABC(G)$ *with equality if and only if G is a t-regular graph;*

(ii) $ABC(G) \le \frac{\sqrt{2s-2}}{s} GA(G)$ *if* $t < 2s - 3 + \sqrt{5s^2 - 14s + 9}$, *with equality if and only if G is an s-regular graph; and* $ABC(G) \le \frac{(s+t)\sqrt{s+t-2}}{2st} GA(G)$ *if* $t \ge 2s - 3 + \sqrt{5s^2 - 14s + 9}$, *with equality if and only if one vertex has degree s and the other vertex has degree t for every edge of G.*

Proof. Let uv be an edge of G. By the symmetry between u and v, we may assume that $s \le d_u \le d_v \le t$. Since G is a connected graph with $n \ge 3$ vertices, we have $d_v \ge 2$. We consider the function

$$f(x, y) = \left(\frac{\sqrt{\frac{x+y-2}{xy}}}{\frac{2\sqrt{xy}}{x+y}} \right)^2 = \frac{(x+y)^2(x+y-2)}{4x^2y^2}$$

with $s \le x \le y \le t$ and $y \ge 2$. Since

$$\begin{aligned} \frac{\partial f(x,y)}{\partial x} &= \frac{(x+y)(x^2 - 2y^2 - xy + 4y)}{4x^3y^2} \\ &= \frac{(x+y)[x(x-y) + 2y(2-y)]}{4x^3y^2} \\ &\le 0, \end{aligned}$$

we see that $f(x, y)$ is strictly monotonously decreasing in x. Hence the minimum value of $f(x, y)$ is $f(y, y)$ for some $\max\{s, 2\} \le y \le t$, and the maximum value of $f(x, y)$ is $f(s, y)$ for some $\max\{s, 2\} \le y \le t$.