ON COMPARISON BETWEEN FIRST GEOMETRIC-ARITHMETIC INDEX AND ATOM-BOND CONNECTIVITY INDEX

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Abstract. The recently introduced first geometric-arithmetic (GA) index and atom bond connectivity (ABC) index are molecular structure descriptors which play a significant role in QSAR/QSPR studies. Das and Trinajstić [Chem. Phys. Lett. 497 (2010) 149-151] compared these two indices for molecular graphs and for general graphs in which the difference between maximum and minimum degree was less than or equal to three. In this paper, GA and ABC indices have been compared for the line graphs of molecular graphs and for general graphs in which the difference between maximum and minimum degree ($\delta > 1$) is less than or equal to $(2\delta - 1)^2$. Moreover, we compare these two indices for some families of trees.

1. Introduction

Let $G = (V, E)$ denote a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$ such that $|E(G)| = m$. Suppose that $d_i$ is the degree of a vertex $v_i \in V(G)$.

Topological indices are numerical parameters of a graph which are invariant under graph isomorphisms. They play a significant role in mathematical chemistry especially in the QSAR/QSPR investigations.

A whole class of newly studied graph invariants are the "geometric-arithmetic indices" whose general definition is as follows:

$$GA_{general} = GA_{general}(G) = \sum_{ij \in E(G)} \frac{\sqrt{Q_iQ_j}}{2(Q_i + Q_j)}$$

where $Q_i$ is some quantity that in a unique manner can be associated with the vertex $v_i$ of the graph $G$. The first GA-index was proposed by Vukičević and Furtula [4] by setting $Q_i$ to be the degree $d_i$ of the vertex $v_i$ of the graph $G$:

$$GA(G) = \sum_{ij \in E(G)} \frac{\sqrt{d_id_j}}{2(d_i + d_j)}$$

Key words and phrases. First geometric-arithmetic index; atom-bond connectivity index; minimum and maximum degree of a graph; line graph.
It has been demonstrated, on the example of octane isomers, that GA index is well-correlated with a variety of physico-chemical properties [4]. A survey of mathematical properties of the GA indices and their applications in QSPR and QSAR is recently given by Das, Gutman and Furtula [6].

Estrada et al. [7] proposed a new index, known as the atom-bond connectivity (ABC) index of graph $G$, which is abbreviated as $ABC(G)$ and defined as

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

The ABC index provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [7, 8]. In [9]-[18], mathematical properties of the ABC index was studied.

A connected graph with maximum vertex degree 4 is known as molecular graph. The line graph $L(G)$ of a graph $G$ has the vertex set $V(L(G)) = E(G)$ where the two distinct vertices of $L(G)$ are adjacent if the corresponding edges of $G$ are adjacent; for detailed properties of a line graph see [1]. Some possible chemical applications of line graphs of molecular graphs were discussed in [19]. Das and Trinajstic [18] compared GA and ABC for molecular graphs and for general graphs in which the difference between maximum and minimum degree, less than or equal to three.

In this work, these two indices have been compared for the line graphs of molecular graphs, for general graphs in which the difference between maximum and minimum degree ($\delta > 1$) is less than or equal to $(2\delta - 1)^2$ and for some families of trees.

2. Preliminaries

The maximum and minimum vertex degree in a graph $G$ are denoted by $\Delta$ and $\delta$ respectively. Also, a vertex of the graph $G$ is said to be pendant if its neighborhood contains exactly one vertex. While, an edge of a graph is said to be pendant if one of its vertices is pendant.

A tree in which exactly one of its vertices has degree greater than two is known as Starlike tree. Let $S(r_1, r_2, \ldots, r_k)$ denote the Starlike tree which has a vertex $v_1$ of degree $k > 2$ such that $S(r_1, r_2, \ldots, r_k) \setminus \{v_1\} = P_{r_1} \cup P_{r_2} \cup \cdots \cup P_{r_k}$. We say that the
Starlike tree \( S(r_1, r_2, \ldots, r_k) \) has \( k \) branches, the lengths of which are \( r_1, r_2, \ldots, r_k \) \((r_1 \geq r_2 \geq \cdots \geq r_k \geq 1)\) respectively, and has \( \sum_{i=1}^{k} r_i + 1 \) vertices.

Denoted by \( K_{1,n} \) and \( K_n \) the Star on \( n + 1 \) vertices and complete graph on \( n \) vertices respectively. A triangle of a graph \( G \) is called odd if there is a vertex of \( G \) adjacent to an odd number of its vertices.

**Lemma 2.1.** \([1]\). A graph \( G \) is a line graph if and only if \( G \) does not have \( K_{1,3} \) as an induced subgraph, and if two odd triangles have a common edge then the subgraph is \( K_4 \) induced by their vertices.

3. Comparison between GA index and ABC index

Denoted by \( T^* \) the tree on eight vertices, obtained by joining the central vertices of two copies \( K_{1,3} \) by an edge (see Figure 1). In \([18]\), the following two main results were proved:

**Theorem 3.1.** \([18]\). Let \( G \) be a molecular graph of order \( n \). Then \( GA(G) > ABC(G) \) for \( G \not\cong K_{1,4}, T^* \).

**Theorem 3.2.** \([18]\). Let \( G \) be a simple graph with maximum degree \( \Delta \) and minimum degree \( \delta \). If \( \Delta - \delta \leq 3 \) and \( G \not\cong K_{1,4}, T^* \), then \( GA(G) > ABC(G) \).

Let \( m_{a,b} \) be the number of edges of a graph \( G \) connecting the vertices of degree \( a \) and \( b \). Firstly, we compare GA index and ABC index for line graph of a molecular graph in the following theorem:

**Theorem 3.3.** Let \( G \) be a molecular graph of order \( n \). Then \( GA(L(G)) > ABC(L(G)) \).

**Proof.** If \( n \leq 4 \), then \( L(G) \) is a molecular graph and hence result follows from theorem 3.1, so we suppose that \( n \geq 5 \). Note that \( 1 \leq d_i \leq 6 \) for all vertices \( v_i \) of \( L(G) \). Hence the edges of \( L(G) \) with possible degree pairs are: \((6,6), (6,5), (6,4), (6,3), (6,2), (6,1), (5,5), (5,4), (5,3), (5,2), (5,1), (4,4), (4,3), (4,2), (4,1), (3,3), (3,2), (3,1), (2,2), (2,1)\). The values of \( \theta_{ij} = \frac{2\sqrt{d_id_j}}{d_i+d_j} \) and \( \phi_{ij} = \sqrt{\frac{d_i+d_j-2}{d_id_j}} \) for all above mentioned degree pairs are given in the Table 1 and Table 2 (table 2 is taken from \([18]\) ). From these tables one can note easily that
Again from (3.1) it follows that $u$, adjacent with $v$, $w$, $t$ of $x$.

If at least one of $m_{i,j}$ is nonzero. Consider the edge $e = xy \in L(G)$ where degree of $x$ and $y$ is two and $c$ ($c = 5, 6$) respectively. Let $l$ denote number of vertices of

$$
\begin{align*}
\theta_{ij} - \phi_{ij} = & \begin{cases} 
\geq \frac{2\sqrt{5}}{7} - \sqrt{\frac{5}{6}} \approx -0.2130 & \text{if } (d_i, d_j) = (4, 1), (5, 1), (6, 1) \\
\approx 0.0495 & \text{if } (d_i, d_j) = (3, 1) \\
\approx 0.1589 & \text{if } (d_i, d_j) = (6, 2) \\
\approx 0.1964 & \text{if } (d_i, d_j) = (5, 2) \\
\approx 0.2357 & \text{if } (d_i, d_j) = (2, 1), (4, 2) \\
\geq \sqrt{\frac{24}{20}} - \frac{1}{\sqrt{2}} \approx 0.2727 & \text{otherwise}
\end{cases}
\end{align*}
$$

If $m_{1,b} = 0$ for all $b \geq 4$, then it follows from (3.1) that $\theta_{ij} - \phi_{ij} > 0$ for all edges $ij \in L(G)$ and hence $GA(L(G)) > ABC(L(G))$.

If $m_{1,b} = 0$ not for all $b \geq 4$. It is claimed that $m_{1,b} \leq \lfloor \frac{|V(L(G))|}{2} \rfloor$. To prove this it is enough to show that no two pendent edges are adjacent. On the contrary, suppose that two pendent edges $e_1 = uw$ and $e_2 = uv$ are adjacent.

| $(d_i, d_j)$ | (6,6) | (6,5) | (6,4) | (6,3) | (6,2) | (6,1) | (5,5) | (5,4) | (5,3) | (5,2) | (5,1) |
|-------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| $\theta_{ij}$ | $\sqrt{\frac{5}{18}}$ | $\sqrt{\frac{3}{10}}$ | $\sqrt{\frac{1}{3\sqrt{2}}}$ | $\sqrt{\frac{1}{6}}$ | $\sqrt{\frac{1}{\sqrt{2}}}$ | $\sqrt{\frac{1}{\sqrt{2}}}$ | $\sqrt{\frac{2}{\sqrt{5}}}$ | $\sqrt{\frac{7}{20}}$ | $\sqrt{\frac{2}{5}}$ | $\frac{1}{\sqrt{2}}$ | $\frac{1}{\sqrt{2}}$ |
| $\phi_{ij}$ | $\sqrt{\frac{5}{18}}$ | $\sqrt{\frac{3}{10}}$ | $\sqrt{\frac{1}{3\sqrt{2}}}$ | $\sqrt{\frac{1}{6}}$ | $\sqrt{\frac{1}{\sqrt{2}}}$ | $\sqrt{\frac{1}{\sqrt{2}}}$ | $\sqrt{\frac{2}{\sqrt{5}}}$ | $\sqrt{\frac{7}{20}}$ | $\sqrt{\frac{2}{5}}$ | $\frac{1}{\sqrt{2}}$ | $\frac{1}{\sqrt{2}}$ |

Table 1. Values of $\theta_{ij}$ and $\phi_{ij}$ for all edges with degrees $(d_i, d_j)$; $5 \leq d_i \leq 6$ and $d_i \geq d_j$

| $(d_i, d_j)$ | (4,4) | (4,3) | (4,2) | (4,1) | (3,3) | (3,2) | (3,1) | (2,2) | (2,1) |
|-------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| $\theta_{ij}$ | $\sqrt{\frac{3}{8}}$ | $\sqrt{\frac{5}{12}}$ | $\sqrt{\frac{1}{\sqrt{2}}}$ | $\sqrt{\frac{3}{4}}$ | $\frac{2}{\sqrt{3}}$ | $\frac{1}{\sqrt{2}}$ | $\sqrt{\frac{2}{3}}$ | $\frac{1}{\sqrt{2}}$ | $\frac{1}{\sqrt{2}}$ |
| $\phi_{ij}$ | $\sqrt{\frac{3}{8}}$ | $\sqrt{\frac{5}{12}}$ | $\sqrt{\frac{1}{\sqrt{2}}}$ | $\sqrt{\frac{3}{4}}$ | $\frac{2}{\sqrt{3}}$ | $\frac{1}{\sqrt{2}}$ | $\sqrt{\frac{2}{3}}$ | $\frac{1}{\sqrt{2}}$ | $\frac{1}{\sqrt{2}}$ |

Table 2. Values of $\theta_{ij}$ and $\phi_{ij}$ for all edges with degrees $(d_i, d_j)$; $2 \leq d_i \leq 4$ and $d_i \geq d_j$

Since $n \geq 5$, order of $L(G)$ is at least 4. This implies that there exists a vertex $t$ adjacent with $u$ in $L(G)$. Then the graph obtained by removing all vertices except $u, v, w, t$ of $L(G)$ is $K_{1,3}$, a contradiction to lemma 2.1. If $m_{2,5} = m_{2,6} = 0$, then again from (3.1) it follows that

$$
(3.2) \quad GA(L(G)) - ABC(L(G)) = \sum_{ij \in E(L(G))} (\theta_{ij} - \phi_{ij}) > 0
$$

If at least one of $m_{2,5}, m_{2,6}$ is nonzero. Consider the edge $e = xy \in L(G)$ where degree of $x$ and $y$ is two and $c$ ($c = 5, 6$) respectively. Let $l$ denote number of vertices of
degree two which are adjacent with \( y \). Then \( 1 \leq l \leq 2 \) for otherwise \( K_{1,3} \) would be an induced subgraph of \( L(G) \). This implies that the vertex \( y \) lies on either of the cliques \( K_{c-1}, K_c \) of \( L(G) \) and hence the edges with possible degree pairs of these cliques in \( L(G) \) are \( (6,6), (6,5), (6,4), (6,3), (5,5), (5,4), (5,3), (4,4), (4,3), (3,3) \). For all these degree pairs, \( \theta_{ij} - \phi_{ij} \geq 0.2727 \). Moreover, corresponding to every clique \( K_d \) \( (d = 4, 5, 6) \), there exist at most \( 2d \) edges with degrees \( (2, k) \), where vertex of degree \( c \) (that is \( y \)) lies on \( K_d \). Since the size of \( K_d \) is \( \frac{d(d-1)}{2} \geq 2d \) for \( d \geq 5 \). Therefore, if \( L(G) \) does not have clique \( K_4 \), then by using \((3.1)\) one can easily see that inequality \((3.2)\) holds. If \( L(G) \) has clique \( K_4 \). It can be easily seen that no edge with degrees \( (2, 6) \) can be incident with any vertex of the clique \( K_4 \). This implies, corresponding to every clique \( K_4 \) there exist at most \( 8 \) edges with degrees \( (2, 5) \) but the size of \( K_4 \) is \( 6 \).

\[
8(0.1964) + 6(0.2727) = 2.291 > 2.130
\]

This completes the proof. \( \square \)

Now, we prove that conclusion of theorem 3.2 remains true if minimum degree is \( k > 1 \) and the difference between maximum and minimum degree, less than or equal to \((2k-1)^2\). To proceed, we need the following lemma:

**Lemma 3.4.** If \( f(x, y) = (x + y)^2 + x^2 - (x + \frac{y}{2})^2(2x + y - 2) \), \( k \leq x \leq k + (2k-1)^2 \) and \( 0 \leq y \leq (2k-1)^2 \) where \( k \geq 2 \) then \( f(x, y) > 0 \).

**Proof.**

**Step 1.** Firstly we take \( x = k \), then

\[
g(y) = f(k, y) = (k + y)^2k^2 - (k + \frac{y}{2})^2(2k + y - 2)
\]

and \( g'(y) > 0 \) implies that \( \alpha < y < \beta \), where

\[
\alpha = \frac{2}{3}(1 - 3k + 2k^2) - \frac{2}{3} \sqrt{1 + 4k^2 - 6k^3 + 4k^4}
\]

and

\[
\beta = \frac{2}{3}(1 - 3k + 2k^2) - \frac{2}{3} \sqrt{1 + 4k^2 - 6k^3 + 4k^4}
\]

this implies that \( g \) is increasing on the interval \((\alpha, \beta)\) and decreasing on \((-\infty, \alpha) \cup (\beta, \infty)\). Since \( \alpha < 0 < \beta < (2k-1)^2 \), so \( g \) is increasing at \( y = 0 \) and decreasing at \( y = (2k-1)^2 \). Moreover, \( g(0) = k^2\{k^2 - 2(k - 1)\} > 0 \) and \( g((2k-1)^2) = 4k^4 + 4k^2 - 2k + 1 > 0 \). It follows that \( g(y) > 0 \) for all \( y \in [0, (2k-1)^2] \).

**Step 2.** Now we take \( y = y_0 \), where \( y_0 \) is any fixed integer in the interval \([0, (2k-1)^2]\). Let \( h(x) = f(x, y_0) \) then

\[
h'(x) = (2x + y_0)(2x^2 + 2 - 3x) + (2x - \frac{3}{2})y_0 > 0
\]

for all \( x \geq k \geq 2 \). Hence \( h(x) = f(x, y_0) \) is increasing on \([k, \infty)\). Combining both the results proved in Step 1 and Step 2, we have the lemma. \( \square \)
Theorem 3.5. Let \( G \) be a simple graph with maximum degree \( \Delta \) and minimum degree \( \delta \geq 2 \). If \( \Delta - \delta \leq (2 \delta - 1)^2 \) then \( GA(G) > ABC(G) \).

Proof. Consider
\[
\Gamma = d_i^2d_j^2 - \frac{1}{4}(d_i + d_j)^2(d_i + d_j - 2),
\]
where \( d_i \) and \( d_j \) are degrees of vertices \( v_i \) and \( v_j \) respectively. Since \( \delta \leq d_i, d_j \leq \Delta \leq \delta + (2 \delta - 1)^2 \) this implies that \( |d_i - d_j| \leq (2 \delta - 1)^2 \). Without loss of generality we can suppose that \( d_i \geq d_j \) then \( d_i = d_j + \theta \) for some \( \theta ; 0 \leq \theta \leq (2 \delta - 1)^2 \) and Eq. (3.3) becomes
\[
\Gamma = (d_j^2 + \theta)^2d_j^2 - \frac{1}{4}(d_i + d_j)^2(d_i + d_j - 2),
\]
where \( \delta \leq d_j \leq \delta + (2 \delta - 1)^2 \) and \( 0 \leq \theta \leq (2 \delta - 1)^2 \)

Now from Lemma 3.4. and Eq. (3.4), we have the theorem. \( \square \)

If the condition \( \Delta - \delta \leq (2 \delta - 1)^2 \) is replaced by \( \Delta - \delta \leq (2 \delta - 1)^2 + 1 \) in theorem 3.5, then the conclusion may not be true. Consider the complete bipartite graph \( K_{r,s} \), if we take \( r = \delta \) and \( s = (2 \delta - 1)^2 + \delta + 1 \) then
\[
GA(K_{r,s}) = \frac{2(\delta(2 \delta - 1)^2 + \delta + 1)^2}{(2 \delta - 1)^2 + \delta + 1} < \sqrt{(2 \delta - 1)^2 + \delta + 1} = ABC(K_{r,s})
\]

Now, consider a graph \( G \) obtained by joining any vertex of \( K_{12} \) to a vertex of \( K_3 \) by an edge. Then \( \Delta = 12, \delta = 2 \) and so \( \Delta - \delta = 10 > (2(2) - 1)^2 \). But \( GA(G) < ABC(G) \). We have the following result:

Theorem 3.6. Let \( G \) be a simple graph with minimum degree \( \delta \geq 2 \).

(i): If \( |d_i - d_j| \leq (2 \delta - 1)^2 \) for all edges \( ij \in E(G) \), then \( GA(G) > ABC(G) \).

(ii): If \( |d_i - d_j| > (2 \delta - 1)^2 \) for all edges \( ij \in E(G) \), then \( GA(G) < ABC(G) \).

Proof. Using similar technique as in Theorem 3.5, one can easily prove the above results. \( \square \)

A stronger version of the above result can be similarly proved:

Theorem 3.7. Let \( G \) be a simple graph with minimum degree \( \delta \geq 2 \) and \( k = \min\{d_i, d_j\} \).

(i): If \( |d_i - d_j| \leq (2k - 1)^2 \) for all edges \( ij \in E(G) \), then \( GA(G) > ABC(G) \).

(ii): If \( |d_i - d_j| > (2k - 1)^2 \) for all edges \( ij \in E(G) \), then \( GA(G) < ABC(G) \).

Let \( \delta_1 \) denotes the minimum non-pendant vertex degree in \( G \). Now, we compare GA index and ABC index for trees.
Theorem 3.8. Let $T$ be a tree such that $m_{1,b} = 0$ for all $b \geq 4$ and $\Delta - \delta_1 \leq (2\delta_1-1)^2$ then $GA(T) > ABC(T)$.

Proof. From (3.5) and theorem 3.5, result follows. \qed

We define a special tree $T_{r,s} (r \geq 5$ and $s \geq 0)$ as follows: Let $S_r(i) (i = 1, 2, ..., s)$ and $S_r(j) (j = 1, 2)$ be star graphs of order $r-1$ and $r$ respectively. Then $T_{r,s}$ is a tree obtained by joining the central vertex of $S_r^{(1)}$ to the central vertex of $S_{r-1}^{(1)}$, central vertex of $S_r^{(2)}$ to the central vertex of $S_{r-1}^{(2)}$, ..., central vertex of $S_r^{(s)}$ to the central vertex of $S_{r-1}^{(s)}$ by edges. $T_{r,0}$ is a tree obtained by joining the central vertices of two copies of $S_r$ by an edge. Then

$$ABC(T_{r,s}) = (2(r-1) + s(r-2)) \sqrt{\frac{r-1}{r}} + (s+1) \sqrt{\frac{2(r+1)}{r}}$$

$$> (2(r-1) + s(r-2)) \frac{2\sqrt{r}}{r+1} + (s+1) = GA(T_{r,s})$$

But, for Starlike tree, we have the following theorem.

Theorem 3.9. Let $S = S(r_1, r_2, ..., r_k)$ a Starlike tree such that

(i): If $r_i \geq 4$ for all $i$, then $GA(S) > ABC(S)$.

(ii): If $r_i \geq 2$ and $\sum_{i=1}^{k} r_i \geq 4$, then $GA(S) > ABC(S)$.

(iii): If $r_i \geq 1$ and $\sum_{i=1}^{k} r_i \geq 8$, then $GA(S) > ABC(S)$.

Proof. (i) The edges of $S$ with possible degree pairs are: $(2, 1), (2, 2), (k, 2)$. From Table 2 we have

$$(3.5) \quad \theta_{ij} - \phi_{ij} \approx \begin{cases} 0.2357 & \text{if } (d_i, d_j) = (2, 1) \\ 0.2929 & \text{if } (d_i, d_j) = (2, 2) \end{cases}$$

Moreover, \((\frac{2\sqrt{2k}}{k+2} - \sqrt{\frac{k+2-2}{2k}}) \rightarrow -\frac{1}{\sqrt{2}} \approx -0.7071 \text{ when } k \rightarrow \infty\). Since $r_i \geq 4$ for all $i$, this implies that there are $k$ edges with degrees $(1, 2)$, $k$ edges with degrees $(2, k)$ and at least $2k$ edges with degrees $(2, 2)$ in $S$. This completes the proof.

Note that \(\frac{2\sqrt{d_id_j}}{d_i+d_j} - \sqrt{\frac{d_i+d_j-2}{d_i+d_j}} \rightarrow -1 \text{ if } (d_i, d_j) = (1, k)\). Using the same technique as in part (i), one can easily prove part (ii) and (iii). \qed

Example 3.10. Let $W'$ be a graph obtained by joining every vertex of the wheel graph $W_{n-1}$ (of order $n-1$) with $K_1$ by an edge. Then

$$GA(W') = (n-2)(\frac{8\sqrt{(n-1)}}{n+3} + 1) + 1$$
\[(n - 2)(\sqrt{\frac{n + 1}{n - 1}} + \sqrt{\frac{3}{8}}) + \frac{\sqrt{2(n - 2)}}{n - 1} = ABC(W')\]

Moreover,
\[GA(W_n) = (n - 1)(1 + \frac{2\sqrt{3(n - 1)}}{n + 2})\]

and
\[ABC(W_n) = (n - 1)(\frac{2}{3} + \sqrt{\frac{n}{3(n - 1)}})\]

GA(W_n) > ABC(W_n) if 4 ≤ n ≤ 194 and GA(W_n) < ABC(W_n) if n ≥ 195

Is there any simple non trivial graph G such that GA(G) = ABC(G)? All our attempts to find such a graph were unsuccessful. We end this section with following conjecture.

**Conjecture 3.11.** If G is any simple non trivial graph, then GA(G) ≠ ABC(G).

**4. Conclusion**

In [18], a comparison between GA index and ABC index for general trees and general graphs was left as an open problem. Theorems 3.3 - 3.9 provide a first step towards the solution of this open problem. The complete solution of the said problem remains a task for future.

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