ROSLAN HASNI

School of Informatics and Applied Mathematics
University Malaysia Terengganu
Kuala Nerus, Terengganu, Malaysia

The Conference on Combinatorics and Its Applications
NTU, Singapore, 14–16 July 2018
Topological indexes or molecular descriptors have been proposed for predicting the values of several physical properties and properties related to biological activities through QSAR.

Graph theory is used for building these topological and new concepts are developed to transform such graphs, which are non-numerical mathematical objects, into related numbers that are topological indexes or molecular descriptors.

Topological indexes have been successfully used for estimating several physical properties including normal boiling temperature and data related to biological activities as well.
Topological indices based on end-vertex degrees of edges has been intensively rising recently. Randić index is one of the best-known topological indices in chemical graph theory.

Fundamental and most studied problems in the theory of topological indices, considered in mathematical chemistry, ask for the

- extremal structures, under certain constraints, that maximize or minimize the given topological index
- best possible lower and upper bounds for the given topological index
- relations between different topological indices
Geometric-Arithmetic (GA) Index

Vukicevic and Furtula (2009) introduced a novel topological index based on the end-vertex degrees of the edges and presented its basic properties. This index is called as *geometric-arithmetic index* (GA) and is defined as follows:

\[
GA(G) = \sum_{uv \in E(G)} \frac{2 \sqrt{d_u d_v}}{d_u + d_v},
\]

where the summation extends over all edges \(uv\) in \(G\) and \(d_u, d_v\) are the degrees of vertices that are connected with edge \(uv\).

From the definition, it consists from geometrical mean of end-vertex degrees of an edge \(uv\) \((\sqrt{d_u d_v})\) as numerator and arithmetic mean of end-vertex degrees of the edge \(uv\) \(((d_u + d_v)/2)\) as denominator.
The following results are due to Vukicevic and Furtula (2009):

**Theorem 1** Let $G$ be a simple graph with $n$ vertices, then

$$0 \leq GA(G) \leq \binom{n}{2}$$

Lower bound is achieved if and only if $G$ is an empty graph and upper bound is achieved if and only if $G$ is a complete graph.
Theorem 2  Let $G$ be a simple graph with $n$ vertices, then

$$\frac{2(n-1)^{3/2}}{n} \leq GA(G) \leq \binom{n}{2}$$

Lower bound is achieved if and only if $G$ is a star and upper bound is achieved if and only if $G$ is a complete graph.
**Theorem 3**  Let $T$ be a tree with $n$ vertices, then

$$
\frac{2(n - 1)^{3/2}}{n} \leq GA(G) \leq \begin{cases} 
0, & n = 1 \\
1, & n = 2 \\
\frac{4\sqrt{2}}{3} + (n - 3), & n \geq 3
\end{cases}
$$

Lower bound is achieved if and only if $T$ is a star and upper bound is achieved if and only if $T$ is a path.
Bounds for GA Index

**Theorem 4** Let $T$ be a chemical tree with $n$ vertices, then

$$\frac{13}{15} n - \frac{17}{15} \leq GA(G) \leq \begin{cases} 
0, & n = 1 \\
1, & n = 2 \\
\frac{4\sqrt{2}}{3} + (n - 3), & n \geq 3 
\end{cases}$$

Lower bound is achieved for trees that contains only vertices of degrees 1 and 4; and upper bound is achieved if and only if $T$ is a path.

A pendant vertex is a vertex of degree one. A pendant edge is an edge incident with a pendant vertex. A path $u_1 u_2 \cdots u_r$ in a graph $G$ is said to be a pendant path at $u_1$ if $d_{u_1} \geq 3$, $d_{u_i} = 2$ for $2, \ldots, r - 1$ and $d_{u_r} = 1$.

**Lemma 1 (Du et. al (2011))** If there are $k$ pendant paths in graph $G$, then

$$GA(G) \leq \left( \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} \right) k + |E(G)| - 2k$$

An $n$-vertex connected graph is a bicyclic graph if it posses $n + 1$ edges.

**Lemma 2 (Du et. al (2011))** If there are $k$ pendant paths in $n$-vertex bicyclic graph $G$, then

$$GA(G) \leq \left( \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} \right) k + n + 1 - 2k$$
Classification:

Let $\mathbf{B}_1^1(n)$ be the set of bicyclic graphs obtained from $C_n$ by adding an edge, where $n \geq 4$.
Let $\mathbf{B}_1^2(n)$ be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles $C_a$ and $C_b$ with $a + b = n$ by an edge, where $n \geq 6$.
Let $\mathbf{B}_2(n)$ be the set of bicyclic graphs obtained from $C_a = v_0v_1\ldots v_{n-1}$ with $4 \leq a \leq n - 2$ by joining $v_0$ and $v_2$ by an edge, and attaching a path on $n - a$ vertices to $v_1$.
Let $\mathbf{B}_1^3(n)$ be the set of bicyclic graphs obtained by joining two non-adjacent vertices of $C_a$ with $4 \leq a \leq n - 1$ by a path of length $n - a + 1$, where $n \geq 5$.
Let $\mathbf{B}_2^3(n)$ be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles $C_a$ and $C_b$ with $a + b < n$ by a path of length $n - a - b + 1$, where $n \geq 7$. 
Let $\mathcal{B}_4(n)$ be the set of $n$-vertex bicyclic graphs obtained by attaching a path on at least two vertices to the two vertices of degree two of the unique 4-vertex bicyclic graph, where $n \geq 8$.

Let $\mathcal{B}_5^1(n)$ be the set of bicyclic graphs obtained from a graph in $\mathcal{B}_1^1(k)$ with $k \geq 5$ or $\mathcal{B}_1^2(k)$ with $k \geq 6$ by attaching a path on $n - k \geq 2$ vertices to a vertex of degree two, whose two neighbors are of degree two and three, where $n \geq 7$.

Let $\mathcal{B}_5^2(n)$ be the set of bicyclic graphs obtained from a graph in $\mathcal{B}_3^1(k)$ with $k \geq 5$ or $\mathcal{B}_3^2(k)$ with $k \geq 7$ by attaching a path on $n - k \geq 2$ vertices to a vertex of degree two, whose two neighbors are both of degree three, where $n \geq 7$.

Let $\mathcal{B}_6(n)$ be the bicyclic graphs obtained from $C_{n-1} = v_0v_1 \ldots v_{n-2}$ by joining $v_0$ and $v_2$ by an edge, and attaching a vertex of degree one to $v_1$, where $n \geq 5$. 
Theorem 5 (Du et. al (2011)) Among the set of $n$-vertex bicyclic graphs,

(i) the graphs in $B_1^1(n)$ for $n \geq 4$ and the graphs in $B_1^2(n)$ for $n \geq 6$ are the unique graphs with the maximum $GA$ index, which is equal to $n - 3 + \frac{8\sqrt{6}}{5}$,

(ii) for $n \geq 6$, the graphs in $B_2(n)$ are the unique graphs with the second maximum $GA$ index, which is equal to $n - 3 + \frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}$,

(iii) the graphs in $B_3^1(n)$ for $n \geq 6$ and the graphs in $B_3^2(n)$ for $n \geq 7$ are the unique graphs with the third maximum $GA$ index, which is equal to $n - 5 + \frac{12\sqrt{6}}{5}$,
(iv) for $n \geq 8$, the graphs in $B_4(n)$ are the unique graphs with the fourth maximum $GA$ index, which is equal to $n - 3 + \frac{4\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}$,

(v) for $n \geq 8$, the graphs in $B_5^1(n)$ or $B_5^2(n)$ are the unique graphs with the fifth maximum $GA$ index, which is equal to $n - 5 + 2\sqrt{6} + \frac{2\sqrt{2}}{3}$,

(vi) for $n \geq 8$, the graphs in $B_6(n)$ are the unique graphs with the sixth maximum $GA$ index, which is equal to $n - 2 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}$. 
Proof of Theorem 5: Three cases, i.e., bicyclic graphs with no pendant path, one pendant path and two pendant paths.

For more maximum values of GA index of bicyclic graphs, we consider the cases with exactly one, two and three pendant paths.

We determine the $n$-vertex bicyclic graphs with the seventh and eighth for $n \geq 9$, the ninth, tenth, eleventh and twelfth for $n \geq 10$, the thirteenth, fourteenth, fifteenth, sixteenth and seventeenth for $n \geq 11$, the eighteenth, nineteenth, twentieth, twenty-first, twenty-second, twenty-third, twenty-fourth and twenty-fifth for $n \geq 12$ maximum GA indices.
Classification:

Let $B^3_7(n)$ be the set of bicyclic graphs obtained from $C_a = v_0 v_1 \ldots v_{a-1}$ with $4 \leq a \leq n - 5$ by joining $v_0$ and $v_2$ by an edge, and attaching a pendant vertex of graph $T_a$ to a vertex of degree two of $C_a$, whose neighbors are both of degree three, where $n \geq 9$.

Let $B^1_8(n)$ be the set of bicyclic graphs obtained from $C_a = v_0 v_1 \ldots v_{a-1}$ with $6 \leq a \leq n - 3$ by joining two non-adjacent vertices by an edge and attaching a path of length at least two to a vertex of degree two whose two neighbors are degree two, where $n \geq 9$.

Let $B^2_8(n)$ be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles $C_a$ and $C_b$ with $a + b < n$ by a path of length $n - a - b - 1$ and attaching a path of length at least two to a vertex of degree two whose two neighbors are of degree two and three, where $n \geq 9$.

Let $B^3_8(n)$ be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles $C_a$ and $C_b$ with $a + b < n$ by an edge, and attaching a path of length at least two to a vertex of degree two whose neighbors are both of degree two, where $n \geq 9$. 
Let $B_8^4(n)$ be the set of bicyclic graphs obtained by joining two non-adjacent vertices of $C_a = v_0 v_1 \ldots v_{a-1}$ with $5 \leq a \leq n - 4$ by a path of length $n - a - 2$, and attaching a path of length at least two to a vertex of degree two whose two neighbors are of degree two and three, where $n \geq 9$.

Let $B_9(n)$ be the set of bicyclic graphs obtained by gluing a vertex of $C_a$ and $C_b$ with $a + b < n$, and attaching three path of length exactly one to a vertex of degree four and to two vertices of degree two whose neighbors are of degree two and three, respectively, where $n \geq 10$.

Let $B_{10}(n)$ be the set of bicyclic graphs obtained from the unique 4-vertex cycle graph $C_4 = v_0 v_1 v_2 v_3 v_0$ by joining $v_0$ and $v_2$ by an edge, and attaching two paths of length exactly one and at least two, respectively, to the two vertices of degree two, where $n \geq 10$. 
Let $B_{11}^1(n)$ be the set of bicyclic graphs obtained by joining two non-adjacent vertices of $C_a = v_0v_1 \ldots v_{a-1}$ with $4 \leq a \leq n - 6$ by a path of length $n - a - 4$, and attaching a path of length exactly one to a vertex of degree two whose two neighbors are of degree three, where $n \geq 10$.

Let $B_{11}^2(n)$ be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles $C_a$ and $C_b$ with $a + b < n$ by an edge and attaching a path of length exactly one to a vertex of degree two whose two neighbors are of degree two and three, where $n \geq 10$.

Let $B_{11}^3(n)$ be the set of bicyclic graphs obtained from $C_a = v_0v_1 \ldots v_{a-1}$ with $5 \leq a \leq n - 5$ by adding an edge and attaching a path of length exactly one to a vertex of degree two whose two neighbors are of degree two and three, where $n \geq 10$.

14 more types of bicyclic graphs to be obtained...
Main Result

**Theorem 6 (Du et. al (2011))** Among the set of $n$-vertex bicyclic graphs,

(i) for $n \geq 9$, the graphs in $B_7^1(n)$, $B_7^2(n)$ and $B_7^3(n)$ are the unique graphs with the seventh maximum $GA$ index, which is equal to $n - 5 + \frac{4\sqrt{2}}{3} + \frac{8\sqrt{6}}{5}$,

(ii) for $n \geq 9$, the graphs in $B_8^1(n)$, $B_8^2(n)$, $B_8^3(n)$ and $B_8^4(n)$ are the unique graphs with the eighth maximum $GA$ index, which is equal to $n - 7 + \frac{2\sqrt{2}}{3} + \frac{14\sqrt{6}}{5}$,

(iii) for $n \geq 10$, the graphs in $B_9(n)$ are the unique graphs with the ninth maximum $GA$ index, which is equal to $n - 8 + \sqrt{3} + \frac{2\sqrt{5}}{3} + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{10}}{7}$,

(iv) for $n \geq 10$, the graphs in $B_{10}(n)$ are the unique graphs with the tenth maximum $GA$ index, which is equal to $n - 2 + \frac{2\sqrt{2}}{3} + \frac{2\sqrt{6}}{5} + \frac{\sqrt{3}}{2}$,

(v) for $n \geq 10$, the graphs in $B_{11}^1(n)$, $B_{11}^2(n)$ and $B_{11}^3(n)$ are the unique graphs with the eleventh maximum $GA$ index, which is equal to $n - 4 + \frac{\sqrt{3}}{3} + \frac{8\sqrt{6}}{5}$,
(vi) for \( n \geq 10 \), the graphs in \( B_{12}(n) \) are the unique graphs with the twelfth maximum GA index, which is equal to \( n - 3 + \frac{8\sqrt{2}}{3} \),

(vii) for \( n \geq 11 \), the graphs in \( B_{13}^1(n) \) and \( B_{13}^2(n) \) are the unique graph with the thirteenth maximum GA index, which is equal to \( n - 5 + 2\sqrt{2} + \frac{6\sqrt{6}}{5} \),

(viii) for \( n \geq 11 \), the graphs in \( B_{14}^1(n) \), \( B_{14}^2(n) \), \( B_{14}^3(n) \) and \( B_{14}^4(n) \) are the unique graph with the fourteenth maximum GA index, which is equal to \( n - 7 + \frac{4\sqrt{2}}{3} + \frac{12\sqrt{6}}{5} \),

(ix) for \( n \geq 11 \), the graphs in \( B_{15}^1(n) \) and \( B_{15}^2(n) \) are the unique graph with the fifteenth maximum GA index, which is equal to \( n - 9 + \frac{2\sqrt{2}}{3} + \frac{18\sqrt{6}}{5} \),

(x) for \( n \geq 11 \), the graphs in \( B_{16}^1(n) \) and \( B_{16}^2(n) \) are the unique graph with the sixteenth maximum GA index, which is equal to \( n - 4 + \frac{2\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + \frac{\sqrt{3}}{2} \).
(xi) for $n \geq 11$, the graphs in $B_{17}^1(n)$, $B_{17}^2(n)$, $B_{17}^3(n)$ and $B_{17}^4(n)$ are the unique graph with the seventeenth maximum GA index, which is equal to $n - 6 + \frac{\sqrt{3}}{2} + \frac{12\sqrt{6}}{5}$,

(xii) for $n \geq 12$, the graphs in $B_{18}^1(n)$, $B_{18}^2(n)$ and $B_{18}^3(n)$ are the unique graph with the eighteenth maximum GA index, which is equal to $n - 7 + 2\sqrt{2} + 2\sqrt{6}$,

(xiii) for $n \geq 12$, the graphs in $B_{19}^1(n)$ and $B_{19}^2(n)$ are the unique graphs with the nineteenth maximum GA index which is equal to $n - 9 + \frac{4\sqrt{2}}{3} + \frac{16\sqrt{6}}{5}$,

(xiv) for $n \geq 12$, the graphs in $B_{20}^1(n)$, $B_{20}^2(n)$ and $B_{20}^3(n)$ are the unique graphs with the twentieth maximum GA index which is equal to $n - 6 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{3}}{7} + \frac{4\sqrt{6}}{5}$,

(xv) for $n \geq 12$, the graphs in $B_{21}^1(n)$ and $B_{22}^2(n)$ are the unique graphs with the twenty-first maximum GA index which is equal to $n - 4 + \frac{\sqrt{3}}{2} + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5}$,
(xvi) for \( n \geq 12 \), the graphs in \( B_{22}^1(n), B_{22}^2(n) \) and \( B_{22}^3(n) \) are the unique graphs with the twenty-second maximum \( GA \) index which is equal to
\[
\begin{align*}
&n - 7 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7},
\end{align*}
\]

(xvii) for \( n \geq 12 \), the graphs in \( B_{23}^1(n) \) and \( B_{23}^2(n) \) are the unique graphs with the twenty-third maximum \( GA \) index which is equal to
\[
\begin{align*}
&n - 6 + \frac{2\sqrt{2}}{3} + \frac{\sqrt{3}}{2} + 2\sqrt{6},
\end{align*}
\]

(xviii) for \( n \geq 12 \), the graphs in \( B_{24}^1(n) \) and \( B_{24}^2(n) \) are the unique graphs with the twenty-fourth maximum \( GA \) index which is equal to
\[
\begin{align*}
&n - 8 + \frac{\sqrt{3}}{2} + \frac{16\sqrt{6}}{5},
\end{align*}
\]

(xix) for \( n \geq 12 \), the graphs in \( B_{25}^1(n), B_{25}^2(n) \) and \( B_{25}^3(n) \) are the unique graphs with the twenty-fifth maximum \( GA \) index which is equal to
\[
\begin{align*}
&n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}.
\end{align*}
\]
Proof of Theorem 6

Let $G$ be an $n$-vertex bicyclic graph different from the graphs mentioned in Theorem 5 with the first six maximum GA indices, where $n \geq 8$.

If there are $k \geq 4$ pendant paths in $G$, then by Lemma 2, we have

$$GA(G) \leq \left( \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} \right) k + n + 1 - 2k$$

$$\leq \left( \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} \right) \cdot 4 + n + 1 - 2 \cdot 4$$

$$< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$$
Case 1. There is no pendant paths in $G$
Case 2. There is exactly one pendant path in $G$
Case 3. There are exactly two pendant paths in $G$
Case 4. There are exactly three pendant paths in $G$
Tabular form for results in Theorem 6 is given below.

<table>
<thead>
<tr>
<th>Ordering</th>
<th>Case/Subcase</th>
<th>Family of bicyclic graphs</th>
</tr>
</thead>
<tbody>
<tr>
<td>7th</td>
<td>3/3.5</td>
<td>$B_{7}^1(n)$, $B_{7}^2(n)$, $B_{7}^3(n)$</td>
</tr>
<tr>
<td>8th</td>
<td>2/2.3</td>
<td>$B_{8}^1(n)$, $B_{8}^2(n)$, $B_{8}^3(n)$, $B_{8}^4(n)$</td>
</tr>
<tr>
<td>9th</td>
<td>4/4.4</td>
<td>$B_{9}(n)$</td>
</tr>
<tr>
<td>10th</td>
<td>3/3.5</td>
<td>$B_{10}(n)$</td>
</tr>
<tr>
<td>11th</td>
<td>2/2.3</td>
<td>$B_{11}^1(n)$, $B_{11}^2(n)$, $B_{11}^3(n)$</td>
</tr>
<tr>
<td>12th</td>
<td>1/1.3</td>
<td>$B_{12}(n)$</td>
</tr>
<tr>
<td>13th</td>
<td>3/3.5</td>
<td>$B_{13}^1(n)$, $B_{13}^2(n)$, $B_{13}^3(n)$, $B_{13}^4(n)$</td>
</tr>
<tr>
<td>14th</td>
<td>2/2.3</td>
<td>$B_{14}^1(n)$, $B_{14}^2(n)$</td>
</tr>
<tr>
<td>15th</td>
<td>3/3.5</td>
<td>$B_{15}^1(n)$, $B_{15}^2(n)$</td>
</tr>
</tbody>
</table>
Bibliography


