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# Correcting a paper on the Randić and geometric–arithmetic indices

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**Abstract:** The Randić index ($R$) and the geometric–arithmetic index ($GA$) are found to be useful tools in QSPR and QSAR studies. In the Journal of Inequalities and Applications 180, 1-7, Lokesha, Shwetha Shetty, Ranjini, Cangul, and Cevik gave "New bounds for Randić and GA indices." In the paper, we first point out that Theorems 1, 2, and 4 are incorrect and in this short note we present the correct inequalities for Randić and GA indices. In the same paper, we provide the equality cases for Theorems 3, 5, and 6.

**Key words:** Randić index, geometric–arithmetic index, Zagreb index

## 1. Introduction

Let $G$ be a simple graph with $n$ vertices and $m$ edges. The degree of a vertex is denoted by $d(v_i)$, for $i = 1, 2, \ldots, n$ such that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$, with the maximum and the minimum vertex degree of $G$ denoted by $\Delta = \Delta(G)$ and $\delta = \delta(G)$, respectively. A vertex $v \in V(G)$ is said to be pendant if its neighborhood contains exactly one vertex, i.e. $d(v) = 1$. Moreover, $p$ and $\delta_1 = \delta_1(G)$ denotes the number of pendant vertices and minimum nonpendant vertex degree in $G$, respectively. A graph $G$ is called bidegreed if its vertex degree is either $\Delta$ or $\delta$ with $\Delta > \delta \geq 1$ and $K_{r,n-r}$ $(1 \leq r \leq n-1)$ denotes the bidegreed bipartite graph with $r$ vertices of degree $\Delta$ and $n-r$ vertices of degree $\delta$.

Molecular descriptors play a remarkable role in mathematical chemistry especially in QSPR/QSAR investigations. Out of them, a special place is reserved for topological descriptors. Nowadays, there exists hundreds of such topological descriptors in the literature. Among the oldest and the most famous and successful topological indices are the Randić and Zagreb indices.

In 1972, Gutman and Trinajstić [3] explored the study of total $\pi$-electron energy on the molecular structure and introduced two vertex degree-based graph invariants. These invariants are defined as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2, \qquad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

In 1975, Randić [5] proposed a topological index $R$ under the name branching index, suitable for

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measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons, defined by

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

In 2009, Vukičević and Furtula [6] introduced a new class of topological index named the geometric-arithmetic index, defined by

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}.$$

Subsequently two of these present authors together with Gutman [2] introduced the second general Zagreb index are defined for $\alpha \in \mathbb{R}$ as

$$M_2^{\alpha}(G) = \sum_{uv\in E(G)} [d(u)d(v)]^{\alpha}.$$

In 2013, Lokesha et al. [4] considered inequalities that determine the bounds for the Randić and geometric–arithmetic indices in terms of $m$, $p$, $\Delta$, $\delta_1$, and $M_2^{-1}(G)$. The authors presented six theorems, where the equality cases are missed out. Unfortunately, Theorems 1, 2, and 4 seem to be incorrect, leading to the present short note.

In order to study and investigate the graph-theoretical properties of these topological indices, we use the software GraphTea [1]. GraphTea is an interactive graph-editing framework to extract information from graphs. There is a module in GraphTea designed specifically for topological indices.

## 2. Main errors and equality cases

The main results of the paper [4] deal with the bounds for the Randić and geometric–arithmetic indices, where Theorems 1 and 4 give the inequality for the lower bounds and Theorem 2 gives the upper bound of the above-mentioned indices. We point out the major errors and give our counterexamples, comments, and corrections.

### 2.1. Theorem 1 of [4]

In Theorem 1 of [4] the following lower bound has been allegedly proved for the Randić index:

$$R(G) \geq \frac{p}{\sqrt{\Delta}} + \frac{2\sqrt{(m-p)\Delta\delta_1}}{\Delta+\delta_1}\sqrt{M_2^{-1}(G) - \frac{p}{\Delta}}. \tag{2.1}$$

Firstly, we comment that the inequality (2.1) is wrong. Consider the molecular graph 2,2-dimethyl butane (see Figure 1), for which the inequality (2.1) is not true. (Refer to the Table for the total number of counterexamples up to 9 vertex connected graphs.)

Since $1 < \delta_1 \leq d(v_i) \leq \Delta$ for $i = 1, 2, \cdots, n$, we have that $\frac{1}{\Delta} \leq \frac{1}{d(v_i)} \leq \frac{1}{\delta_1}$.

$$M_2^{-1}(G) = \sum_{v_iv_j\in E(G): d(v_i), d(v_j)\neq 1} \frac{1}{d(v_i)d(v_j)} + \sum_{v_iv_j\in E(G): d(v_j)=1} \frac{1}{d(v_i)}$$

$$\leq \sum_{v_iv_j\in E(G): d(v_i), d(v_j)\neq 1} \frac{1}{d(v_i)d(v_j)} + \frac{p}{\delta_1}.$$

**Table.** Number of counter examples for Theorems 1, 2, and 4.

| Parameters | | Counterexamples | | |
|---|---|---|---|---|
| $n$ | Count | Theorem 1 | Theorem 2 | Theorem 4 |
| 3 | 2 | 0 | 0 | 1 |
| 4 | 6 | 0 | 1 | 5 |
| 5 | 21 | 2 | 6 | 20 |
| 6 | 112 | 9 | 36 | 111 |
| 7 | 853 | 57 | 272 | 851 |
| 8 | 11117 | 376 | 3108 | 11107 |
| 9 | 261080 | 3675 | 56407 | 260995 |

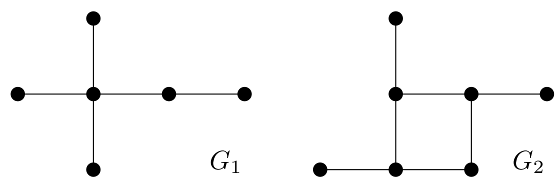


**Figure 1**. $G_1$ : 2,2 dimethyl butane and $G_2$ : 1,2,3 trimethyl cyclobutane.

Since $M_2^{-1}(G)$ is wrongly determined in [4] as

$$M_2^{-1}(G) \leq \sum_{v_iv_j \in E(G): d(v_i), d(v_j) \neq 1} \frac{1}{d(v_i)d(v_j)} + \frac{p}{\Delta},$$

this leads to the counterexample from above. The corrected version of the inequality (2.1) is given by

$$R(G) \geq \frac{p}{\sqrt{\Delta}} + \frac{2\sqrt{(m-p)\Delta\delta_1}}{\Delta + \delta_1}\sqrt{M_2^{-1}(G) - \frac{p}{\delta_1}}. \tag{2.2}$$

Secondly, still the inequality (2.2) holds only for the graphs satisfying $M_2^{-1}(G) - \frac{p}{\delta_1} \geq 0$ and the equality holds if and only if $G$ is regular or a bidegreed graph with one vertex set of degree one. In analogy, corollary 1 of [4] is to be changed as follows.

**Corollary 2.1** *Let $T$ be a tree with $n$ vertices, $p$ pendent vertices, $m$ edges, maximal degree $\Delta$, and minimal nonpendent vertex degree $\delta_1$ and satisfying the condition $M_2^{-1}(T) - \frac{p}{\delta_1} \geq 0$. Then*

$$R(T) \geq \frac{p}{\sqrt{\Delta}} + \frac{2\sqrt{(n-1-p)\Delta\delta_1}}{\Delta + \delta_1}\sqrt{M_2^{-1}(T) - \frac{p}{\delta_1}} \tag{2.3}$$

*equality holds if and only if $T$ is a bidegreed tree.*

### 2.2. Theorem 2 of [4]

In Theorem 2 the following upper bound was allegedly proved for the Randić index:

$$R(G) \leq \frac{p}{\sqrt{\delta_1}} + \sqrt{(m-p)\left(M_2^{-1}(G) - \frac{p}{\delta_1}\right)}. \tag{2.4}$$

Firstly, we comment that the inequality (2.4) is incorrect. Consider the molecular graph 1,2,3-trimethyl cyclobutane (see Figure 1), for which the inequality (2.4) fails.

Using similar arguments for the case of Theorem 1, we have

$$M_2^{-1}(G) \geq \sum_{v_iv_j \in E(G): d(v_i), d(v_j) \neq 1} \frac{1}{d(v_i)d(v_j)} + \frac{p}{\Delta}.$$

However, the wrong assumption in the proof of Theorem 2 leads to the incorrect inequality (2.4). For any simple graph $G$, it is obvious that $M_2^{-1}(G) - \frac{p}{\Delta} \geq 0$. Therefore, the corrected inequality can be expressed as

$$R(G) \leq \frac{p}{\sqrt{\delta_1}} + \sqrt{(m-p)\left(M_2^{-1}(G) - \frac{p}{\Delta}\right)}. \tag{2.5}$$

Secondly, the equality of (2.5) holds if and only if $G$ is regular or a bidegreed graph with one vertex set of degree one or $K_{r,n-r}$.

### 2.3. Theorem 3 of [4]

In Theorem 3, a new upper bound for the Randić index was provided without the equality case.

**Theorem 2.2** [4] *Let $G$ be a simple connected graph of order $n$ with $m$ edges, and let $p$, $\Delta$, and $\delta_1$ denote the number of pendant vertices, maximum vertex degree, and minimum nonpendant vertex degree of $G$, respectively. Then*

$$R(G) \leq \frac{p}{\sqrt{\delta_1}} + \frac{(m-p)}{\delta_1} \tag{2.6}$$

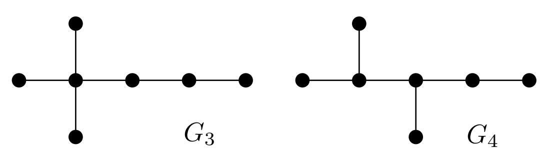


**Figure 2**. $G_3$ : 2,2 dimethyl pentane and $G_4$ : 2,3 dimethyl pentane.

**Remark 2.3** *The equality of (2.6) holds if and only if $G$ is regular or a bidegreed graph with one vertex set of degree one. The bounds in (2.5) and (2.6) are incomparable. For the molecular graph 2,3 dimethyl pentane (refer to Figure 2) (2.5) is better than (2.6) and for the molecular graph 2,2 dimethyl pentane (2.6) is better than (2.5).*

### 2.4. Theorem 4 of [4]

In Theorem 4, the lower bound for the geometric–arithmetic index was provided without the equality case.

$$GA(G) \geq \frac{2p\sqrt{\delta_1}}{\Delta + 1} + 2\sqrt{2}\frac{\delta_1\Delta}{(\Delta^2 + \delta_1^2)}\sqrt{\frac{(m-p)}{\Delta}\,(M_2^1(G) - p\delta_1)}. \tag{2.7}$$

First, we comment that the inequality (2.7) is incorrect and we give a corrected version of it.

**Theorem 2.4** *Let $G$ be a simple connected graph of order $n$ with $m$ edges and let $p$, $\Delta$, and $\delta_1$ denote the number of pendant vertices, maximum vertex degree, and minimum nonpendant vertex degree of $G$, respectively. Then*

$$GA(G) \geq \frac{2p\sqrt{\delta_1}}{\Delta+1} + \frac{2\delta_1}{(\Delta^2+\delta_1^2)}\sqrt{(m-p)\left(M_2^1(G)-p\Delta\right)} \tag{2.8}$$

*equality holds if and only if $G$ is regular or a bidegreed graph with one vertex set of degree one.*

**Proof** For $2 \leq \delta_1 \leq d(v_i) \leq \Delta$, we get $\frac{\delta_1}{\Delta} \leq \frac{2\sqrt{d(v_i)d(v_j)}}{d(v_i)+d(v_j)} \leq \frac{\Delta}{\delta_1}$.
Using the Pólya–Szegö inequality, we have

$$\begin{aligned}
\left(\sum_{v_iv_j\in E(G):d(v_i),d(v_j)\neq 1} \frac{2\sqrt{d(v_i)d(v_j)}}{(d(v_i)+d(v_j))}\right)^2 &\geq \frac{4\Delta^2\delta_1^2(m-p)}{\left(\Delta^2+\delta_1^2\right)^2}\left(\sum_{v_iv_j\in E(G):d(v_i),d(v_j)\neq 1} \frac{4d(v_i)d(v_j)}{\left(d(v_i)+d(v_j)\right)^2}\right) \\
&\geq \frac{4\Delta^2\delta_1^2(m-p)}{\left(\Delta^2+\delta_1^2\right)^2}\left(\sum_{v_iv_j\in E(G):d(v_i),d(v_j)\neq 1} \frac{4d(v_i)d(v_j)}{4\Delta^2}\right) \\
&= \frac{4\delta_1^2(m-p)}{\left(\Delta^2+\delta_1^2\right)^2}\left(\sum_{v_iv_j\in E(G):d(v_i),d(v_j)\neq 1} d(v_i)d(v_j)\right) \\
&\geq \frac{4\delta_1^2(m-p)}{\left(\Delta^2+\delta_1^2\right)^2}\left(M_2^1(G)-p\Delta\right)
\end{aligned}$$

It is easy to see that

$$\begin{aligned}
GA(G) &= \sum_{v_iv_j\in E(G):d(v_i),d(v_j)\neq 1} \frac{2\sqrt{d(v_i)d(v_j)}}{(d(v_i)+d(v_j))} + \sum_{v_iv_j\in E(G):d(v_j)=1} \frac{2\sqrt{d(v_i)}}{(d(v_i)+1)} \\
&\geq \sum_{v_iv_j\in E(G):d(v_i),d(v_j)\neq 1} \frac{2\sqrt{d(v_i)d(v_j)}}{(d(v_i)+d(v_j))} + \frac{2p\sqrt{\delta_1}}{\Delta+1}
\end{aligned}$$

completes the proof. □

**Corollary 2.5** *Let $T$ be a tree of order $n$ and with the assumptions in Theorem 2.4 one has the inequality*

$$GA(T) \geq \frac{2p\sqrt{\delta_1}}{\Delta+1} + \frac{2\delta_1}{(\Delta^2+\delta_1^2)}\sqrt{(n-1-p)\left(M_2^1(T)-p\Delta\right)} \tag{2.9}$$

*and the equality holds if and only if $T$ is a bidegreed tree.*

### 2.5. Theorems 5 and 6 of [4]

Theorems 5 and 6 give the upper bounds for the geometric–arithmetic index and the equality cases are missing for both the inequalities

$$GA(G) \leq \frac{2p\sqrt{\Delta}}{1+\delta_1} + \frac{1}{\delta_1}\sqrt{(m-p)\,(M_2^1(G) - p\Delta)}, \tag{2.10}$$

$$GA(G) \leq \frac{2p\sqrt{\Delta}}{1+\delta_1} + \frac{(m-p)\Delta}{\delta_1}. \tag{2.11}$$

Note that equality holds in the above inequalities if and only if $G$ is regular or a bidegreed graph with one vertex set of degree one.

### 2.6. Computational results

In the Table, we present the computational results for the connected graphs on $n = 3$ to $n = 9$ vertices using GraphTea [1]. The first two columns contain $n$ and the number of connected graphs of order $n$. The next three columns contain the number of graphs, for which the inequalities of Theorems 1, 2, and 4 are incorrect, respectively.

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## References

[1] Ali Rostami M, Martin Bücker H, Azadi A. Illustrating a Graph Coloring Algorithm Based on the Principle of Inclusion and Exclusion Using GraphTea. LNCS, Springer 2014; 8719: 514-517.

[2] Britto Antony Xavier G, Suresh E, Gutman I. Counting relations for general Zagreb indices. Kragujevac J Math 2014; 38: 95-103.

[3] Gutman I, Trinajstić N. Graph theory and molecular orbitals. Total $\pi$-electron energy of alternant hydrocarbons. Chem Phys Lett 1972; 17: 535-538.

[4] Lokesha V, Shwetha Shetty B, Ranjini PS, Cangul IN, Cevik AS. New bounds for Randić and GA indices. J Inequal Appl 2013; 180: 1-7.

[5] Randić M. On characterization of molecular branching. J Am Chem Soc 1975; 97: 6609-6615.

[6] Vukičević D, Furtula B. Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. J Math Chem 2009; 46: 1369-1376.