Relationships between Randić index and other topological indices

Z. Du[1,2,*] A. Jahanbani[3] and S.M. Sheikholeslami[3]

[1] School of Software, South China Normal University, Foshan, Guangdong 528225, China

[2] School of Mathematics and Statistics, Zhaoqing University, Zhaoqing 526061, China
zhibindu@126.com

[3] Department of Mathematics, Azarbaijan Shahid Madani University, Tabriz, Iran
Akbar.jahanbani92@gmail.com   s.m.sheikholeslami@azaruniv.ac.ir

Abstract: Let G be a graph with vertex set $V(G)$ and edge set $E(G)$, and let d_u denote the degree of vertex $u \in V(G)$. The Randić index of G is defined as $R(G) = \sum_{uv \in E(G)} 1/\sqrt{d_u d_v}$. In this paper, we investigate the relationships between Randić index and several topological indices.

Keywords: Randić index, Zagreb indices, ABC index, Geometric-Arithmetic index, Augmented Zagreb index

AMS Subject classification: 05C50

1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The integers $n = |V(G)|$ and $m = |E(G)|$ are the *order* and the *size* of the graph G, respectively. The *open neighborhood* of vertex v is $N(v) = \{u \in V(G) \mid uv \in E(G)\}$ and the *degree* of v is $d_v = |N(v)|$. The *minimum* and *maximum degree* of a graph G are denoted by δ and Δ, respectively.

Molecular descriptors play a significant role in mathematical chemistry, especially in QSPR/QSAR investigations. Among them, special place is reserved for the so-called topological descriptors. A topological index is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947 when H.

---

* *Corresponding author*

Wiener developed the most widely known topological descriptor, namely the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin (see, for instance, [8, 30]).

Topological indices based on vertex-degree play a vital role in mathematical chemistry and some of them are recognized tools in chemical research. An excellent survey about the degree-based topological indices can be found in [12].

The molecular structure-descriptor, put forward in 1975 by Milan Randić [26], is defined by

$$R = R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

For any real number α, the general Randić index, R_α, is defined in [3] as

$$R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha.$$

The Randić index, sometimes called connectivity index, has been successfully related to physical and chemical properties of organic molecules and become one of the most popular molecular descriptors. More results about the Randić index can refer to the survey [19].

Among the several hundred presently existing graph-based molecular structure descriptors [32, 33], the Randić index is certainly the most widely applied in chemistry and pharmacology, in particular for designing quantitative structure-property and structure-activity relations. For more information, you can see the books [17, 29] and the surveys written by Randić himself [27, 28]. Initially, the Randić index was studied only by chemists, but recently it has also attracted the attention of mathematicians, for instance, we cite [2, 3, 6].

The Randić index found chemical applications and became a popular topic of research in mathematics and mathematical chemistry, for more information you can see [23, 26, 27]. Randić proposed this index in order to quantitatively characterize the degree of molecular branching. According to him, the degree of branching of the molecular skeleton is a critical factor for some molecular properties such as boiling points of hydrocarbons and the retention volumes and the retention times obtained from chromatographic studies (all citations are taken from [26]).

In this paper, considering the importance of Randić index, we obtain some lower and upper bounds for it and investigate its relationships with other topological indices. We make use of the following inequalities throughout this paper.

Proposition A. (Jensen's inequality [21]) Let $a = (a_i)_{i=1}^n$ and $p = (p_i)_{i=1}^n$ be two sequences of positive numbers. Then, for any real number r with $r \leqslant 0$ or $r \geqslant 1$,

$$\sum_{i=1}^n p_i a_i^r \geqslant \sum_{i=1}^n p_i \left(\frac{\sum_{i=1}^n p_i a_i}{\sum_{i=1}^n p_i} \right)^r.$$

Proposition B.   ([25]) Let $a = (a_i)_{i=1}^n$ and $b = (b_i)_{i=1}^n$ be two sequences of positive numbers. For any $r \geqslant 0$,

$$\sum_{i=1}^n \frac{a_i^{r+1}}{b_i^r} \geqslant \frac{\left(\sum_{i=1}^n a_i\right)^{r+1}}{\left(\sum_{i=1}^n b_i\right)^r}.$$

Lemma 1.   [22] Let $n \geqslant 1$ be an integer and $a_1, a_2, \ldots, a_n$ be some nonnegative numbers such that $a_1 \geqslant a_2 \geqslant \cdots \geqslant a_n$. Then

$$(a_1 + \cdots + a_n)(a_1 + a_n) \geqslant a_1^2 + \cdots + a_n^2 + n a_1 a_n.$$

Lemma 2.   [31] Let $a_1, a_2, \ldots, a_n > 0$. Then

$$n \sum_{i=1}^n a_i - \left(\sum_{i=1}^n \sqrt{a_i}\right)^2 \leq n(n-1) \left(\frac{1}{n} \sum_{i=1}^n a_i - \left(\prod_{i=1}^n a_i\right)^{\frac{1}{n}}\right).$$

Theorem 1.   [7] Let $a = (a_i)_{i=1}^n$ and $b = (b_i)_{i=1}^n$ be two decreasing nonnegative sequences with $a_1, b_1 \neq 0$, and $w = (w_i)_{i=1}^n$ be a nonnegative sequence. Then the following inequality is valid

$$\sum_{i=1}^n w_i a_i^2 \sum_{i=1}^n w_i b_i^2 \leqslant \max\left\{b_1 \sum_{i=1}^n w_i a_i, a_1 \sum_{i=1}^n w_i b_i\right\} \sum_{i=1}^n w_i a_i b_i.$$

2.   Bounds

In this section, we present lower and upper bounds for Randić index. We begin with a simple inequality.

Lemma 3.   Let $x \geqslant y$ be two positive numbers. Then

$$\frac{(x-y)^2}{8x} \leqslant \frac{x+y}{2} - \sqrt{xy} \leqslant \frac{(x-y)^2}{8y}.$$

Proof.   Since the proofs of the two inequalities are similar, we only prove the left inequality. Since $\frac{x+y}{2} - \sqrt{xy} = \frac{(\sqrt{x}-\sqrt{y})^2}{2}$ and

$$\frac{(x-y)^2}{8x} = \frac{(\sqrt{x}-\sqrt{y})^2(\sqrt{x}+\sqrt{y})^2}{8x},$$

it is enough to prove that

$$\frac{(\sqrt{x}-\sqrt{y})^2(\sqrt{x}+\sqrt{y})^2}{8x} \leqslant \frac{(\sqrt{x}-\sqrt{y})^2}{2}$$

or equivalently,

$$(\sqrt{x}+\sqrt{y})^2 \leqslant 4x.$$

In fact, we have that

$$(\sqrt{x}+\sqrt{y})^2 \leqslant (\sqrt{x}+\sqrt{x})^2 = 4x,$$

as desired. $\square$

Theorem 2. *Let G be a graph of size $m \geqslant 1$ and maximum degree Δ. Then*

$$R(G) \leqslant R^2_{\frac{-1}{4}}(G) - \frac{m(m-1)}{\Delta}.$$

Proof. Setting $a_{uv} = \frac{1}{\sqrt{d_u d_v}}$ for all edges $uv \in E(G)$. Applying Lemma 2 and the definitions, we have

$$m \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} - \left(\sum_{uv \in E(G)} \frac{1}{\sqrt[4]{d_u d_v}} \right)^2 \leqslant m(m-1) \left(\frac{1}{m} \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} - \left(\prod_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \right)^{\frac{1}{m}} \right).$$

Hence,

$$R(G) \leqslant R^2_{\frac{-1}{4}}(G) - \frac{m(m-1)}{\Delta}.$$

The proof is completed. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

For any graph G of order n, the Randić matrix of G, denoted by $\mathbf{R} = (r_{ij})$, is defined in [5] as follows:

$$r_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}} & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent} \\ 0 & \text{otherwise.} \end{cases}$$

In [5], it is proved that

$$tr(\mathbf{R}^2) = 2 \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

Theorem 3. *Let G be a graph of size $m \geqslant 1$ with maximum degree Δ and minimum degree δ. Then*

$$\sqrt{\frac{1}{2} tr(\mathbf{R}^2) + \frac{m(m-1)}{\Delta^2}} \leqslant R(G) \leqslant \sqrt{\frac{1}{2} tr(\mathbf{R}^2) + \frac{m(m-1)}{\delta^2}}.$$

Proof. Since $\delta \leqslant d_{v_i} \leqslant \Delta$ for all vertices $v_i \in V(G)$, we have

$$
\begin{aligned}
(R(G))^2 &= \left(\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \right)^2 \\
&= \sum_{uv \in E(G)} \frac{1}{d_u d_v} + \sum_{uv \neq zw} \frac{1}{\sqrt{d_u d_v}} \frac{1}{\sqrt{d_z d_w}} \\
&\leqslant \sum_{uv \in E(G)} \frac{1}{d_u d_v} + \frac{m(m-1)}{\delta^2} \\
&= \frac{1}{2} tr(\mathbf{R}^2) + \frac{m(m-1)}{\delta^2}.
\end{aligned}
$$

Likewise, we have

$$
\begin{aligned}
(R(G))^2 &= \left(\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \right)^2 \\
&= \sum_{uv \in E(G)} \frac{1}{d_u d_v} + \sum_{uv \neq zw} \frac{1}{\sqrt{d_u d_v}} \frac{1}{\sqrt{d_z d_w}} \\
&\geqslant \sum_{uv \in E(G)} \frac{1}{d_u d_v} + \frac{m(m-1)}{\Delta^2} \\
&= \frac{1}{2} tr(\mathbf{R}^2) + \frac{m(m-1)}{\Delta^2}.
\end{aligned}
$$

The result follows easily. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Theorem 4. *Let G be a graph with maximum degree Δ and minimum degree δ. Then*

$$
\frac{\delta tr(\mathbf{R}^2)}{2} \leqslant R(G) \leqslant \frac{\Delta tr(\mathbf{R}^2)}{2}.
$$

Proof.   We know that $\delta^2 \leqslant d_u d_v \leqslant \Delta^2$ for all edges $uv \in E(G)$, $\delta \leqslant d_i \leqslant \Delta$ for all vertices $v_i \in V(G)$. By the definition of Randić index, we have

$$
\begin{aligned}
tr(\mathbf{R}^2) &= 2 \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \frac{1}{\sqrt{d_u d_v}} \\
&\leqslant \frac{2}{\delta} \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\
&= \frac{2R(G)}{\delta}.
\end{aligned}
$$

Therefore, we have

$$
\frac{\delta tr(\mathbf{R}^2)}{2} \leqslant R(G).
$$

Analogously above, we have

$$
\begin{aligned}
tr(\mathbf{R}^2) &= 2 \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \frac{1}{\sqrt{d_u d_v}} \\
&\geqslant \frac{2}{\Delta} \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\
&= \frac{2R(G)}{\Delta}.
\end{aligned}
$$

Hence

$$
\frac{\Delta tr(\mathbf{R}^2)}{2} \geqslant R(G).
$$

The result follows. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

3. Randić index versus other topological indices

In this section, we investigate the relationships between Randić index and other topological indices. The first and second Zagreb indices are vertex-degree-based graph invariants defined as

$$M_1 = M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

and

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

The quantity M_1 was first considered in 1972 [16], whereas M_2 in 1975 [14]. The bounds for Zagreb indices can refer to [4].

The sigma index of G, is defined in [15] as

$$\sigma = \sigma(G) = \sum_{uv \in E(G)} (d_u - d_v)^2.$$

Applying Lemma 3, we establish an upper bound for Randić index in terms of the first Zagreb index and the sigma index.

Theorem 5. *Let G be a non-trivial graph with maximum degree Δ. Then*

$$R(G) \leqslant \frac{M_1(G)}{2} - \frac{\sigma(G)}{8\Delta}.$$

Proof. By definitions, we have

$$
\begin{aligned}
R(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\
&\leqslant \sum_{uv \in E(G)} \sqrt{d_u d_v} \\
&\leqslant \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{2} - \frac{(d_u - d_v)^2}{8d_u} \right) \\
&= \sum_{uv \in E(G)} \frac{d_u + d_v}{2} - \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{8d_u} \\
&\leqslant \sum_{uv \in E(G)} \frac{d_u + d_v}{2} - \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{8\Delta} \\
&= \frac{M_1(G)}{2} - \frac{\sigma(G)}{8\Delta},
\end{aligned}
$$

and the proof is completed. $\square$

Next we present an upper bound for Randić index in terms of the first Zagreb index.

Theorem 6. *Let G be a non-trivial graph with minimum degree δ. Then*

$$R(G) \leqslant \frac{M_1(G)}{2\delta^2}.$$

Proof. By using geometric arithmetic inequality for two positive real numbers x and y, we have that

$$\frac{x+y}{2} \geqslant \sqrt{xy} \geqslant \frac{2}{\frac{1}{x} + \frac{1}{y}}. \tag{1}$$

Using Inequality (1) and the fact $\delta \leqslant d_u \leqslant \Delta$, we have

$$\begin{aligned}
R(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\
&\leqslant \sum_{uv \in E(G)} \frac{1}{\frac{2}{\frac{1}{d_u} + \frac{1}{d_v}}} \\
&= \sum_{uv \in E(G)} \frac{1}{\frac{2}{\frac{d_u + d_v}{d_u d_v}}} \\
&= \frac{1}{2} \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u d_v} \\
&\leqslant \frac{M_1(G)}{2\delta^2},
\end{aligned}$$

as desired. $\square$

By a closer look at the proof of Theorem 6, we can obtain the following result.

Corollary 1. *For any non-trivial connected graph G with maximum degree Δ,*

$$R(G) \leqslant \Delta R_{-1}(G).$$

The generalization of Zagreb index was introduced in [13] as follows

$$M_{\alpha,\beta}(G) = \sum_{uv \in E(G)} \frac{(d_u d_v)^\alpha}{(d_u + d_v)^\beta}.$$

In [36], the general sum-connectivity index was defined by

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha.$$

We now give a lower bound for Randić index in terms of the generalization of Zagreb index and the general sum-connectivity index.

Theorem 7. *Let G be a non-trivial graph. Then*

$$R(G) \geqslant \frac{\chi^2_{-1}(G)}{M_{\frac{1}{2},2}(G)}.$$

Proof. Put $r = 1$, $a_{uv} = \frac{1}{d_u+d_v}$ and $b_{uv} = \frac{1}{\sqrt{d_u d_v}}$ for each $uv \in E(G)$. Applying Proposition B and definitions we have

$$
\begin{aligned}
M_{\frac{1}{2},2}(G) &= \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{(d_u + d_v)^2} \\
&= \sum_{uv \in E(G)} \frac{\frac{1}{(d_u+d_v)^2}}{\frac{1}{\sqrt{d_u d_v}}} \\
&\geqslant \frac{\left(\sum_{uv \in E(G)} \frac{1}{d_u + d_v} \right)^2}{\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}} \\
&= \frac{\chi^2_{-1}(G)}{R(G)},
\end{aligned}
$$

and this leads to the desired bound. $\qquad\square$

Next we present an upper bound for Randić index in terms of the general Randić index.

Theorem 8. *Let G be a non-trivial graph with m edges. Then*

$$R(G) \leqslant \sqrt[3]{m^2 R_{-\frac{3}{2}}(G)}.$$

Proof. Setting $r = 3$, $a_{uv} = \frac{1}{\sqrt{d_u d_v}}$ and $p_{uv} = 1$ for each $uv \in E(G)$. Applying Proposition A and definitions we have

$$
\begin{aligned}
R_{-\frac{3}{2}}(G) &= \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d_u d_v}} \right)^3 \\
&\geqslant \sum_{i=1}^{m} 1 \left(\frac{\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}}{\sum_{uv \in E(G)} 1} \right)^3 \\
&= \frac{1}{m^2} \left(\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \right)^3 \\
&= \frac{1}{m^2} \left(R(G) \right)^3,
\end{aligned}
$$

and this leads to the desired bound.   □

Next we present a lower bound for Randić index in terms of the general sum-connectivity index.

Theorem 9. *Let G be a non-trivial graph. Then*

$$R(G) \geqslant \chi_{-\frac{3}{2}}(G).$$

Proof. For two real numbers x and y, we have that

$$xy = \frac{1}{4}\left((x+y)^2 - (x-y)^2\right). \tag{2}$$

By Equality (2) and definition of the Randić index, we have

$$
\begin{aligned}
R(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\
&= \sum_{uv \in E(G)} \frac{1}{\sqrt{\frac{1}{4}\left((d_u + d_v)^2 - (d_u - d_v)^2\right)}} \\
&= \sum_{uv \in E(G)} \frac{2}{\sqrt{((d_u + d_v)^2 - (d_u - d_v)^2)}} \\
&\geqslant \sum_{uv \in E(G)} \frac{2}{\sqrt{(d_u + d_v)^2}} \\
&\geqslant \sum_{uv \in E(G)} \frac{1}{\sqrt{(d_u + d_v)^3}} = \chi_{-\frac{3}{2}}(G).
\end{aligned}
$$

The result follows.   □

The atom-bond connectivity index or ABC index, is defined in [8] as

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

Here we present a lower bound for Randić index in terms of the atom-bond connectivity index.

Theorem 10. *Let G be a non-trivial graph with m edges, maximum degree Δ, and minimum degree $\delta \geqslant 1$. Then*

$$R(G) \geqslant \frac{\left(m^{\frac{\sqrt[4]{2\delta - 2}}{\Delta}}\right)^2}{ABC(G)}.$$

Proof. Setting $r = 2$, $a_{uv} = (d_u + d_v - 2)^{\frac{1}{4}}$ and $p_{uv} = \frac{1}{\sqrt{d_u d_v}}$ for each $uv \in E(G)$ and applying Proposition A and definitions, we obtain

$$
\begin{aligned}
ABC(G) &= \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\
&= \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d_u d_v}} \right) \left((d_u + d_v - 2)^{\frac{1}{4}} \right)^2 \\
&\geqslant \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \left(\frac{\sum\limits_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} (d_u + d_v - 2)^{\frac{1}{4}}}{\sum\limits_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}} \right)^2 \\
&= \frac{\left(\sum\limits_{uv \in E(G)} \frac{\sqrt[4]{d_u + d_v - 2}}{\sqrt{d_u d_v}} \right)^2}{\sum\limits_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}} \\
&= \frac{\left(\sum\limits_{uv \in E(G)} \frac{\sqrt[4]{d_u + d_v - 2}}{\sqrt{d_u d_v}} \right)^2}{R(G)} \\
&\geqslant \frac{\left(\sum\limits_{uv \in E(G)} \frac{\sqrt[4]{d_u + d_v - 2}}{\Delta} \right)^2}{R(G)} \\
&\geqslant \frac{\left(\sum\limits_{uv \in E(G)} \frac{\sqrt[4]{2\delta - 2}}{\Delta} \right)^2}{R(G)} \\
&= \frac{\left(m \frac{\sqrt[4]{2\delta - 2}}{\Delta} \right)^2}{R(G)},
\end{aligned}
$$

and this implies the desired bound.   □

The inverse indeg index, denoted by $ISI(G)$, was defined in [34] as

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

Next we present a lower bound for Randić index in terms of the general sum-connectivity index and inverse sum indeg index.

Theorem 11. *For any non-trivial graph of G,*

$$R(G) \geqslant \sqrt{\frac{\left(\chi_{-\frac{1}{3}}(G)\right)^3}{ISI(G)}}.$$

Proof. Put $r = 2$, $a_{uv} = \frac{1}{\sqrt[3]{d_u+d_v}}$ and $b_{uv} = \frac{1}{\sqrt{d_u d_v}}$ for each $uv \in E(G)$. Applying Proposition B and definitions we have

$$
\begin{aligned}
ISI(G) &= \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v} \\
&= \sum_{uv \in E(G)} \frac{\left(\frac{1}{\sqrt[3]{d_u+d_v}}\right)^3}{\left(\frac{1}{\sqrt{d_u d_v}}\right)^2} \\
&\geqslant \frac{\left(\displaystyle\sum_{uv \in E(G)} \frac{1}{\sqrt[3]{d_u + d_v}}\right)^3}{\left(\displaystyle\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}\right)^2} \\
&\geqslant \frac{\left(\chi_{-\frac{1}{3}}(G)\right)^3}{(R(G))^2},
\end{aligned}
$$

and this leads to the desired bound. □

The augmented Zagreb index was defined in [10] as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3.$$

Next result relates the Randić index to the augmented Zagreb index.

Theorem 12. *Let G be a non-trivial graph with m edges, maximum degree $\Delta \geqslant 2$, and minimum degree δ. Then*

$$R(G) \geqslant \sqrt{\frac{\frac{m^3 \delta^6}{\Delta^2}}{(2\Delta - 2)^3 \, AZI(G)}}.$$

Proof. Put $r = 2$, $a_{uv} = \frac{d_u d_v}{d_u+d_v-2}$ and $b_{uv} = \frac{1}{\sqrt{d_u d_v}}$ for each $uv \in E(G)$. Applying

Proposition B and definitions, we have

$$
\begin{aligned}
\Delta^2 AZI(G) &\geqslant \sum_{uv \in E(G)} \frac{\left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3}{\left(\frac{1}{d_u d_v}\right)} \\
&= \sum_{uv \in E(G)} \frac{\left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3}{\left(\frac{1}{\sqrt{d_u d_v}}\right)^2} \\
&\geqslant \frac{\left(\displaystyle\sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v - 2}\right)^3}{\left(\displaystyle\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}\right)^2} \\
&= \frac{\left(\displaystyle\sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v - 2}\right)^3}{(R(G))^2} \\
&\geqslant \frac{\left(\frac{m\delta^2}{2\Delta - 2}\right)^3}{(R(G))^2},
\end{aligned}
$$

and this leads to the desired bound. □

The sum-connectivity F-index and the general first F-index of a graph G were defined in [18] as

$$
SF(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u^2 + d_v^2}}
$$

and

$$
F_1^a(G) = \sum_{uv \in E(G)} \left(d_u^2 + d_v^2\right)^a,
$$

where a is a real number.

The forgotten topological index has been introduced by Furtula and Gutman [11] as

$$
F(G) = \sum_{uv \in E(G)} \left(d_u^2 + d_v^2\right).
$$

Now we find a relationship between the Randić index and the product of forgotten topological index and general first F-index.

Theorem 13. *Let G be a non-trivial graph with minimum degree δ. Then*

$$R(G) \leqslant \sqrt{\frac{F_1^{-1}(G)F(G)}{\delta^2}}.$$

Proof. Set $r = 1$, $a_{uv} = \frac{1}{\sqrt{d_u d_v}}$ and $b_{uv} = \frac{1}{d_u^2 + d_v^2}$ for each $uv \in E(G)$. Applying Proposition B and definitions, we have

$$\begin{aligned}
\frac{F(G)}{\delta^2} &= \frac{1}{\delta^2} \sum_{uv \in E(G)} (d_u^2 + d_v^2) \\
&\geqslant \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u d_v} \\
&= \sum_{uv \in E(G)} \frac{\left(\frac{1}{\sqrt{d_u d_v}}\right)^2}{\frac{1}{d_u^2 + d_v^2}} \\
&\geqslant \frac{\left(\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}\right)^2}{\sum_{uv \in E(G)} \frac{1}{d_u^2 + d_v^2}} \\
&= \frac{(R(G))^2}{F_1^{-1}(G)},
\end{aligned}$$

and this leads to the desired bound. $\qquad\square$

Next we present a lower bound for Randić index in terms of the sum-connectivity F-index.

Theorem 14. *Let G be a non-trivial graph. Then*

$$R(G) \geqslant \sqrt{2}\, SF(G).$$

Proof. For two real numbers x and y, we have that

$$xy \leqslant \frac{x^2}{2} + \frac{y^2}{2}. \tag{3}$$

By definitions of the Randić index and Equality (3), we have

$$
\begin{aligned}
R(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\
&\geqslant \sum_{uv \in E(G)} \frac{1}{\sqrt{\frac{d_u^2}{2} + \frac{d_v^2}{2}}} \\
&= \sum_{uv \in E(G)} \frac{1}{\sqrt{\frac{d_u^2 + d_v^2}{2}}} \\
&= \sum_{uv \in E(G)} \frac{\sqrt{2}}{\sqrt{d_u^2 + d_v^2}} \\
&= \sqrt{2}\, SF(G).
\end{aligned}
$$

Now we get the desired result. $\square$

The (first) geometric-arithmetic index of a graph was defined in [35] as

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

Some recent results on geometric-arithmetic index of graphs can be found in [24]. Next we present a lower bound for Randić index in terms of the (first) geometric-arithmetic index.

Theorem 15. *Let G be a non-trivial graph with m edges and maximum degree Δ. Then*

$$
R(G) \geqslant \frac{m^2}{\Delta GA(G)}.
$$

Proof. Set $r = 1$, $a_{uv} = \frac{1}{\sqrt{d_u + d_v}}$ and $b_{uv} = \frac{1}{\sqrt{d_u d_v}}$ for each $uv \in E(G)$. By Proposition B and definitions, we have

$$
\begin{aligned}
\frac{GA(G)}{2} &= \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{d_u + d_v} \\
&= \sum_{uv \in E(G)} \frac{\left(\frac{1}{\sqrt{d_u + d_v}}\right)^2}{\frac{1}{\sqrt{d_u d_v}}} \\
&\geqslant \frac{\left(\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}\right)^2}{\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}} \\
&\geqslant \frac{m^2}{2\Delta R(G)},
\end{aligned}
$$

and this leads to the desired bound. □

The harmonic index, denoted by $H(G)$, was defined in [9] as

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

The Albertson index, $Alb(G)$, used as an irregularity measure of a graph, was defined in [1] as

$$Alb(G) = \sum_{uv \in E(G)} |d_u - d_v|.$$

Theorem 16. *[20] Let G be a simple connected graph with $m \geqslant 1$ edges. Then*

$$GA(G) \leqslant \sqrt{H(G)ISI(G)}.$$

Theorem 17. *[20] Let G be a simple connected graph with m edges. Then*

$$GA(G) \leqslant \sqrt{m\left(m - \frac{(Alb(G))^2}{F(G) + 2M_2(G)}\right)}.$$

By Theorems 15 and 16, we can see the relationship between Randić index, the inverse indeg index and the harmonic index as following.

Corollary 2. *Let G be a simple connected graph with $m \geqslant 1$ edges and maximum degree Δ. Then*

$$R(G) \geqslant \frac{m^2}{\Delta\sqrt{H(G)ISI(G)}}.$$

Also, by Theorems 15 and 17, we can see the relationship between Randić index, Albertson index, F-index and the second Zagreb index as following.

Corollary 3. *Let G be a simple connected graph with $m \geqslant 1$ edges and maximum degree Δ. Then*

$$R(G) \geqslant \frac{m^2}{\Delta\sqrt{m\left(m - \frac{(Alb(G))^2}{F(G)+2M_2(G)}\right)}}.$$

Theorem 18. *Let G be a graph with minimum degree $\delta > 2$. Then*

$$R(G) \geqslant \delta R_{-1}(G).$$

Proof. For $a_{uv} = b_{uv} := \frac{1}{\sqrt{d_u d_v}}$, and $w_{uv} := 1$, for all edges $uv \in E(G)$. Applying Theorem 1 and the definitions, we have

$$\sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d_u d_v}} \right)^2 \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d_u d_v}} \right)^2$$

$$\leqslant \max \left\{ \frac{1}{\delta} \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}, \frac{1}{\delta} \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \right\} \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

Hence, by definitions, it is equivalent to

$$R(G) \geqslant \delta R_{-1}(G).$$

The proof is completed. □

References

[1] M.O. Albertson, *The irregularity of a graph*, Ars Combin. **46** (1997), 219–225.

[2] O. Araujo and J.A. De La Peña, *The connectivity index of a weighted graph*, Linear Algebra Appl. **283** (1998), no. 1-3, 171–177.

[3] B. Bollobás and P. Erdős, *Graphs of extremal weights*, Ars Combin. **50** (1998), 225–233.

[4] B. Borovicanin, K.C. Das, B. Furtula, and I. Gutman, *Bounds for Zagreb indices*, MATCH Commun. Math. Comput. Chem. **78** (2017), no. 1, 17–100.

[5] S.B. Bozkurt, A.D. Güngör, I. Gutman, and A.S. Cevik, *Randić matrix and Randić energy*, MATCH Commun. Math. Comput. Chem. **64** (2010), 239–250.

[6] C. Delorme, O. Favaron, and D. Rautenbach, *On the Randić index*, Discrete Math. **257** (2002), no. 1, 29–38.

[7] S.S. Dragomir, *A survey on Cauchy-Bunyakovsky-Schwarz type discrete inequalities*, J. Inequal. Pure Appl. Math. **4** (2003), no. 3, 1–142.

[8] E. Estrada, L. Torres, L. Rodríguez, and I. Gutman, *An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes*, Indian J. Chem. **A 37** (1998), 849–855.

[9] S. Fajtlowicz, *On conjectures of Graffiti-II*, Congr. Numer. **60** (1987), 187–197.

[10] B. Furtula, A. Graovac, and D. Vukičević, *Augmented Zagreb index*, J. Math. Chem. **48** (2010), no. 2, 370–380.

[11] B. Furtula and I. Gutman, *A forgotten topological index*, J. Math. Chem. **53** (2015), no. 4, 1184–1190.

[12] I. Gutman, *Degree-based topological indices*, Croat. Chem. Acta **86** (2013), no. 4, 351–361.

[13] I. Gutman, E. Milovanović, and I. Milovanović, *Beyond the Zagreb indices*, AKCE Int. J. Graphs Comb. (2018), in press.

[14] I. Gutman, B. Ruščić, N. Trinajstić, and C.F. Wilcox Jr, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys. **62** (1975), no. 9, 3399–3405.

[15] I. Gutman, M. Togan, A. Yurttas, A.S. Cevik, and I.N. Cangul, *Inverse problem for sigma index*, MATCH Commun. Math. Comput. Chem. **79** (2018), no. 2, 491–508.

[16] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals. Total $\pi-$electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), no. 4, 535–538.

[17] L.B. Kier and L.H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New York, 1976.

[18] V.R. Kulli, *F-indices of chemical networks*, Int. J. Math. Archive **10** (2019), no. 3, 21–30.

[19] X. Li and Y. Shi, *A survey on the Randić index*, MATCH Commun. Math. Comput. Chem. **59** (2008), no. 1, 127–156.

[20] I.Ž. Milovanović, E.I. Milovanović, and M.M. Matejić, *On upper bounds for the geometric–arithmetic topological index*, MATCH Commun. Math. Comput. Chem. **80** (2018), no. 1, 109–127.

[21] D.S. Mitrinović, J.E. Pečarić, and A.M. Fink, *Classical and New Inequalities in Analysis*, Springer, Netherlands, 1993.

[22] M.R. Oboudi, *A new lower bound for the energy of graphs*, Linear Algebra Appl. **580** (2019), 384–395.

[23] L. Pogliani, *From molecular connectivity indices to semiempirical connectivity terms: Recent trends in graph theoretical descriptors*, Chem. Rev. **100** (2000), no. 10, 3827–3858.

[24] A. Portilla, J.M. Rodríguez, and J.M. Sigaretta, *Recent lower bounds for geometric-arithmetic index*, Discrete Math. Lett. **1** (2019), 59–82.

[25] J. Radon, *Theorie und Anwendungen der absolut additiven Mengenfunktionen*, Sitzungsber. Acad. Wissen. Wien. **112** (1913), 1295–1438.

[26] M. Randić, *Characterization of molecular branching*, J. Am. Chem. Soc. **97** (1975), no. 23, 6609–6615.

[27] _____ , *The connectivity index 25 years after*, J. Mol. Graphics Model. **20** (2001), no. 1, 19–35.

[28] _____ , *On history of the Randić index and emerging hostility toward chemical graph theory*, MATCH Commun. Math. Comput. Chem. **59** (2008), no. 1, 5–124.

[29] M. Randić, M. Novič, and D. Plavšić, *Solved and Unsolved Problems of Structural Chemistry*, CRC Press, Boca Raton, 2016.

[30] P.S. Ranjini, V. Lokesha, A.R. Bindusree, and M.P. Raju, *New bounds on Zagreb indices and the Zagreb co-indices*, Bol. Soc. Parana. Mat. SPM **31** (2013), no. 1, 51–55.

[31] P.B. Sarasija and R. Binthiya, *Bounds on the Seidel energy of strongly quotient graphs*, J. Chem. Pharm. Sci. **10** (2017), no. 1, 1–4.

[32] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, John Wiley & Sons, 2008.

[33] _____, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, 2009.

[34] D. Vukičević, *Bond additive modeling 2. Mathematical properties of max-min rodeg index*, Croat. Chem. Acta. **83** (2010), no. 3, 261–273.

[35] D. Vukičević and B. Furtula, *Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges*, J. Math. Chem. **46** (2009), no. 4, 1369–1376.

[36] B. Zhou and N. Trinajstić, *On general sum-connectivity index*, J. Math. Chem. **47** (2010), no. 1, 210–218.