# ON THE SUM-CONNECTIVITY INDEX 

Shilin Wang, Bo Zhou* and Nenad Trinajstić


#### Abstract

The sum-connectivity index of a simple graph $G$ is defined in mathematical chemistry as $$
R^{+}(G)=\sum_{u v \in E(G)}\left(d_{u}+d_{v}\right)^{-1 / 2}
$$ where $E(G)$ is the edge set of $G$ and $d_{u}$ is the degree of vertex $u$ in $G$. We give a best possible lower bound for the sum-connectivity index of a graph (a triangle-free graph, respectively) with $n$ vertices and minimum degree at least two and characterize the extremal graphs, where $n \geq 11$.


## 1 Introduction

Let $G$ be a simple graph with vertex set $V(G)$ and edge set $E(G)$ [1]. For $u \in V(G)$, $d_{u}(G)$ or $d_{u}$ denotes the degree of $u$ in $G$. Let $N(u)$ be the set of neighbors of vertex $u$ in $G$. Then $d_{u}=|N(u)|$.

The Randić connectivity index of a graph $G$, proposed by Randić in 1975, is defined as [2]

$$
R(G)=\sum_{u v \in E(G)}\left(d_{u} d_{v}\right)^{-1 / 2}
$$

It is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies [3-8]. Its mathematical properties [9, 10] and generalizations/variants [11-13] have also been studied extensively. We also call it the product-connectivity index.

[^0]Motivated by Randićs definition of the product-connectivity index, the sumconnectivity index of a graph $G$ was proposed in [14], which is defined as

$$
R^{+}(G)=\sum_{u v \in E(G)}\left(d_{u}+d_{v}\right)^{-1 / 2}
$$

The applications of the sum-connectivity index have been investigated in [15, 16]. Some basic mathematical properties of the sum-connectivity index have been established in [14, 17-19].

Bollobás and Erdös [20] showed that for a graph $G$ with $n$ vertices and without isolated vertices, $R(G) \geq \sqrt{n-1}$ with equality if and only if $G$ is the star. Then Delorme et al. [21] gave a best possible lower bound for the product-connectivity index of a graph with $n \geq 6$ vertices and minimum degree at least two. Later Liu et al. [22] found a best possible lower bound for the product-connectivity index of a triangle-free graph with $n \geq 6$ vertices and minimum degree at least two.

In [14], it was shown that for a graph $G$ with $n \geq 5$ vertices and without isolated vertices, $R^{+}(G) \geq \frac{n-1}{\sqrt{n}}$ with equality if and only if $G$ is the star. For $n=4$, this is not true since for the union of two copies of path on two vertices, its sum-connectivity index is $\sqrt{2}$, less than $\frac{3}{2}$. In this paper, we establish a best possible lower bound for the sum-connectivity index of a graph (triangle-free graph, respectively) with $n \geq 11$ vertices and minimum degree at least two and characterize the extremal graphs.

## 2 Preliminaries

For a graph $G$ with $u \in V(G)(e \in E(G)$, respectively), $G-u$ ( $G-e$, respectively) means the graph obtained feom $G$ by deleting $u$ and its incident edges ( $e$, respectively).

For an edge $e=u v$ of a graph $G$, its weight is defined to be $\left(d_{u}+d_{v}\right)^{-1 / 2}$. The sum-connectivity index of $G$ is the sum of weights over all its edges.

Lemma 2.1. If $e$ is an edge of maximal weight in $G$, then $R^{+}(G-e)<R^{+}(G)$.
Proof. Let $e=u v$. Since $u v$ is an edge of maximal weight in $G$, we have $d_{w} \geq d_{v}$ for $w \in N(u)$ and $d_{w} \geq d_{u}$ for $w \in N(v)$. Obviously, for positive $a, \frac{1}{\sqrt{x+a}}-\frac{1}{\sqrt{x+a-1}}$ and $\frac{x-1}{\sqrt{x}}$ are both increasing for $x \geq 1$. Then

$$
\begin{aligned}
& R^{+}(G)-R^{+}(G-e) \\
= & \frac{1}{\sqrt{d_{u}+d_{v}}}+\sum_{w \in N(u) \backslash\{v\}}\left(\frac{1}{\sqrt{d_{u}+d_{w}}}-\frac{1}{\sqrt{d_{u}+d_{w}-1}}\right) \\
& +\sum_{w \in N(v) \backslash\{u\}}\left(\frac{1}{\sqrt{d_{v}+d_{w}}}-\frac{1}{\sqrt{d_{v}+d_{w}-1}}\right) \\
\geq & \frac{1}{\sqrt{d_{u}+d_{v}}}+\left(d_{u}-1\right)\left(\frac{1}{\sqrt{d_{u}+d_{v}}}-\frac{1}{\sqrt{d_{u}+d_{v}-1}}\right)
\end{aligned}
$$

$$
\begin{aligned}
& +\left(d_{v}-1\right)\left(\frac{1}{\sqrt{d_{v}+d_{u}}}-\frac{1}{\sqrt{d_{v}+d_{u}-1}}\right) \\
= & \frac{d_{u}+d_{v}-1}{\sqrt{d_{u}+d_{v}}}-\frac{d_{u}+d_{v}-2}{\sqrt{d_{u}+d_{v}-1}} \\
> & 0 .
\end{aligned}
$$

The result follows.

$$
\text { For } x \geq 3 \text {, let } r(x)=2 \sqrt{x+1}+\frac{1}{\sqrt{2 x-2}}-\frac{6}{\sqrt{x+1}}
$$

Lemma 2.2. For $n \geq 11,2 \sqrt{n}-\frac{4}{\sqrt{n}}-r(n)>0$.
Proof. For $11 \leq n \leq 15$, the result can be checked by direct calculation. Suppose that $n \geq 16$. For $a, b>0$, it is easily seen that $\frac{1}{a}+\frac{1}{b} \geq \frac{4}{a+b}$ with equality if and only if $a=b$. This implies that

$$
-\frac{2}{\sqrt{n}+\sqrt{n+1}}>-\frac{1}{2}\left(\frac{1}{\sqrt{n}}+\frac{1}{\sqrt{n+1}}\right) .
$$

Then

$$
\begin{aligned}
& 2 \sqrt{n}-\frac{4}{\sqrt{n}}-r(n) \\
= & 2 \sqrt{n}-\frac{4}{\sqrt{n}}-2 \sqrt{n+1}-\frac{1}{\sqrt{2(n-1)}}+\frac{6}{\sqrt{n+1}} \\
= & -\frac{2}{\sqrt{n}+\sqrt{n+1}}-\frac{4}{\sqrt{n}}-\frac{1}{\sqrt{2(n-1)}}+\frac{6}{\sqrt{n+1}} \\
> & -\frac{1}{2}\left(\frac{1}{\sqrt{n}}+\frac{1}{\sqrt{n+1}}\right)-\frac{4}{\sqrt{n}}-\frac{1}{\sqrt{2(n-1)}}+\frac{6}{\sqrt{n+1}} \\
= & -\frac{9}{2 \sqrt{n}}+\frac{11}{2 \sqrt{n+1}}-\frac{1}{\sqrt{2(n-1)}} \\
= & \left(-\frac{9}{2 \sqrt{n}}+\frac{9}{2 \sqrt{n+1}}\right)+\left(\frac{1}{\sqrt{2(n+1)}}-\frac{1}{\sqrt{2(n-1)}}\right) \\
& +\frac{\sqrt{2}-1}{\sqrt{2(n+1})} \\
= & \frac{\sqrt{2}-1}{2 \sqrt{2(n+1)}}+\left(-\frac{9}{2 \sqrt{n}}+\frac{9}{2 \sqrt{n+1}}\right) \\
& +\frac{\sqrt{2}-1}{2 \sqrt{2(n+1)}}+\left(\frac{1}{\left.\sqrt{2(n+1)}-\frac{1}{\sqrt{2(n-1)}}\right)}\right. \\
= & \frac{1}{2 \sqrt{2(n+1)}}\left(\sqrt{2}-1-\frac{9 \sqrt{2}}{\sqrt{n}(\sqrt{n+1}+\sqrt{n})}\right)
\end{aligned}
$$

$$
\begin{aligned}
& +\frac{1}{2 \sqrt{2(n+1)}}\left(\sqrt{2}-1-\frac{4}{\sqrt{n-1}(\sqrt{n+1}+\sqrt{n-1})}\right) \\
\geq & \frac{1}{2 \sqrt{2(n+1)}}\left(\sqrt{2}-1-\frac{9 \sqrt{2}}{\sqrt{16}(\sqrt{17}+\sqrt{16})}\right) \\
& +\frac{1}{2 \sqrt{2(n+1)}}\left(\sqrt{2}-1-\frac{4}{\sqrt{15}(\sqrt{17}+\sqrt{15})}\right) \\
> & 0 .
\end{aligned}
$$

The result follows.
Lemma 2.3. For $x \geq 3+i, r(x)-r(x-i)$ is decreasing in $x$, where $i=2,3$.
Proof. For $x \geq 3$, it is easily seen that $6 \sqrt{2}\left(\frac{x-1}{x+1}\right)^{5 / 2} \geq 6 \sqrt{2}\left(\frac{3-1}{3+1}\right)^{5 / 2}>1$, implying that $\frac{3}{4 \sqrt{2}}(x-1)^{-5 / 2}<\frac{9}{2}(x+1)^{-5 / 2}$. Then

$$
\begin{aligned}
r^{\prime \prime}(x) & =-\frac{1}{2}(x+1)^{-3 / 2}+\frac{3}{4 \sqrt{2}}(x-1)^{-5 / 2}-\frac{9}{2}(x+1)^{-5 / 2} \\
& <-\frac{1}{2}(x+1)^{-3 / 2} \\
& <0
\end{aligned}
$$

By the Lagrange mean-value theorem, $r^{\prime}(x)-r^{\prime}(x-i)<0$ for $x \geq 3+i$, and thus the result follows.

Let $f(x, y)=\frac{1}{\sqrt{x+y}}-\frac{1}{\sqrt{x+y-2}}+\frac{x-1}{\sqrt{x+2}}-\frac{x-2}{\sqrt{x+1}}+\frac{y-1}{\sqrt{y+2}}-\frac{y-2}{\sqrt{y+1}}$, where $x, y \geq 2$.
Lemma 2.4. For $x, y \geq 3, f(x, y)$ is decreasing in $x$ and $y$.
Proof. Let $g(x)=(x+2) x^{-3 / 2}-(x+1)^{-3 / 2}$ for $x \geq 4$. Then

$$
g^{\prime}(x)=-\left(\frac{1}{2} x+3\right) x^{-5 / 2}+\frac{3}{2}(x+1)^{-5 / 2}<0
$$

i.e., $g(x)$ is decreasing in $x$. It is easily seen that

$$
\begin{aligned}
\frac{\partial f(x, y)}{\partial x}= & \frac{1}{2}(x+5)(x+2)^{-3 / 2}-\frac{1}{2}(x+4)(x+1)^{-3 / 2} \\
& -\frac{1}{2}(x+y)^{-3 / 2}+\frac{1}{2}(x+y-2)^{-3 / 2}
\end{aligned}
$$

and thus

$$
\frac{\partial}{\partial y}\left(\frac{\partial f(x, y)}{\partial x}\right)=-\frac{3}{4}(x+y-2)^{-5 / 2}+\frac{3}{4}(x+y)^{-5 / 2}<0
$$

implying that

$$
\frac{\partial f(x, y)}{\partial x} \leq \frac{\partial f(x, 3)}{\partial x}
$$

$$
\begin{aligned}
& =\frac{1}{2}(x+5)(x+2)^{-3 / 2}-\frac{1}{2}(x+3)(x+1)^{-3 / 2}-\frac{1}{2}(x+3)^{-3 / 2} \\
& =\frac{1}{2}(g(x+2)-g(x+1)) \\
& <0
\end{aligned}
$$

Similarly, $\frac{\partial f(x, y)}{\partial y}<0$. Now the result follows.
Let $K_{a, b}$ be the complete bipartite graph with $a$ and $b$ vertices in its two partite sets, respectively. For $n \geq 4$, let $K_{2, n-2}^{*}$ be the graph obtained from $K_{2, n-2}$ by joining an edge between the two vertices of degree $n-2$. Obviously, $R^{+}\left(K_{2, n-2}^{*}\right)=$ $r(n)$. Let $\delta(G)$ be the minimum degree of the graph $G$.

Lemma 2.5. Let $G$ be a graph with $n$ vertices and $\delta(G)=2$. Let $u$ be a vertex of degree two with two adjacent neighbors, both of degree at least three. Then $R^{+}(G)-$ $R^{+}(G-u) \geq f(n-1, n-1)$ with equality if and only if $G=K_{2, n-2}^{*}$.

Proof. Let $N(u)=\{v, w\}$. Obviously, $\frac{1}{\sqrt{x}}-\frac{1}{\sqrt{x-1}}$ is increasing for $x>1$. We have

$$
\begin{aligned}
& R^{+}(G)-R^{+}(G-u) \\
= & \frac{1}{\sqrt{d_{v}+2}}+\frac{1}{\sqrt{d_{w}+2}}+\frac{1}{\sqrt{d_{v}+d_{w}}}-\frac{1}{\sqrt{d_{v}+d_{w}-2}} \\
& +\sum_{z \in N(v) \backslash\{u, w\}}\left(\frac{1}{\sqrt{d_{v}+d_{z}}}-\frac{1}{\sqrt{d_{v}+d_{z}-1}}\right) \\
& +\sum_{z \in N(w) \backslash\{u, v\}}\left(\frac{1}{\sqrt{d_{w}+d_{z}}}-\frac{1}{\sqrt{d_{w}+d_{z}-1}}\right) \\
\geq & \frac{1}{\sqrt{d_{v}+2}}+\frac{1}{\sqrt{d_{w}+2}}+\frac{1}{\sqrt{d_{v}+d_{w}}}-\frac{1}{\sqrt{d_{v}+d_{w}-2}} \\
& +\left(d_{v}-2\right)\left(\frac{1}{\sqrt{d_{v}+2}}-\frac{1}{\sqrt{d_{v}+2-1}}\right) \\
& +\left(d_{w}-2\right)\left(\frac{1}{\sqrt{d_{w}+2}}-\frac{1}{\sqrt{d_{w}+2-1}}\right) \\
= & f\left(d_{v}, d_{w}\right),
\end{aligned}
$$

and thus $R^{+}(G)-R^{+}(G-u) \geq f\left(d_{v}, d_{w}\right)$ with equality if and only if $d_{z}=2$ for $z \in N(v) \backslash\{u, w\}$ or $z \in N(w) \backslash\{u, v\}$. By Lemma 2.4, $R^{+}(G)-R^{+}(G-u) \geq$ $f(n-1, n-1)$ with equality if and only if $d_{v}=d_{w}=n-1$ and $d_{z}=2$ for $z \in N(v) \backslash\{u, w\}$ or $z \in N(w) \backslash\{u, v\}$, i.e., $G=K_{2, n-2}^{*}$.

Lemma 2.6. Let $G$ be a triangle-free graph with $n$ vertices and $\delta(G)=2$. Let $u$ be $a$ vertex of degree two in $G$. Then $R^{+}(G)-R^{+}(G-u) \geq 2\left(\frac{n-2}{\sqrt{n}}-\frac{n-2-1}{\sqrt{n-1}}\right)$ with equality if and only if $G=K_{2, n-2}$.

Proof. Let $N(u)=\left\{v_{1}, v_{2}\right\}$. Since $G$ is a triangle-free graph, $d_{v_{1}}, d_{v_{2}} \leq n-2$ and $v_{1} v_{2} \notin E(G)$. Note that $\frac{x}{\sqrt{\delta+x}}-\frac{x-1}{\sqrt{\delta+x-1}}$ is decreasing for $x \geq 1$. We have

$$
\begin{aligned}
& R^{+}(G)-R^{+}(G-u) \\
= & \sum_{i=1}^{2}\left(\frac{1}{\sqrt{2+d_{v_{i}}}}+\sum_{z \in N\left(v_{i}\right) \backslash\{u\}}\left(\frac{1}{\sqrt{d_{z}+d_{v_{i}}}}-\frac{1}{\sqrt{d_{z}+d_{v_{i}}-1}}\right)\right) \\
\geq & \sum_{i=1}^{2}\left[\frac{1}{\sqrt{2+d_{v_{i}}}}+\left(d_{v_{i}}-1\right)\left(\frac{1}{\sqrt{2+d_{v_{i}}}}-\frac{1}{\sqrt{2+d_{v_{i}}-1}}\right)\right] \\
= & \sum_{i=1}^{2}\left(\frac{d_{v_{i}}}{\sqrt{2+d_{v_{i}}}}-\frac{d_{v_{i}}-1}{\sqrt{2+d_{v_{i}}-1}}\right) \\
\geq & 2\left(\frac{n-2}{\sqrt{2+(n-2)}}-\frac{(n-2)-1}{\sqrt{2+(n-2)-1}}\right) \\
= & 2\left(\frac{n-2}{\sqrt{n}}-\frac{n-3}{\sqrt{n-1}}\right)
\end{aligned}
$$

with equalities if and only if $d_{v_{1}}=d_{v_{2}}=n-2$ and $d_{z}=2$ for $z \in N\left(v_{i}\right) \backslash\{u\}$ with $i=1,2$, i.e., $G=K_{2, n-2}$.

## 3 Result

Now we prove our main results.
Theorem 3.1. Let $G$ be a graph with $n \geq 11$ vertices and $\delta(G) \geq 2$. Then $R^{+}(G) \geq$ $r(n)$ with equality if and only if $G=K_{2, n-2}^{*}$.

Proof. Assume that $G$ is a counterexample with minimal number of vertices for which $R^{+}(G)$ is minimal. If $\delta(G) \geq 3$, then by Lemma 2.1, the deletion of an edge of maximal weight yields a graph $G^{\prime}$ of minimal degree at least two such that $R^{+}\left(G^{\prime}\right)<R^{+}(G)$, which is a contradiction to the choice of $G$. Hence $\delta(G)=2$.
Claim 1. The neighbors of every vertex of degree two are adjacent.
Suppose that the claim is false. Let $u$ be a vertex of degree two with $N(u)=$ $\{v, w\}$ and $v w \notin E(G)$. Then $G_{1}=G-u+v w$ is not a counterexample, and thus $R^{+}\left(G_{1}\right) \geq r(n-1)$.

Let $t(x, y)=\frac{1}{\sqrt{2+x}}+\frac{1}{\sqrt{2+y}}-\frac{1}{\sqrt{x+y}}$, where $x, y \geq 2$. Then $\frac{\partial t(x, y)}{\partial x}=-\frac{1}{2}(2+$ $x)^{-3 / 2}+\frac{1}{2}(x+y)^{-3 / 2}$, and thus $\frac{\partial}{\partial y}\left(\frac{\partial t(x, y)}{\partial x}\right)=-\frac{3}{4}(x+y)^{-5 / 2}<0$, implying that $\frac{\partial t(x, y)}{\partial x} \leq \frac{\partial t(x, 2)}{\partial x}=0$. Similarly, $\frac{\partial t(x, y)}{\partial y} \leq 0$. Since $2 \leq d_{v}, d_{w} \leq n-2$, we have $t\left(d_{v}, d_{w}\right) \geq t(n-2, n-2)$. By Lemma 2.2, we have

$$
R^{+}(G)=R^{+}\left(G_{1}\right)+\frac{1}{\sqrt{2+d_{v}}}+\frac{1}{\sqrt{2+d_{w}}}-\frac{1}{\sqrt{d_{v}+d_{w}}}
$$

$$
\begin{aligned}
& =R^{+}\left(G_{1}\right)+t\left(d_{v}, d_{w}\right) \\
& \geq r(n-1)+t(n-2, n-2) \\
& =2 \sqrt{n}-\frac{4}{\sqrt{n}} \\
& >r(n)
\end{aligned}
$$

which is a contradiction. Claim 1 follows.
Claim 2. Every pair of adjacent vertices of degree two has no common neighbor.
Suppose that the claim is false. Let $u_{1}$ and $u_{2}$ be two adjacent vertices of degree two and $u_{3}$ a common neighbor of them. Obviously, $2 \leq d_{u_{3}} \leq n-1$.

Suppose that $d_{u_{3}}=2$. Then $G_{2}=G-u_{1}-u_{2}-u_{3}$ is not a counterexample, and thus $R^{+}\left(G_{2}\right) \geq r(n-3)$. By Lemma 2.3, $r(n)-r(n-3) \leq r(11)-r(8)=1.1525<\frac{3}{2}$, implying that

$$
R^{+}(G)=R^{+}\left(G_{2}\right)+\frac{3}{2} \geq r(n-3)+\frac{3}{2}>r(n)
$$

which is a contradiction.
Now suppose that $d_{u_{3}} \geq 4$. Then $G_{3}=G-u_{1}-u_{2}$ is not a counterexample, and thus $R^{+}\left(G_{3}\right) \geq r(n-2)$. Then

$$
\begin{aligned}
R^{+}(G)= & R^{+}\left(G_{3}\right)+\sum_{v \in N\left(u_{3}\right) \backslash\left\{u_{1}, u_{2}\right\}}\left(\frac{1}{\sqrt{d_{v}+d_{u_{3}}}}-\frac{1}{\sqrt{d_{v}+d_{u_{3}}-2}}\right) \\
& +\frac{2}{\sqrt{2+d_{u_{3}}}}+\frac{1}{2} \\
\geq & r(n-2)+\left(d_{u_{3}}-2\right)\left(\frac{1}{\sqrt{2+d_{u_{3}}}}-\frac{1}{\sqrt{2+d_{u_{3}}-2}}\right) \\
& +\frac{2}{\sqrt{2+d_{u_{3}}}}+\frac{1}{2} \\
= & r(n-2)+\frac{d_{u_{3}}}{\sqrt{2+d_{u_{3}}}}-\frac{d_{u_{3}}-2}{\sqrt{d_{u_{3}}}}+\frac{1}{2} .
\end{aligned}
$$

It is easily seen that $\frac{a}{\sqrt{2+a}}-\frac{a-2}{\sqrt{a}}$ is decreasing for $a \geq 2$. If $11 \leq n \leq 20$, then $d_{u_{3}} \leq n-1$, and by Lemma 2.3 and direct calculation, we have

$$
\begin{aligned}
R^{+}(G)-r(n) & \geq(r(n-2)-r(n))+\left(\frac{d_{u_{3}}}{\sqrt{2+d_{u_{3}}}}-\frac{d_{u_{3}}-2}{\sqrt{d_{u_{3}}}}\right)+\frac{1}{2} \\
& \geq(r(11-2)-r(11))+\left(\frac{19}{\sqrt{2+19}}-\frac{19-2}{\sqrt{19}}\right)+\frac{1}{2} \\
& >0
\end{aligned}
$$

It is easily seen that $\frac{a-2}{\sqrt{a}}$ is increasing for $a \geq 2$. If $n \geq 21$, then by Lemma 2.3 and direct calculation, we have

$$
R^{+}(G)-r(n) \geq(r(n-2)-r(n))+\left(\frac{d_{u_{3}}}{\sqrt{2+d_{u_{3}}}}-\frac{d_{u_{3}}-2}{\sqrt{d_{u_{3}}}}\right)+\frac{1}{2}
$$

$$
\begin{aligned}
& \geq(r(21-2)-r(21))+\frac{1}{2} \\
& >\quad 0
\end{aligned}
$$

Thus $R^{+}(G) \geq r(n)$, which is a contradiction.
Suppose that $d_{u_{3}}=3$. Denote by $u_{4}$ the neighbor of $u_{3}$ in $G$ different from $u_{1}$ and $u_{2}$, where $2 \leq d_{u_{4}} \leq n-3$. First suppose that $d_{u_{4}}=2$. Denote by $u_{5}$ the neighbor of $u_{4}$ in $G$ different from $u_{3}$. By Claim $1, u_{3} u_{5} \in E(G)$. Since $d_{u_{3}}=3$, the neighbors of $u_{3}$ are $u_{1}, u_{2}, u_{4}$, which is a contradiction. Then $d_{u_{4}} \neq 2$. Next suppose that $3 \leq d_{u_{4}} \leq n-3$. Then $G_{4}=G-u_{1}-u_{2}-u_{3}$ is not a counterexample, and thus $R^{+}\left(G_{4}\right) \geq r(n-3)$. By Lemma 2.3, $r(n)-r(n-3) \leq r(11)-r(8)<\frac{1}{2}+\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{5}}$. Then

$$
\begin{aligned}
R^{+}(G)= & R^{+}\left(G_{4}\right)+\sum_{v \in N\left(u_{4}\right) \backslash\left\{u_{3}\right\}}\left(\frac{1}{\sqrt{d_{v}+d_{u_{4}}}}-\frac{1}{\sqrt{d_{v}+d_{u_{4}}-1}}\right) \\
& +\frac{1}{\sqrt{3+d_{u_{4}}}}+\frac{1}{2}+\frac{2}{\sqrt{5}} \\
\geq & r(n-3)+\left(d_{u_{4}}-1\right)\left(\frac{1}{\sqrt{2+d_{u_{4}}}}-\frac{1}{\sqrt{2+d_{u_{4}}-1}}\right) \\
& +\frac{1}{\sqrt{3+d_{u_{4}}}}+\frac{1}{2}+\frac{2}{\sqrt{5}} \\
= & r(n-3)+\frac{1}{\sqrt{3+d_{u_{4}}}}-\frac{1}{\sqrt{2+d_{u_{4}}}}+\frac{1}{2}+\frac{2}{\sqrt{5}} \\
& +\left(\frac{d_{u_{4}}}{\sqrt{2+d_{u_{4}}}}-\frac{d_{u_{4}}}{\sqrt{1+d_{u_{4}}}}\right) \\
> & r(n-3)+\frac{1}{\sqrt{3+d_{u_{4}}}}-\frac{1}{\sqrt{2+d_{u_{4}}}}+\frac{1}{2}+\frac{2}{\sqrt{5}} \\
\geq & r(n-3)+\frac{1}{\sqrt{3+3}}-\frac{1}{\sqrt{2+3}}+\frac{1}{2}+\frac{2}{\sqrt{5}} \\
= & r(n-3)+\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{5}}+\frac{1}{2} \\
> & r(n),
\end{aligned}
$$

which is a contradiction.
Now Claim 2 follows.
Let $v \in V(G)$ be a vertex of degree two with neighbors $v_{1}$ and $v_{2}$. By Claim 1, $v_{1}$ and $v_{2}$ are adjacent. By Claim 2, $d_{v_{1}}, d_{v_{2}} \geq 3$. By Lemma 2.5,

$$
\begin{aligned}
R^{+}(G) & \geq R^{+}(G-v)+f(n-1, n-1) \\
& \geq r(n-1)+\frac{1}{\sqrt{2(n-1)}}-\frac{1}{\sqrt{2(n-2)}}+\frac{2(n-2)}{\sqrt{n+1}}-\frac{2(n-3)}{\sqrt{n}} \\
& =r(n)
\end{aligned}
$$

On the sum-connectivity index
with equality if and only if $G=K_{2, n-2}^{*}$, which is a contradiction.
It is easily checked that $R^{+}\left(K_{2,8}\right)=\frac{16}{\sqrt{2+8}}=5.05964<5.05988=2 \sqrt{10+1}+$ $\frac{1}{\sqrt{20-2}}-\frac{6}{\sqrt{10+1}}$. Thus the condition $n \geq 11$ in Theorem 1 is necessary.

Theorem 3.2. Let $G$ be a triangle-free graph of order $n \geq 11$ with $\delta(G) \geq 2$. Then $R^{+}(G) \geq \frac{2(n-2)}{\sqrt{n}}$ with equality if and only if $G=K_{2, n-2}$.
Proof. Assume that $G$ is a counterexample with minimal number of vertices for which $R^{+}(G)$ is minimal. By Lemma 2.1, we have $\delta(G)=2$. Let $V_{2}$ be the set of vertices of degree two in $G$. Suppose that there exists a vertex $z \in V_{2}$ with $N(z) \cap V_{2}=\emptyset$. Let $N(z)=\left\{z_{1}, z_{2}\right\}$. Then $z_{i} \notin V_{2}$ for $i=1,2$. Note that $2 \leq \delta(G-z) \leq \frac{n-1}{2}$ as $G-z$ is triangle-free. By the assumption of $G$, we have $R^{+}(G) \geq \frac{2(n-1-2)}{\sqrt{n-1}}$. By Lemma 2.6, we have

$$
\begin{aligned}
R^{+}(G) & \geq R^{+}(G-z)+2\left(\frac{n-2}{\sqrt{n}}-\frac{n-2-1}{\sqrt{n-1}}\right) \\
& \geq \frac{2(n-2-1)}{\sqrt{n-1}}+2\left(\frac{n-2}{\sqrt{n}}-\frac{n-2-1}{\sqrt{n-1}}\right) \\
& =\frac{2(n-2)}{\sqrt{n}}=R^{+}\left(K_{2, n-2}\right)
\end{aligned}
$$

with equalities if and only if $G=K_{2, n-2}$, which is a contradiction to the choice of $G$. Thus $N(z) \cap V_{2} \neq \emptyset$ for any $z \in V_{2}$.

Choose a vertex $u \in V_{2}$ such that $\left|N(u) \cap V_{2}\right|$ is as small as possible. Let $N(u)=\left\{u_{1}, u_{2}\right\}$ with $u_{1} \in V_{2}$ and $d_{u_{2}} \geq 2$.
Claim 1. $N\left(u_{1}\right) \cap N\left(u_{2}\right) \backslash\{u\} \neq \emptyset$.
Suppose that the claim is false. Then $G_{1}=G-u+u_{1} u_{2}$ is not a counterexample, i.e., $R^{+}\left(G_{1}\right) \geq \frac{2(n-3)}{\sqrt{n-1}}$. It is easily seen that $\frac{2(n-3)}{\sqrt{n-1}}-\frac{2(n-2)}{\sqrt{n}}$ is increasing for $n \geq 11$, implying that $\frac{2(n-3)}{\sqrt{n-1}}-\frac{2(n-2)}{\sqrt{n}} \geq \frac{2(11-3)}{\sqrt{11-1}}-\frac{2(11-2)}{\sqrt{11}}>-\frac{1}{2}$. Thus

$$
\begin{aligned}
R^{+}(G) & =R^{+}\left(G_{1}\right)+\frac{1}{\sqrt{2+d_{u_{2}}}}+\frac{1}{2}-\frac{1}{\sqrt{2+d_{u_{2}}}} \\
& \geq \frac{2(n-3)}{\sqrt{n-1}}+\frac{1}{2} \\
& >\frac{2(n-2)}{\sqrt{n}}
\end{aligned}
$$

which is a contradiction. Claim 1 follows.
Let $v$ be the neighbor of $u_{1}, u_{2}$ different from $u$. For $u_{1} \in V_{2}$, by Claim 1, we have $N\left(u_{1}\right) \cap N\left(u_{2}\right)=\{u, v\}$. Since $G$ is a triangle-free graph, we have $d_{v}+d_{u_{2}} \leq n$. Claim 2. $v \in V_{2}$.

Suppose that the claim is false. Suppose that $u_{2} \notin V_{2}$. We have $3 \leq d_{v}, d_{u_{2}} \leq$ $n-3$ as $G$ is triangle-free. Since $G_{2}=G-u-u_{1}$ is not a counterexample, we
have $R^{+}\left(G_{2}\right) \geq \frac{2(n-4)}{\sqrt{n-2}}$. Let $g(x)=\frac{2}{\sqrt{x-2}}+\frac{2(x-3)}{\sqrt{x-1}}$ with $x \geq 11$. Then $g^{\prime \prime}(x)=$ $\frac{3}{2}(x-2)^{-5 / 2}-\left(\frac{1}{2} x+\frac{5}{2}\right)(x-1)^{-5 / 2}<0$, implying that $g(x)-g(x+1)$ is increasing for $x \geq 11$.

By Lemma 2.4, we have $f\left(d_{v}, d_{u_{2}}\right) \geq f(n-3, n-3)$, and thus

$$
\left.\begin{array}{rl}
R^{+}(G)= & R^{+}\left(G_{2}\right)+\frac{1}{2}+\frac{1}{\sqrt{2+d_{v}}}+\frac{1}{\sqrt{2+d_{u_{2}}}}+\frac{1}{\sqrt{d_{v}+d_{u_{2}}}} \\
& -\frac{1}{\sqrt{d_{v}+d_{u_{2}-2}}} \\
& +\sum_{w \in N(v) \backslash\left\{u_{1}, u_{2}\right\}}\left(\frac{1}{\sqrt{d_{w}+d_{v}}}-\frac{1}{\sqrt{d_{w}+d_{v}-1}}\right) \\
& +\sum_{w \in N\left(u_{2}\right) \backslash\{u, v\}}\left(\frac{1}{\sqrt{d_{w}+d_{u_{2}}}}-\frac{1}{\sqrt{d_{w}+d_{u_{2}-1}}}\right) \\
\geq & \frac{2(n-4)}{\sqrt{n-2}}+\frac{1}{2}+\frac{1}{\sqrt{2+d_{v}}}+\frac{1}{\sqrt{2+d_{u_{2}}}}+\frac{1}{\sqrt{d_{v}+d_{u_{2}}}} \\
& -\frac{1}{\sqrt{d_{v}+d_{u_{2}-2}}} \\
& +\left(d_{v}-2\right)\left(\frac{1}{\sqrt{2+d_{v}}}-\frac{1}{\sqrt{1+d_{v}}}\right) \\
= & \frac{2(n-4)}{\sqrt{n-2}}+\frac{1}{2}+f\left(d_{u_{2}}-2\right)\left(\frac{1}{\sqrt{2+d_{u_{2}}}}-\frac{1}{\left.\sqrt{1+d_{u_{2}}}\right)}\right) \\
\geq & \frac{2(n-4)}{\sqrt{n-2}+\frac{1}{2}+f(n-3, n-3)} \\
= & \frac{2(n-2)}{\sqrt{n}}+\frac{1}{2}+\left(\frac{2}{\sqrt{n-2}}-\frac{2(n-2)}{\sqrt{n}}+\frac{2(n-4)}{\sqrt{n-1}}\right) \\
& +\left(\frac{1}{\sqrt{2(n-3)}}-\frac{1}{\sqrt{2(n-4)}}\right) \\
& +\left(\frac{2(n-2)}{\sqrt{n}}+\frac{1}{2}+(g(n)-g(n+1))\right. \\
\sqrt{2(n-3)}-\frac{1}{\sqrt{2(n}}+\frac{1}{2}+(g(11)-g(11+1)) \\
& +(11-3) \\
\sqrt{2(n-4)}) \\
\sqrt{2 \cdot(11-4)}
\end{array}\right)
$$

$$
>\frac{2(n-2)}{\sqrt{n}}
$$

which is a contradiction.
Now suppose that $u_{2} \in V_{2}$. Then $3 \leq d_{v} \leq n-2$ and $G_{3}=G-u-u_{1}-u_{2}$ is not a counterexample, and thus $R^{+}\left(G_{3}\right) \geq \frac{2(n-5)}{\sqrt{n-3}}$. Let $h(x)=\frac{x-2}{\sqrt{x}}$ with $x \geq 2$. Then $h^{\prime \prime}(x)=-\frac{3}{2}\left(\frac{1}{6} x+1\right) x^{-5 / 2}<0$, implying that $h(x-3)-h(x)=\frac{x-5}{\sqrt{x-3}}-\frac{x-2}{\sqrt{x}}$ and $h(x-3)-h(x-2)=\frac{x-5}{\sqrt{x-3}}-\frac{x-4}{\sqrt{x-2}}$ are both increasing in $x$. Then

$$
\begin{aligned}
R^{+}(G)= & R^{+}\left(G_{3}\right)+1+\frac{2}{\sqrt{2+d_{v}}} \\
& +\sum_{w \in N(v) \backslash\left\{u_{1}, u_{2}\right\}}\left(\frac{1}{\sqrt{d_{w}+d_{v}}}-\frac{1}{\sqrt{d_{w}+d_{v}-2}}\right) \\
\geq & \frac{2(n-5)}{\sqrt{n-3}}+1+\frac{2}{\sqrt{2+d_{v}}}+\left(d_{v}-2\right)\left(\frac{1}{\sqrt{2+d_{v}}}-\frac{1}{\sqrt{d_{v}}}\right) \\
= & \frac{2(n-5)}{\sqrt{n-3}}+1+\frac{d_{v}}{\sqrt{2+d_{v}}}-\frac{d_{v}-2}{\sqrt{d_{v}}} \\
\geq & \frac{2(n-5)}{\sqrt{n-3}}+1+\frac{n-2}{\sqrt{(n-2)+2}}-\frac{(n-2)-2}{\sqrt{n-2}} \\
= & \frac{2(n-2)}{\sqrt{n}}+\left(\frac{n-5}{\sqrt{n-3}}-\frac{n-2}{\sqrt{n}}\right)+\left(\frac{n-5}{\sqrt{n-3}}-\frac{n-4}{\sqrt{n-2}}\right)+1 \\
\geq & \frac{2(n-2)}{\sqrt{n}}+\left(\frac{11-5}{\sqrt{11-3}}-\frac{11-2}{\sqrt{11}}\right)+\left(\frac{11-5}{\sqrt{11-3}}-\frac{11-4}{\sqrt{11-2}}\right)+1 \\
> & \frac{2(n-2)}{\sqrt{n}},
\end{aligned}
$$

which is a contradiction. Claim 2 follows.
Claim 3. $u_{2} \notin V_{2}$.
Suppose that the claim is false. Then $G_{4}=G-u-u_{1}-u_{2}-v$ is not a counterexample. It is easily seen that $\frac{2(n-6)}{\sqrt{n-4}}-\frac{2(n-2)}{\sqrt{n}} \geq \frac{2 \cdot(11-6)}{\sqrt{11-4}}-\frac{2 \cdot(11-2)}{\sqrt{11}}>-2$, and thus $R^{+}(G)=R^{+}\left(G_{4}\right)+2 \geq \frac{2(n-6)}{\sqrt{n-4}}+2>\frac{2(n-2)}{\sqrt{n}}$, which is a contradiction.

By Claims 2 and 3, we have $v \in V_{2}$ and $3 \leq d_{u_{2}} \leq n-2$ as $G$ is triangle-free. Now we will complete our proof by considering the following two cases.
Case 1. $d_{u_{2}} \geq 4$. Then $G-u-u_{1}-v$ is not a counterexample. Replacing $u_{2}$ by $v$ in the proof of the Claim 2 for the case $u_{2} \in V_{2}$, we may derive a contradiction.
Case 2. $d_{u_{2}}=3$. Let $N\left(u_{2}\right) \backslash\{u, v\}=\{x\}$ and $y \in N(x) \backslash\left\{u_{2}\right\}$. If $d_{x}=2$, then $N(y) \cap N\left(u_{2}\right) \backslash\{x\}=\emptyset$ as $d_{u}=d_{v}=2$. Thus we can derive a contradiction by the same argument as in the proof of Case 1 by setting $u_{2}=y$. Hence $d_{x} \geq 3$. Note that $G_{5}=G-u-u_{1}-u_{2}-v$ is not a counterexample. Then $R^{+}\left(G_{5}\right) \geq \frac{2(n-6)}{\sqrt{n-4}}$. Since $\frac{1}{\sqrt{3+d}}-\frac{1}{\sqrt{2+d}}$ is increasing for $3 \leq d \leq n-4$, noting the properties of $h(x)$
used above, we have

$$
\begin{aligned}
R^{+}(G)= & R^{+}\left(G_{5}\right)+1+\frac{2}{\sqrt{5}}+\frac{1}{\sqrt{3+d_{x}}} \\
& +\sum_{w \in N(x) \backslash\left\{u_{2}\right\}}\left(\frac{1}{\sqrt{d_{x}+d_{w}}}-\frac{1}{\sqrt{d_{x}+d_{w}-1}}\right) \\
\geq & \frac{2(n-6)}{\sqrt{n-4}}+1+\frac{2}{\sqrt{5}}+\frac{1}{\sqrt{3+d_{x}}} \\
& +\left(d_{x}-1\right)\left(\frac{1}{\sqrt{d_{x}+2}}-\frac{1}{\sqrt{d_{x}+2-1}}\right) \\
= & \frac{2(n-6)}{\sqrt{n-4}}+1+\frac{2}{\sqrt{5}}+\frac{1}{\sqrt{3+d_{x}}}+\frac{d_{x}-1}{\sqrt{d_{x}+2}}-\frac{d_{x}-1}{\sqrt{d_{x}+1}} \\
> & \frac{2(n-6)}{\sqrt{n-4}}+1+\frac{2}{\sqrt{5}}+\frac{1}{\sqrt{3+d_{x}}}-\frac{1}{\sqrt{d_{x}+2}} \\
\geq & \frac{2(n-6)}{\sqrt{n-4}}+1+\frac{2}{\sqrt{5}}+\frac{1}{\sqrt{3+3}}-\frac{1}{\sqrt{3+2}} \\
> & \frac{2(n-2)}{\sqrt{n}},
\end{aligned}
$$

which is a contradiction.
The proof of our theorem is completed.
It is easily checked that for the cycle $C_{10}$ (on 10 vertices), $R^{+}\left(C_{10}\right)=\frac{10}{2}<$ $\frac{2(10-2)}{\sqrt{10}}$. Thus the condition $n \geq 11$ in Theorem 2 is necessary.

## References

[1] N. Trinajstić, Chemical Graph Theory, revised edn., CRC Press, Boca Raton. 1992.
[2] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97 (1975), 6609-6615.
[3] L.B. Kier, L.H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.
[4] L.B. Kier, L.H. Hall, Molecular Connectivity in Structure-Activity Analysis, Research Studies Press/Wiley, Letchworth/New York, 1986.
[5] J. Devillers, A.T. Balaban (eds.), Topological Indices and Related Descriptors in $Q S A R$ and $Q S P R$, Gordon and Breach, Amsterdam, 1999.
[6] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.
[7] R. Todeschini, V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley-VCH, Weinheim, 2009.
[8] M.V. Diudea (ed.), QSPR/QSAR Studies by Molecular Descriptors, Nova, Huntington, 2001.
[9] X. Li, I. Gutman, Mathematical Aspects of Randić-Type Molecular Structure Descriptors, Univ. Kragujevac, Kragujevac, 2006.
[10] I. Gutman, B. Furtula (eds.), Recent Results in the Theory of Randic Index, Univ. Kragujevac, Kragujevac, 2008.
[11] L. Pogliani, From molecular connectivity indices to semiempirical connectivity terms: Recent trends in graph theoretical descriptors, Chem. Rev. 100 (2000), 3827-3858.
[12] M. Randić, The connectivity index 25 years later, J. Mol. Graph. Model. 20 (2001), 19-35.
[13] R. García-Domenech, J. Gálvez, J.V. de Julián-Ortiz, L. Pogliani, Some new trends in chemical graph theory, Chem. Rev. 108 (2008), 1127-1169.
[14] B. Zhou, N. Trinajstić, On a novel connectivity index, J. Math. Chem. 46 (2009), 1252-1270.
[15] B. Lučić, S. Nikolić, N. Trinajstić, B. Zhou, S. Ivaniš Turk, Sum-Connectivity index, in: I. Gutman, B. Furtula (eds.), Novel Molecular Structure Descriptors - Theory and Applications I, Univ. Kragujevac, Kragujevac, 2010, pp. 101-136.
[16] B. Lučić, N. Trinajstić, B. Zhou, Comparison between the sum-connectivity index and product-connectivity index for benzenoid hydrocarbons, Chem. Phys. Lett. 475 (2009), 146-148.
[17] Z. Du, B. Zhou, N. Trinajstić, Minimum sum-connectivity indices of trees and unicyclic graphs of a given matching number, J. Math. Chem. 47 (2010), 842855.
[18] R. Xing, B. Zhou, N. Trinajstić, Sum-connectivity index of molecular trees, J. Math. Chem. 48 (2010), 583-591.
[19] Z. Du, B. Zhou, On sum-connectivity index of bicyclic graphs, Bull. Malays. Math. Sci. Soc., in press.
[20] B. Bollobás, P. Erdös, Graphs of extremal weights, Ars Combin. 50 (1998), 225-233.
[21] C. Delorme, O. Favaron, D. Rautenbach, On the Randić index, Discrete Math. 257 (2002), 29-38.
[22] H. Liu, M. Lu, F. Tian, On the Randić index, J. Math. Chem. 38 (2005), 345-354.

Shilin Wang and Bo Zhou:
Department of Mathematics, South China Normal University, Guangzhou 510631,
China
E-mail: zhoubo@scnu.edu.cn
Nenad Trinajstić:
The Rudjer Bošković Institute, P. O. Box 180, HR-10002 Zagreb, Croatia
E-mail: trina@irb.hr


[^0]:    * Corresponding author

    2010 Mathematics Subject Classifications. 05C07, 05C35, 05C90, 92E10.
    Key words and Phrases. Sum-connectivity index, product-connectivity index, Randić connectivity index, triangle-free graph, minimum degree.

    Received: Required
    Communicated by Dragan Stevanović
    This work was supported by the National Natural Science Foundation of China (Grant No. 11071089) and the Ministry of Science, Education and Sports of Croatia (Grant No. 098-1770495-2919).

