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ON A VARIATION OF RANDIĆ INDEX

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On a variation of Randić index

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Abstract

Randić index, R, also known as the connectivity or branching index, is an important topological index in chemistry. In order to attack some conjectures concerning Randić index, Dvořák et al. [5] introduced a modification of this index, denoted by R'. In this paper we present some of the basic properties of R'. We determine graphs with minimal and maximal values of R', as well as graphs with minimal and maximal values of R' among the trees and unicyclic graphs. We also show that if G is a triangle-free graph on n vertices with minimum degree δ, then $R'(G) \geq \delta$. Moreover, equality holds only for the complete bipartite graph $K_{\delta,n-\delta}$.

1 Introduction

Molecular descriptors are invariants that are calculated from the topological information contained in the structure of the graph of a molecule [14]. Topological information of a molecule comprises the position and sometimes the type of the atoms defined in relation to the bonds that connect them. Such topological descriptors correlate with certain compound properties and activities. In studying branching properties of alkanes, several numbering schemes for the edges of the associated hydrogen-suppressed graph were proposed based on the degrees of the endvertices of an edge. In 1975 Randić [13] introduced the topological connectivity index $R(G)$ of a graph G defined as the sum of weights $(\deg_G(u)\deg_G(v))^{-\frac{1}{2}}$ over all edges uv of G, i.e.,

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

where $\deg_G(v)$ is the degree of the vertex v in G. Originally this index was named "branching index" or "molecular connectivity index" and it has been proved to be suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Nowadays

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this parameter is known as *Randić index*. Later, in 1998 Bollobás and Erdös [1] generalized this index by replacing $-\frac{1}{2}$ with any real number α to obtain the *general Randić index* R_α. Thus,

$$R_\alpha(G) = \sum_{uv \in E(G)} (\deg_G(u)\deg_G(v))^\alpha.$$

Randić has shown that there exists a correlation of the Randić index with several physico-chemical properties of alkanes such as boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapor pressure, Kovats constants, calculated surface areas and others [9, 13]. According to Caprossi and Hansen [2], Randić index together with its generalizations is certainly the molecular-graph-based structure-descriptor, that found many applications in organic chemistry, medicinal chemistry, and pharmacology, and therefore is an interesting topic in graph theory. For more results concerning Randić index see [11].

Recently Dvořák et al. [5] have shown that for every connected graph G we have $R(G) \geq \mathrm{rad}(G)/2$, where $\mathrm{rad}(G)$ is the radius of G. The main idea in their work was introducing a new index $R'(G)$ defined as:

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{\deg_G(u), \deg_G(v)\}}.$$

Although no application of the index R' in chemistry is known so far, still this index turns out to be very useful, especially from mathematical point of view, as it is much easier to follow during graph modifications than Randić index. Using this index, Cygan et al. [4] proved that for any connected graph G of maximum degree four which is not a path with even number of vertices, $R(G) \geq \mathrm{rad}(G)$. As a consequence, they resolve the conjecture $R(G) \geq \mathrm{rad}(G) - 1$ given by Fajtlowicz [6] in 1988 for the case when G is a chemical graph. They actually showed that for all connected chemical graphs G the inequality $R'(G) \geq \mathrm{rad}(G) - \frac{1}{2}$ holds.

Motivated by some already known results concerning Randić index, in this paper we present some basic properties of the newly introduced index R'. We show that for every graph G on n vertices, $R'(G)$ is at least 1 but no more than $\frac{n}{2}$, and these bounds are attained by stars and regular graphs, respectively. Then we determine graphs with minimal and maximal value of R' among all trees and unicyclic graphs. It turns out that the same trees and unicyclic graphs attain minimal (maximal) values of R' and Randić index. In the last part we prove that if G is a triangle-free graph on n vertices with minimum degree δ, then $R'(G) \geq \delta$. Equality holds only for complete bipartite graph $K_{\delta,n-\delta}$.

Now, we define terms and symbols used in the sequel. Let $G = (V(G), E(G))$ be a simple graph on $n = |V(G)|$ vertices and $m = |E(G)|$ edges. The degree of a vertex v in G is denoted by $\deg_G(v)$, and the set of neighbors of v in G is denoted by $N_G(v)$. By $\delta(G)$ and $\Delta(G)$ we denote the minimum and maximum degree in G, respectively. The set of vertices of degree a in G is denoted by $V_a(G)$. *A diameter* of connected graph G, $\mathrm{diam}(G)$, is the maximum distance between vertices of G, i.e., $\mathrm{diam}(G) = \max\{d_G(u,v) \,|\, u,v \in V(G)\}$.

Let v be a vertex of a graph G. The graph $G - v$ is obtained from G when v and all edges incident to v are removed. By $G^{\div}$ we denote a graph obtained from G by adding one edge joining two vertices of degree 1. If G is a tree then $G^{\div}$ is a unicyclic graph. Observe that $G^{\div}$ is not determined uniquely. A *subdivision* of an edge is a replacement of this edge by a path of positive length. Of course, all internal vertices of this new path have degrees 2. A graph H is a *subdivision* of G if H arises by subdivision of some of the edges of G.

A star with n vertices, S_n, is called an n*–star*. Similarly, a path P_n and a cycle C_n are called an n*–path* and an n*–cycle*, respectively, if they have n vertices.

2 Basic properties of R'

Here we present some basic properties of R'. From the definition of R', it is obvious that if G is not connected, then $R'(G)$ is the sum of the R' indices of its components. Therefore, in what follows we consider only connected graphs. We start with upper and lower bounds for R' in general graphs.

Proposition 2.1. *For every graph G on n vertices the inequality $R'(G) \le R(G) \le \frac{n}{2}$ holds. Moreover, $R'(G) = \frac{n}{2}$ if and only if G is a regular graph.*

Proof. From the definitions of R and R' it is obvious that $R(G) \ge R'(G)$. It is known that among all connected graphs of order n, regular graphs attain the maximum Randić index [3]. Since $R'(G) = R(G) = \frac{n}{2}$ if G is a regular graph, we obtain the result. □

To obtain a lower bound for R' we need the following lemma. Recall that all our graphs are connected.

Lemma 2.2. *Let G be a graph on at least 2 vertices. Further, let S be an independent set of vertices of G, such that for every $u, v \in V(G)$, where $v \in S$ and $uv \in E(G)$, we have $\deg_G(u) \le \deg_G(v)$. Denote by E_S those edges xy of G for which neither x nor y is in S. Then*

$$R'(G) = |S| + \sum_{uv \in E_S} \frac{1}{\max\{\deg_G(u), \deg_G(v)\}}.$$

Proof. Let $v \in S$. Denote by E_v the edges of G incident to v. Then $\{E_v : v \in S\} \cup \{E_S\}$ is a partition of $E(G)$. Since every edge of E_v contributes to $R'(G)$ precisely $1/\deg_G(v)$ and since there are $\deg_G(v)$ edges in E_v, we have

$$\begin{aligned} R'(G) &= \sum_{v \in S} \left(\sum_{uv \in E_v} \frac{1}{\max\{\deg_G(u), \deg_G(v)\}} \right) + \sum_{uv \in E_S} \frac{1}{\max\{\deg_G(u), \deg_G(v)\}} \\ &= |S| + \sum_{uv \in E_S} \frac{1}{\max\{\deg_G(u), \deg_G(v)\}}. \end{aligned}$$

□

Since the contribution of every edge to R' is positive, Lemma 2.2 can be used to bound R'.

Corollary 2.3. *Let G be a graph on at least 2 vertices. Further, let S be an independent set of vertices of G, such that for every $u, v \in V(G)$, where $v \in S$ and $uv \in E(G)$, we have $\deg_G(u) \le \deg_G(v)$. Then $R'(G) \ge |S|$.*

We can now obtain the following consequence of Corollary 2.3 and Lemma 2.2.

Corollary 2.4. *For every graph G on at least 2 vertices we have $R'(G) \ge 1$. Moreover, $R'(G) = 1$ if and only if G is the star S_n.*

Proof. Let S consist of a single vertex v of maximum degree in G. Then $\deg_G(u) \leq \deg_G(v)$ for every $uv \in E(G)$, so that $R'(G) \geq 1$ for every graph G on at least 2 vertices by Corollary 2.3.

On the other hand, if $R'(G) = 1$ then all the edges of G must be incident to v, by Lemma 2.2. Hence, if $R'(G) = 1$ then G is a star. □

By using different methods, Bollobás and Erdös [1], and Pavlović and Gutman [12] independently showed that among all graphs of order n without isolated vertices, the star S_n attains the minimum Randić index as well, and $R(S_n) = \sqrt{n-1}$.

Lemma 2.2 gives an interesting bound for trees with small diameter.

Corollary 2.5. *Let T be a tree of order n, $n \geq 3$, and let v be an internal vertex of T with minimal degree. Denote $k = \deg_T(v)$ and denote by l the number of leaves adjacent to v. Then, $R'(G) \geq k - l + \frac{l}{k}$.*

Proof. Denote $T_0 = T - v$. Then T_0 is a disconnected graph and $k-l$ components of T_0 have at least one edge. Denote these components by $T_1, T_2, \ldots, T_{k-l}$. As v is the internal vertex with minimal degree, each T_i, $1 \leq i \leq k-l$, contains a vertex u_i such that $\deg_T(u_i) \geq \deg_T(x)$ for every vertex x such that $xu_i \in E(T)$. As $u_iu_j \notin E(T)$ for $1 \leq i < j \leq k-l$, the set $S = \{u_1, u_2, \ldots, u_{k-l}\}$ satisfies the assumptions of Lemma 2.2. Since the pendant edges incident with v contain none of $u_1, u_2, \ldots, u_{k-l}$, we have $R'(T) \geq (k-l) + \frac{l}{k}$ by Lemma 2.2. □

Observe that all trees in Table 1 attain the bound of Corollary 2.5. Next lemma shows that removing a vertex of degree 1 decreases the value of R'.

Lemma 2.6. *Let G_1 be a graph on at least 3 vertices and let $v \in V(G_1)$ such that $\deg_{G_1}(v) = 1$. Denote $G_2 = G_1 - v$. Let u be the unique neighbor of v. Denote $a = \deg_{G_1}(u)$ and denote by l the number of neighbors of u whose degree is at least a. Then*

$$R'(G_1) - R'(G_2) = \frac{l}{a(a-1)}.$$

Proof. When v is removed, the degree of u decreases by 1 while the vertices of $V(G_1) \setminus \{u, v\}$ have the same degree in G_2 as in G_1. Hence, only edges incident with u affect the difference $R'(G_1) - R'(G_2)$. Let $x_1, x_2, \ldots, x_l$ be neighbors of u such that $\deg_{G_1}(x_i) \geq \deg_{G_1}(u)$ for $i = 1, 2, \ldots, l$. Then

$$\begin{aligned}
R'(G_1) - R'(G_2) =& \frac{a-l}{a} + \left(\frac{1}{\deg_{G_1}(x_1)} + \frac{1}{\deg_{G_1}(x_2)} + \cdots + \frac{1}{\deg_{G_1}(x_l)}\right) \\
& - \left(\frac{a-l-1}{a-1} + \left(\frac{1}{\deg_{G_2}(x_1)} + \frac{1}{\deg_{G_2}(x_2)} + \cdots + \frac{1}{\deg_{G_2}(x_l)}\right)\right) \\
=& \frac{a-l}{a} - \frac{a-l-1}{a-1} = \frac{l}{a(a-1)},
\end{aligned}$$

which completes the proof. □

Using the previous result we describe a situation when a leaf is removed from his position and it is attached to another leaf. Next lemma shows that in this case the value of R' is not decreasing.

Lemma 2.7. *Let a graph G_1 have at least four vertices, let v be a vertex of degree 1 in G_1 and let u be its neighbor. Denote $a = \deg_{G_1}(u)$ and denote by l the number of neighbors of u whose degree is at least a. Denote $G_2 = G_1 - v$. Let w be a vertex of degree 1 in G_2 and let G_3 be a graph obtained by attaching a pendant edge to w. Then*

$$R'(G_3) - R'(G_1) = \frac{1}{2} - \frac{l}{a(a-1)} \geq 0.$$

Proof. By Lemma 2.6, $R'(G_1) - R'(G_2) = \frac{l}{a(a-1)}$. Now we calculate $R'(G_3) - R'(G_2)$. Since G_2 has at least 3 vertices, there is a unique neighbor of w whose degree is at least 2 in G_3. Since the degree of w is 2 in G_3, by Lemma 2.6 we have $R'(G_3) - R'(G_2) = \frac{1}{2}$. Hence,

$$R'(G_3) - R'(G_1) = \Big(R'(G_3) - R'(G_2)\Big) - \Big(R'(G_1) - R'(G_2)\Big) = \frac{1}{2} - \frac{l}{a(a-1)} \geq \frac{1}{2} - \frac{1}{a} \geq 0,$$

as $a > l \geq 0$ and $a \geq 2$. □

3 Trees and unicyclic graphs

Here we determine trees and unicyclic graphs attaining the smallest (the greatest) values of R'. We start with their definition.

By $D_{k,n}$ we denote a double star on n vertices, i.e., a tree having one vertex of degree k, one vertex of degree $n-k$ and $n-2$ leaves. By $S_{k,n}$ we denote a tree of order n which is a subdivision of the star S_k. Hence, $S_{k,n}$ has one vertex of degree $k-1$, every other vertex has degree either 1 or 2. Observe that the graph of double star $D_{3,6}$ resembles the letter H. Therefore by $H_{k,n}$ we denote a subdivision of $D_{3,6}$ on n vertices in which the vertices of degree 3 are joined by a path of length k

By $B^S_{k,n}$ we denote a unicyclic graph obtained from a triangle by identifying centers of two stars, S_k and S_{n-k-1}, with two different vertices of the triangle. Observe that $B^S_{k,n}$ has one vertex of degree $k+1$, one vertex of degree $n-k$, one vertex of degree 2 and $n-3$ vertices of degree 1. Note that $B^S_{k,n} = B^S_{l,n}$ for $l = n-k-1$. Analogously, by B^P_n (and D^P_n) we denote a unicyclic graph on n vertices obtained from a triangle (a quadrangle) by identifying endvertices of two paths with two different vertices of the triangle (with two nonadjacent vertices of the quadrangle). Then both B^P_n and D^P_n have 2 vertices of degree 3, 2 vertices of degree 1 and $n-4$ vertices of degree 2. Finally, by Y^P_n we denote a unicyclic graph on n vertices obtained from a triangle by identifying endvertices of three distinct paths with three distinct vertices of the triangle. Then Y^P_n has 3 vertices of degree 3, 3 vertices of degree 1 and $n-6$ vertices of degree 2.

First we discuss trees on n vertices, $n \geq 2$, with smallest value of R'. By Corollary 2.4, the star S_n attains the minimal value of R' and $R'(S_n) = 1$. For the next smallest values of R' we use the following proposition.

Proposition 3.1. *Let T be a tree on at least 2 vertices. Then, $R'(T) \geq 2$ if and only if* $\operatorname{diam}(T) > 3$. *Moreover, if* $\operatorname{diam}(T) = 3$ *then* $R'(T) = 2 - \frac{1}{a}$, *where a is the smallest degree in T which is greater than 1.*

Proof. We distinguish three cases. Suppose first that $\operatorname{diam}(T) \leq 2$. Since T has at least 2 vertices, T is a star S_n and $R'(S_n) = 1$ by Corollary 2.4.

Suppose now that $\mathrm{diam}(T) = 3$. Then T has exactly 2 vertices, say u and v, whose degree is greater than 1, and moreover, these two vertices are adjacent. All the other vertices have degree 1. Hence, T is a double star. Assume that $\deg_T(u) \geq \deg_T(v)$. Then

$$R'(T) = \sum_{ux \in E(T)} \frac{1}{\deg_T(u)} + \sum_{vy \in E(T) \setminus \{vu\}} \frac{1}{\deg_T(v)} = 2 - \frac{1}{\deg_T(v)}.$$

Finally, suppose that $\mathrm{diam}(T) \geq 4$. Then there are vertices x and y such that $d_G(x, y) = 4$. Therefore, there is a path $P : xv_1v_2v_3y$ of length 4 in T. Applying Lemma 2.6, we can remove vertices from T, one by one, until we obtain the path P. By Lemma 2.6, $R'(T) \geq R'(P)$. Since for $S = \{v_1, v_3\}$ we get $R'(P) = 2$ by Lemma 2.2, we have $R'(T) \geq 2$. □

By Proposition 3.1, if T is not a star and $R'(T) < 2$, then $\mathrm{diam}(T) = 3$. Hence, the trees with smallest values of R' and the corresponding values of R' are given in Table 1, where $k = \lfloor n/2 \rfloor$. We remark that the next value of $R'(T)$ is 2 but there are more types of trees attaining this value.

G	S_n	$S_{n-1,n}$	$D_{3,n}$	$D_{4,n}$	$D_{5,n}$	$\ldots$	$D_{k,n}$
$R'(G)$	1	3/2	5/3	7/4	9/5	$\ldots$	$(2k-1)/k$

Table 1. Trees with smallest values of R'.

For unicyclic graphs we use the following proposition.

Proposition 3.2. *Let C be the unique cycle in a unicyclic graph G. If the length of C is at least 4, or if G has a vertex at distance at least 2 to C, or if the length of C is 3 and all the vertices of C have degrees at least 3 in G, then $R'(G) \geq 2$. On the other hand, $R'(S_n^{\div}) = \frac{3}{2}$ and $R'(B_{k,n}^S) = \frac{2k+1}{k+1}$, where $2 \leq k \leq n-k-1$.*

Proof. Denote $G_0 = G$. Remove a vertex of degree 1 from G_0 and denote the resulting graph by G_1. Repeat removing of vertices of degree 1 to obtain G_2, G_3, ... until we get a graph $G_r = C$. By Lemma 2.6, we have $R'(G_0) \geq R'(G_1) \geq \cdots \geq R'(G_r)$. By Proposition 2.1, if C has length c then $R'(G_r) = R'(C) = \frac{c}{2}$. Hence, if $c \geq 4$ then $R'(G_r) \geq 2$ and consequently $R'(G) \geq 2$. In what follows suppose that C has length 3. Then $R'(G_r) = R'(C) = \frac{3}{2}$.

If $G = S_n^{\div}$ then all vertices of degree 1 are adjacent to one vertex, say u, of C. Since there is a unique edge which is not incident with u in G and both endvertices of this edge have degrees 2, we have $R'(S_n^{\div}) = \frac{3}{2}$ by Lemma 2.2.

If there is a vertex at distance at least 2 from C, then there is G_t, $0 \leq t < r$, such that to obtain G_{t+1} we remove a vertex adjacent to a vertex of degree 2. Then $R'(G_t) - R'(G_{t+1}) = \frac{1}{2}$, by Lemma 2.6, and hence $R'(G) \geq 2$. Thus, in the following we may assume that all the vertices of $V(G) - V(C)$ have degree 1 and are adjacent to a vertex of C.

Suppose that there are exactly two vertices of C, say u and v, whose degrees are greater than 2. Assume that $\deg_G(u) \geq \deg_G(v)$. Then all the edges of G are incident to u or v, so that

$$R'(G) = \sum_{ux \in E(T)} \frac{1}{\deg_T(u)} + \sum_{vy \in E(T) \setminus \{vu\}} \frac{1}{\deg_T(v)} = 2 - \frac{1}{\deg_T(v)},$$

i.e., $R'(B_{k,n}^S) = \frac{2k+1}{k+1}$ with $2 \leq k \leq n-k-1$. Observe that in any case $R'(G) \geq 2 - \frac{1}{3}$.

Finally, suppose that all the vertices of C have degree at least 3 in G. Then there is G_{t+1} such that $G_{t+1} = B^S_{k,n}$ for some k. By Lemma 2.6 we have $R'(G_t) - R'(G_{t+1}) = \frac{1}{3}$. As $R'(G_{t+1}) \geq 2 - \frac{1}{3}$, we have $R'(G) \geq 2$. □

By Proposition 3.2, in Table 2 we have unicyclic graphs with greatest values of R' and the corresponding values of R'. In the last column $k = \lfloor (n-1)/2 \rfloor$. We remark that the next value of R' in a unicyclic graph is 2, but as it can be seen from the proof of Proposition 3.2, there are more types of unicyclic graphs G for which $R'(G) = 2$.

Gao and Lu [8] show that among all unicyclic graphs, $S_n^{\div}$ also attains minimum for Randić index.

G	$S_n^{\div}$	$B^S_{2,n}$	$B^S_{3,n}$	$B^S_{4,n}$	$B^S_{5,n}$	$\dots$	$B^S_{k,n}$
$R'(G)$	3/2	5/3	7/4	9/5	11/6	$\dots$	$(2k+1)/(k+1)$

Table 2. Unicyclic graphs with smallest values of R'.

Now we turn our attention to trees with greatest values of R'. Caporossi et al. [3] prove that among all trees on n vertices, the path P_n attains the maximum value of Randić index. In the same paper they prove that $S_{4,n}$ attains the second maximum value of Randić index. Next proposition shows that the same holds for R' as well.

G	P_n	$S_{4,n}$	$H_{1,n}$	$H_{k,n}$, $S_{5,n}$
$R'(G)$	$(n-1)/2$	$(n-2)/2$	$(n-2)/2 - 1/3$	$(n-3)/2$

Table 3. Trees with greatest values of R'.

Proposition 3.3. *The trees listed in Table 3 attain the greatest values of R'. All the remaining trees on n vertices have R' smaller than $(n-3)/2$.*

Proof. Let $T = T_0$ be any tree on n vertices different from the trees present in Table 3, and let P^0 be a longest path in T_0. Take a leaf u_0 which is not on P^0, remove it from T_0, join it by an edge to an endvertex of P^0 and denote the resulting graph by T_1. Repeating this process we get a sequence of trees $T_0, T_1, \dots, T_r$, such that $T_r = P_n$. By Lemma 2.7, we have $R'(T_0) \leq R'(T_1) \leq \dots \leq R'(T_r)$. Moreover, by Lemma 2.7 again, if u_i is adjacent to a vertex of degree 2 in T_i, $0 \leq i < r$, then $R'(T_i) = R'(T_{i+1})$, otherwise $R'(T_i) < R'(T_{i+1})$. Since u_{r-1} is adjacent to a vertex of degree 3 in T_{r-1}, the path $P_n = T_r$ is the unique tree on n vertices achieving the maximum value of R'. As $\Delta(P_n) = 2$ and every edge of P_n is incident to a vertex of degree 2, we have $R'(P_n) = \frac{n-1}{2}$.

From the discussion above it is obvious that the tree with the second greatest value of R' is T_{r-1}. By Lemma 2.7 we have that if a leaf incident to a vertex of degree 2 is removed and joined to another leaf, then the value of the R' index is not changing. Hence, all trees with one vertex of degree 3, and all others of degree 2 and 1 attain the second greatest value of R'. Let s be the greatest value, $0 \leq s < r-1$, such that u_s is adjacent to a vertex of degree at least 3. Then $T_{s+1}, T_{s+2}, \dots, T_{r-1}$ all are subdivisions of S_4. Since $R'(S_{4,n}) = \frac{n-2}{2}$, we have $R'(T_{s+1}) = R'(T_{s+2}) = \dots = R'(T_{r-1}) = \frac{n-2}{2}$ and $R'(T_s) < R'(T_{s+1})$.

Now, we are going backwards in the sequence of trees $T_s, T_{s-1}, \dots, T_0$. Since $S_{4,n}$, a subdivision of the star S_4, attains the second greatest value of R', it is clear that the third greatest value will be attained for tree with two vertices, v_1 and v_2, of degree 3, or one vertex of degree 4 and all others of degree 2 and 1. So, candidates for graph attaining the third greatest value of R' are $H_{1,n}$, if v_1 and v_2 are adjacent, $H_{k,n}$ where $k \geq 2$, if v_1 and v_2 are nonadjacent, and $S_{5,n}$.

Let t be the greatest value, $0 \leq t < s$, such that u_t is adjacent to a vertex of degree at least 3. Denote by v_t the unique neighbor of u_t in T_t. As $R'(H_{1,n}) = \frac{n-2}{2} - \frac{1}{3}$ and $R'(H_{k,n}) = R'(S_{5,n}) = \frac{n-3}{2}$ if $k \geq 2$, to finish the proof it suffices to show that $R'(T_t) < \frac{n-3}{2}$. Since $R'(T_t) < R'(T_s)$, we can assume that $T_s = H_{1,n}$. If the degree of v_t is 4, then $R'(T_s) - R'(T_t) = R'(T_{t+1}) - R'(T_t) = \frac{1}{2}$, by Lemma 2.7, as no neighbor of v_t has degree at least 4 in T_t. Thus, $R'(T_t) = (\frac{n-2}{2} - \frac{1}{3}) - \frac{1}{2} < \frac{n-3}{2}$. On the other hand if the degree of v_t is 3, then $R'(T_s) - R'(T_t) \geq \frac{1}{2} - \frac{1}{6}$, by Lemma 2.7, as at most one neighbor of v_t has degree at least 3 in T_t. Thus, $R'(T_t) \leq (\frac{n-2}{2} - \frac{1}{3}) - \frac{1}{2} + \frac{1}{6} < \frac{n-3}{2}$. □

Finally, we consider unicyclic graphs with the greatest values of R'. Caparossi et al. [3] also considered the maximum values of Randić index in the class of unicyclic graphs. They show that among all unicyclic graphs of order n the cycle C_n attains the maximum value and $S^{\div}_{4,n}$ attains the second maximum value of Randić index. We show that the same holds for R'.

G	C_n	$S^{\div}_{4,n}$	$H^{\div}_{1,n}$, B^P_n	$H^{\div}_{k,n}$, $S^{\div}_{5,n}$, D^P_n, Y^P_n
$R'(G)$	$n/2$	$(n-1)/2$	$(n-1)/2 - 1/3$	$(n-2)/2$

Table 4. Unicyclic graphs with greatest values of R'.

Proposition 3.4. *The unicyclic graphs listed in Table 4 attain the greatest values of R'. All the remaining unicyclic graphs on n vertices have R' smaller than $(n-2)/2$.*

Proof. First observe that if $R'(G) = \ell$ then $R'(G^{\div}) = \ell + \frac{1}{2}$. Therefore $R'(C_n) = R'(P^{\div}_n) = \frac{n}{2}$, $R'(S^{\div}_{4,n}) = \frac{n-1}{2}$, $R'(H^{\div}_{1,n}) = \frac{n-1}{2} - \frac{1}{3}$ and $R'(H^{\div}_{k,n}) = R'(S^{\div}_{5,n}) = \frac{n-2}{2}$ if $k \geq 2$. As B^P_n has 5 edges incident to vertices of degree 3 while every other vertex is incident to a vertex of degree 2, we have $R'(B^P_n) = \frac{5}{3} + \frac{n-5}{2}$. Finally, as both D^P_n and Y^P_n have 6 edges incident to vertices of degree 3 while every other vertex is incident to a vertex of degree 2, we have $R'(D^P_n) = R'(Y^P_n) = \frac{6}{3} + \frac{n-6}{2}$.

Let G be a unicyclic graph with the unique cycle C. If the length of C is n then $G = C_n$. Hence, suppose that the length of C is smaller than n. Denote $G_0 = G$ and denote by P^0 a longest path in G_0. Then at least one vertex of P^0 has degree 1. Let u_0 be a vertex of degree 1 which is not on P^0. Remove u_0 from G_0, join it by an edge to an endvertex of P^0 which degree is 1 and denote the resulting graph by G_1. Repeating this process we get a sequence of unicyclic graphs $G_0, G_1, \dots, G_r$ with $R'(G_0) \leq R'(G_1) \leq \cdots \leq R'(G_r)$, by Lemma 2.7. Observe that G_r consists of the cycle C with a path, attached to C by an endvertex. Analogously as in the proof of Proposition 3.3 we get $R'(G_{r-1}) < R'(G_r)$. As $G_r = S^{\div}_{4,n}$, among unicyclic graphs with cycles of length strictly smaller than n, $S^{\div}_{4,n}$ has the greatest value of R'.

Now consider G_{r-1} and denote by v_{r-1} the unique vertex adjacent to u_{r-1}. If $\deg_{G_{r-1}}(v_{r-1})$ is 4, then $G_{r-1} = S^{\div}_{5,n}$. Now, suppose that $\deg_{G_{r-1}}(v_{r-1}) = 3$. Denote by w the other vertex of degree 3 in G_{r-1}. We distinguish six cases:

- $v_{r-1} \in V(C)$, $d_{G_{r-1}}(w, v_{r-1}) = 1$ *and* $C = C_3$: Then $G_{r-1} = B^P_n$.

- $v_{r-1} \in V(C)$, $d_{G_{r-1}}(w, v_{r-1}) = 1$ *and* $C \neq C_3$: Then $G_{r-1} = H^{\div}_{1,n}$.

- $v_{r-1} \in V(C)$, $d_{G_{r-1}}(w, v_{r-1}) = 2$ *and* $C = C_4$: Then $G_{r-1} = D^P_n$.

- $v_{r-1} \in V(C)$ *and either* $d_{G_{r-1}}(w, v_{r-1}) > 2$ *or* $d_{G_{r-1}}(w, v_{r-1}) = 2$ *and* $C \neq C_4$: Then $G_{r-1} = H^{\div}_{k,n}$ for $k \geq 2$.

- $v_{r-1} \notin V(C)$ *and* $d_{G_{r-1}}(w, v_{r-1}) = 1$: Then $G_{r-1} = H^{\div}_{1,n}$.

- $v_{r-1} \notin V(C)$ *and* $d_{G_{r-1}}(w, v_{r-1}) > 1$: Then $G_{r-1} = H^{\div}_{k,n}$ for $k \geq 2$.

Observe that in any case, G_{r-1} is a graph presented in Table 4.

Let t be the greatest value, $0 \leq t < r-1$, such that u_t is adjacent to a vertex, say v_t, of degree at least 3. Then $R'(G_{t+1}) = R'(G_{t+2}) = \cdots = R'(G_{r-1})$ and $R'(G_t) < R'(G_{t+1})$ by Lemma 2.7. To finish the proof we have to find all G_t with $R'(G_t) \geq \frac{n-2}{2}$ in the case when $G_{r-1} = H^{\div}_{1,n}$ or $G_{r-1} = B^P_n$, see Table 4. If $\deg_{G_t}(v_t) = 4$ then $R'(G_{r-1}) - R'(G_t) = R'(G_{t+1}) - R'(G_t) = \frac{1}{2}$ as there is no vertex in $G_t - v_t$ of degree at least 4. Hence, assume that $\deg_{G_t}(v_t) = 3$. Observe that $R'(G_{t+1}) = \frac{n-1}{2} - \frac{1}{3}$ and so $\frac{n-2}{2} - R'(G_{t+1}) = \frac{1}{6}$. Hence, if $R'(G_t) \geq \frac{n-2}{2}$, then $\frac{1}{2} - \frac{l}{a(a-1)} \leq \frac{1}{6}$ by Lemma 2.7, where $a = \deg_{G_t}(v_t)$ and l is the number of neighbors of v_t whose degree is at least 3. This gives $l = 2$ and $R'(G_{t+1}) - R'(G_t) = \frac{1}{6}$. Therefore $G_{t+1} = B^P_n$ and v_t is a vertex of $C = C_3$. Consequently, $G_t = Y^P_n$, which finishes the proof. $\square$

4 Triangle-free graphs

Favaron et al. [7], showed that for any triangle-free graph G with m edges, we have $R(G) \geq \sqrt{m}$. Later Li and Liu [10] proved the following: For any triangle-free graph G of order n and minimum degree $\delta(G) = k \geq 1$, we have $R(G) \geq \sqrt{k(n-k)}$. Equality holds if and only if $G = K_{k,n-k}$.

In this section we show that if a graph G on n vertices has maximum degree at most $n - \delta(G)$, then the lower bound for $R'(G)$ is $\delta(G)$. Consequently, this gives a bound for triangle-free graphs, and this bound is attained by $K_{k,n-k}$.

Theorem 4.1. *Let G be a simple graph on n vertices with $\delta(G) = k$, $k \geq 1$, $\Delta(G) \leq n - k$, $n > 2k$, and such that when satisfying all these conditions, $R'(G)$ is as small as possible. Then $R'(G) = k$ and $G = K_{k,n-k}$.*

In order to prove Theorem 4.1, we extend it to graphs with multiple edges. Hence, suppose that G is a graph on n vertices, possibly with multiple edges, with $\delta(G) = k$, $k \geq 1$, $\Delta(G) \leq n - k$, $n > 2k$, not necessarily connected, and such that when satisfying all these conditions, the parameter $R'(G)$ is as small as possible. In the following two lemmas we prove that G is a bipartite graph with bipartition $(V_{n-k}(G), V_k(G))$. Observe that since $R'(K_{k,n-k}) = k$, we already have $R'(G) \leq k$.

Lemma 4.2. *If $|V(G)| \leq |V_{n-k}(G)| + |V_k(G)| + 1$, then $|V(G)| = |V_{n-k}(G)| + |V_k(G)|$ and G is a bipartite graph with bipartition $(V_{n-k}(G), V_k(G))$.*

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Proof. First assume that $|V(G)| = |V_{n-k}(G)| + |V_k(G)| + 1$. Let v be the vertex such that $k < \deg_G(v) < n-k$. Then v has neighbors only in $V_k(G)$ and $V_{n-k}(G)$. Denote $l = \deg_G(v)$ and $\alpha = |N_G(v) \cap V_k(G)|$. Then $|N_G(v) \cap V_{n-k}(G)| = l - \alpha$. Further, denote $a = |V_k(G)|$ and $b = |V_{n-k}(G)|$. Finally, assume that there are s and t edges whose both endvertices are in $V_{n-k}(G)$ and $V_k(G)$, respectively. Counting the number of edges in two ways, namely through their endvertices of "higher", respectively "smaller" degree gives

$$|E(G)| = b(n-k) - s + \alpha + t = ak - t + (l - \alpha) + s.$$

Since $a + b = n - 1$, after dividing by n we obtain

$$b = k - \frac{2\alpha}{n} + \frac{l-k}{n} + \frac{2s}{n} - \frac{2t}{n}.$$

Now we evaluate $R'(G)$. There are $b(n-k) - s$ edges with an endvertex in $V_{n-k}(G)$, α edges connecting v with a vertex of $V_k(G)$ and t edges connecting two vertices of $V_k(G)$. Hence,

$$R'(G) = \frac{b(n-k) - s}{n-k} + \frac{\alpha}{l} + \frac{t}{k},$$

and after substituting for b the previous expression we obtain

$$R'(G) = k + \alpha\frac{n-2l}{nl} + \frac{l-k}{n} + s\frac{n-2k}{n(n-k)} + t\frac{n-2k}{nk}.$$

Since $n - 2k > 0$, we have $s\frac{n-2k}{n(n-k)} + t\frac{n-2k}{nk} \geq 0$, and as $l > k$, we have $\frac{l-k}{n} > 0$. Consider two cases.

- $n \geq 2l$: Then $\alpha\frac{n-2l}{nl} \geq 0$, so that $R'(G) \geq k + \frac{l-k}{n} > k$.
- $n < 2l$: Since $\alpha \leq l$, we have $\alpha\frac{n-2l}{nl} \geq l\frac{n-2l}{nl}$. As $l < n-k$, we have $R'(G) \geq k + \frac{n-2l}{n} + \frac{l-k}{n} = k + \frac{n-k-l}{n} > k$.

In both cases we have a contradiction as $R'(G) \leq k$.

Now consider the case $|V(G)| = |V_{n-k}(G)| + |V_k(G)|$. Using the notation as above we get

$$|E(G)| = b(n-k) - s + t = ak - t + s.$$

Since $a + b = n$, after dividing by n we obtain

$$b = k + \frac{2s}{n} - \frac{2t}{n}.$$

For $R'(G)$ we get

$$R'(G) = \frac{b(n-k) - s}{n-k} + \frac{t}{k},$$

and after substituting for b the previous expression we obtain

$$R'(G) = k + s\frac{n-2k}{n(n-k)} + t\frac{n-2k}{nk}.$$

Obviously, $R'(G) \geq k$ with equality only if $s = t = 0$. Hence, G is a bipartite graph with bipartition $(V_{n-k}(G), V_k(G))$, as required. $\square$

We remark that, although G is bipartite if the assumptions of Lemma 4.2 are satisfied, G can possibly have multiple edges and does not need to be connected. This assumption is important as in the proof of the next lemma we possibly create multiple edges and we may disconnect the graph.

Lemma 4.3. *We have* $|V(G)| = |V_{n-k}(G)| + |V_k(G)|$.

Proof. By Lemma 4.2, we cannot have $|V(G)| = |V_{n-k}(G)| + |V_k(G)| + 1$. Thus, by way of contradiction, suppose that there are $u, v \in V(G)$, such that $k < \deg_G(u) \le \deg_G(v) < n-k$. Moreover, assume that among the vertices of $V(G) \setminus (V_k(G) \cup V_{n-k}(G))$, the vertex u has the smallest degree and v has the greatest degree. Denote $A(u) = \{wu \in E(G); \deg_G(w) < \deg_G(u)\}$ and $A(v) = \{vz \in E(G); \deg_G(v) < \deg_G(z)\}$. Let $a = \min\{|A(u)|, |A(v)|\}$. Remove a edges $wu \in A(u)$ and replace them by a edges wv; remove a edges $vz \in A(v)$ and replace them by a edges uz; and denote the resulting graph by G_0. Then $\deg_G(x) = \deg_{G_0}(x)$ for every $x \in V(G)$. Since $\deg_G(u) \le \deg_G(v)$, we have $R'(G_0) \le R'(G)$.
Denote $A_0(u) = \{wu \in E(G_0); \deg_{G_0}(w) < \deg_{G_0}(u)\}$ and $A_0(v) = \{vz \in E(G_0); \deg_{G_0}(v) < \deg_{G_0}(z)\}$. Then either $A_0(u) = \emptyset$ or $A_0(v) = \emptyset$. Consider two cases:

- $A_0(u) \neq \emptyset$: Choose $wu \in A_0(u)$, remove this edge from G_0, replace it by wv and denote the resulting graph by G_1. Now $\deg_{G_1}(u) = \deg_{G_0}(u) - 1$ and $\deg_{G_1}(v) = \deg_{G_0}(v) + 1$. Since $A_0(u) \neq \emptyset$, we have $A_0(v) = \emptyset$, and as v has the maximum degree among the vertices of $V(G) \setminus (V_k(G) \cup V_{n-k}(G))$, edges incident with v in G_0 contribute by 1 to $R'(G_0)$, and analogously edges incident with v in G_1 contribute by 1 to $R'(G_1)$. Therefore, to count $R'(G_0) - R'(G_1)$ it suffices to consider the edges incident with u. Denote $l = |A_0(u)|$ and $d = \deg_{G_0}(u)$. As u has the minimum degree among the vertices of $V(G) \setminus (V_k(G) \cup V_{n-k}(G))$, we have $R'(G_1) = R'(G_0) - \frac{l}{d} + \frac{l-1}{d-1}$. Since $-\frac{l}{d} + \frac{l-1}{d-1} = \frac{l-d}{d(d-1)} \le 0$, we have $R'(G_1) \le R'(G_0)$ with equality only if $d = l$.

- $A_0(u) = \emptyset$: Choose $uw \in E(G_0)$, such that $uw \neq uv$, remove this edge from G_0, replace it by vw and denote the resulting graph by G_1. Analogously as in the previous case, $\deg_{G_1}(u) = \deg_{G_0}(u) - 1$ and $\deg_{G_1}(v) = \deg_{G_0}(v) + 1$. As $A_0(u) = \emptyset$ and u has the minimum degree among the vertices of $V(G) \setminus (V_k(G) \cup V_{n-k}(G))$, the edges incident with u contribute to R' by the same value in G_0 as in G_1, with the possible exception of the edge uw, which is now replaced by vw, and its contribution to $R'(G_1)$ is not greater as its contribution to $R'(G_0)$. Denote $l = |\{vz \in E(G_0); \deg_{G_0}(z) \le \deg_{G_0}(v)\}|$ and $d = \deg_{G_0}(v)$. Then $R'(G_1) \le R'(G_0) - \frac{l}{d} + \frac{l}{d+1} \le R'(G_0)$ with equality only if $l = 0$ (and $\deg_{G_0}(w) > \deg_{G_0}(v)$).

Now define $A_1(u)$ and $A_1(v)$ analogously as $A_0(u)$ and $A_0(v)$. Observe that if $A_0(u) \neq \emptyset$ then $A_1(v) = \emptyset$ and if $A_0(u) = \emptyset$ then $A_1(u) = \emptyset$. Hence, repeat the process described in the previous cases to obtain $G_2, G_3, \ldots$ until we get a graph G_r such that either $\deg_{G_r}(u) = k$ or $\deg_{G_r}(v) = n-k$. In this way we decreased the number of vertices x which degree is in the open interval $(k, n-k)$.

Now repeat the process with other pair of vertices whose degree is in the interval $(k, n-k)$ and yet another and so on. At the end we have either a single vertex with degree in $(k, n-k)$, which contradicts Lemma 4.2, or exactly two such vertices. Thus, we can assume that G has exactly two vertices, say u and v, with $k < \deg(u) \le \deg(v) < n-k$. By Lemma 4.2, we have $u \in V_k(G_r)$ and $v \in V_{n-k}(G_r)$. If $R'(G_r) < R'(G)$, that finishes the proof of the lemma. So, we may assume that $R'(G) = R'(G_0) = \cdots = R'(G_r)$. Analogously as above, consider two cases:

- $A_0(u) \neq \emptyset$: Then $A_0(v) = \emptyset$ and $\deg_{G_0}(u) = d = l$, see the analogous case above, so that both u and v have neighbors only in $V_k(G_0)$. This means that also in G_r the vertex u has neighbors only in $V_k(G_r)$. Hence, $V_k(G_r)$ is not an independent set, which contradicts Lemma 4.2.

- $A_0(u) = \emptyset$: Then $l = 0$, see the analogous case above, so that $uv \notin E(G_0)$ and both u and v have neighbors only in $V_{n-k}(G_0)$. This means that in G_r the vertex v has neighbors only in $V_{n-k}(G_r)$. Hence, $V_{n-k}(G_r)$ is not an independent set, which contradicts Lemma 4.2. □

Observe that in the final contradiction of the previous proof we use the fact that Lemma 4.2 is stated for graphs which may be disconnected and which may have multiple edges.

Proof of Theorem 4.1. By Lemmas 4.2 and 4.3, G is a bipartite graph with bipartition $(V_{n-k}(G), V_k(G))$, possibly with multiple edges.

Denote $a = |V_k(G)|$ and $b = |V_{n-k}(G)|$. Then $|E(G)| = ak = b(n-k)$, so that $(a+b)k = bn$. As $a + b = n$, we get $b = k$ and consequently $a = n - k$. Hence, $R'(G) = \frac{b(n-k)}{n-k} = b = k$. Since there is a unique simple graph satisfying $|V_k(G)| = n - k$ and $|V_{n-k}(G)| = k$, namely $K_{k,n-k}$, the theorem is proved. □

Corollary 4.4. *Let G be a triangle-free graph on n vertices with $\delta(G) = k$, $k \geq 1$. Then $R'(G) \geq k$ with equality if and only if $G = K_{k,n-k}$.*

Proof. Suppose that there is a vertex v in G such that $\deg_G(v) > n - k$. Let u be a neighbor of v. Since G is triangle-free, $N_G(u) \cap N_G(v) = \emptyset$, so that $N_G(u) \subseteq V(G) \setminus N_G(v)$. Hence, $\deg_G(u) < k$, a contradiction. Thus, $\Delta(G) \leq n - k$. As $\delta(G) \leq \Delta(G)$, we have $k \leq n - k$, so that $n \geq 2k$. Now, consider two cases:

- $n > 2k$: By Theorem 4.1 we have $R'(G) \geq k$ with equality if and only if $G = K_{k,n-k}$.

- $n = 2k$: As $n-k = k$, G is a regular graph. Since $|E(G)| = \frac{kn}{2}$, we have $R'(G) = \frac{kn}{2k} = k$. Choose two vertices, say u and v, such that $uv \in E(G)$. Since both $N_G(u)$ and $N_G(v)$ are disjoint independent sets of k vertices each, we have $G = K_{k,k}$. □

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