Filomat 28:9 (2014), 1849–1853
DOI 10.2298/FIL1409849L

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

On the Variation of the Randić Index with Given Girth and Leaves

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Abstract. The variation of Randić index $R'(G)$ of a graph G is defined by $R'(G) = \sum_{uv} \frac{1}{\max\{d_u, d_v\}}$, where d_u is the degree of a vertex u in G and the summation extends over all edges uv of G. In this work, we characterize the extremal trees achieving the minimum value of R' for trees with given number of vertices and leaves. Furthermore, we characterize the extremal graphs achieving the minimum value of R' for connected graphs with given number of vertices and girth.

1. Introduction

The *Randić index* $R = R(G)$ of a graph G is defined as follows:

$$R = R(G) = \sum_{uv \in E(G)} \left(d_u \cdot d_v\right)^{-\frac{1}{2}}$$

where d_u denotes the degree of a vertex u and the summation runs over all edges uv of G. This topological index was first proposed by Randić [14] in 1975. Originally this index was named *branching index* or *molecular connectivity index* and it has been shown to be suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Nowadays this parameter is known as *Randić index*. Later, in 1998 Bollobás and Erdös [3] generalized this index by replacing $-\frac{1}{2}$ with any real number α to obtain the general Randić index R_α. Thus,

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

Chemists have shown that there exists a correlation between 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 [10, 11, 14]. According to Caporossi and Hansen [5], Randić index together with its

2010 *Mathematics Subject Classification*. Primary 05C05; Secondary 05C35, 92E10, 95C38.
Keywords. variation of Randić index; leaf; girth.
Received: 14 September 2012; Accepted: 17 August 2014
Communicated by Francesco Belardo
Research supported by the national natural Science foundation of China (No.11101097), the Training Program for Outstanding Young Teachers in University of Guangdong Province of 2014, and Foundation for Distinguished Young Talents in Higher Education of Guangdong, China (No.2013LYM0027).
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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. In fact, it is one of the most popular molecular descriptors to which three books [10–12] are devoted.

There are many open conjectures concerning the Randić index, see the survey of Li and Shi [13] for examples, some of which had been proved only for some special cases, e.g., trees, unicyclic graphs and bicyclic graphs etc. They do not seem to be easy to be resolved for general graphs [6]. Therefore, Dvořák et al. [8] introduced a modification of this index, denoted by R', in order to resolve some conjectures concerning Randić index,

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

It is easy to see that $R(G) \geq R'(G)$ for any graph G, and the equality holds if and only if every connected component of G is regular and nontrivial.

Though no application of the index R' in chemistry and pharmacology 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 the Randić index. Using this index, Dvořák et al. [8] have shown that for any connected graph G, $R'(G) \geq D(G)/2$, where $D(G)$ is the diameter of G. Thus, they have asymptotically resolved the second claim of the conjecture of Aouchiche et al. [1]: for any connected graph on $n \geq 3$ vertices, $R(G) - D(G) \geq \sqrt{2} - \frac{n+1}{2}$ and $\frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}$, with equalities if and only if G is a path. Using again this index, Cygan et al. [7] have shown that for any connected graph G of maximum degree four which is not a path with even number of vertices, $R(G) \geq r(G)$. As a consequence, they resolve the conjecture $R(G) \geq r(G) - 1$ given by Fajtlowicz [9] in 1988 for the case when G is a chemical graph. For reasons mentioned above, it is meaningful to study the index R'. As a matter of fact, Andova et al. [2] determined 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.

In this work we present some basic properties of the index R' with respect to edge deletions. We characterize the extremal trees achieving the minimum value of R' with given number of leaves for trees of n vertices. Furthermore, we characterize the extremal graphs achieving the minimum value of R' for connected graphs with n vertices and girth g.

All the graphs considered in this paper are simple undirected ones. For a graph G, a *leaf* is a vertex with degree one in G. The *girth* of G is the minimum length of its cycles. If the graph does not contain any cycles (i.e. it's an acyclic graph), its girth is defined to be infinity. A graph is called *cyclic* if it is not acyclic. The *neighborhood* of a vertex u is denoted by $N(u)$. For undefined terminology and notations we refer the reader to [4].

2. Basic Properties of R'

In this section, we present some basic properties of the index R' with respect to edge deletions. For an edge uv of a graph G, we denote by ℓ^u_{uv} the number of vertices in $N(u)\backslash\{v\}$ with degree less than d_u.

We say u is a *strictly local maximum vertex* (*local maximum vertex*) if $d_u > d_w$ ($d_u \geq d_w$) for any $w \in N(u)$. Similarly, we say v is a *local minimum vertex* if $d_v \leq d_w$ for any $w \in N(v)$. Note that for a local minimum vertex v, we have $\ell^v_{vw} = 0$ for every vertex $w \in N(v)$.

Lemma 2.1. *Let uv be an edge of a graph G such that v is a local minimum vertex. Then*

$$R'(G) - R'(G - uv) = \frac{d_u - \ell^u_{uv} - 1}{d_u(d_u - 1)} \geq 0,$$

where the equality holds if and only if $\ell^u_{uv} = d_u - 1$.

Proof. Since v is a local minimum vertex, we have $\ell_{uv}^{v} = 0$. By definition, we have

$$R'(G) - R'(G - uv) = \frac{1}{d_u} + \frac{\ell_{uv}^{u}}{d_u} - \frac{\ell_{uv}^{u}}{d_u - 1} = \frac{d_u - \ell_{uv}^{u} - 1}{d_u(d_u - 1)}.$$

Since $d_u \geq \ell_{uv}^{u} + 1$, the result follows immediately.

From Lemma 2.1, we can see that deleting edges incident to a local minimum vertex might not increase the value of R'. The latter fact was observed by Dvořák et al. in [8].

3. Trees with a Given Number of Leaves

In this section, we characterize trees achieving the minimum value of R' with n vertices and ℓ leaves. First, we define a class of trees, namely $\mathcal{T}_n^{\ell}$, which is the class of extremal trees of our problem.

Definition. For $n \geq 3$, define $\mathcal{T}_n^{2} = \{P_n\}, \mathcal{T}_n^{n-1} = \{S_n\}$. Then $\mathcal{T}_n^{\ell}$ can be defined inductively as follows: a tree of $\mathcal{T}_n^{\ell}$ can be formed either by adding a new vertex with an edge connecting to a leaf of a tree in $\mathcal{T}_{n-1}^{\ell}$ or by adding a new vertex with an edge connecting to a local maximum vertex of a tree in $\mathcal{T}_{n-1}^{\ell-1}$.

For example, an $n-$vertex comet formed by connecting $\ell - 1$ isolated vertices to the same leaf of path $P_{n+1-\ell}$, is a tree in $\mathcal{T}_n^{\ell}$.

Theorem 3.1. *For a tree T of n ($n \geq 3$) vertices and ℓ leaves,*

$$R'(T) \geq \frac{n - \ell + 1}{2},$$

with equality if and only if $T \in \mathcal{T}_n^{\ell}$.

Proof. We apply the induction on n. For $n \leq 4$, it is easy to verify that the result is true. Thus, we assume $n \geq 5$ and the result is true for smaller n in the following.

Let v be a leaf of T and $uv \in E(T)$. Note that a leaf is always a local minimum vertex. We divide the proof into two cases: i.e., **Case** 1. $d_u = 2$; **Case** 2. $d_u \geq 3$.

Case 1. $d_u = 2$.

Let $T' = T - v$, then T' is a tree of $n - 1$ vertices and ℓ leaves. By induction,

$$R'(T) = R'(T') + \frac{1}{2} \geq \frac{(n-1) - \ell + 1}{2} + \frac{1}{2} = \frac{n - \ell + 1}{2},$$

where the equality holds if and only if $R'(T') = \frac{n-\ell}{2}$, i.e., $T' \in \mathcal{T}_{n-1}^{\ell}$, which means that $T \in \mathcal{T}_n^{\ell}$.

Case 2. $d_u \geq 3$.

Let $T' = T - v$, then T' is a tree of $n - 1$ vertices and $\ell - 1$ leaves. By induction and Lemma 2.1, we have

$$\begin{aligned} R'(T) &= R'(T') + \frac{d_u - \ell_{uv}^{u} - 1}{d_u(d_u - 1)} \\ &\geq \frac{(n-1) - (\ell - 1) + 1}{2} + \frac{d_u - \ell_{uv}^{u} - 1}{d_u(d_u - 1)} \\ &\geq \frac{n - \ell + 1}{2}, \end{aligned}$$

where the equality holds if and only if $R'(T') = \frac{n-\ell+1}{2}$ and $\ell_{uv}^{u} = d_u - 1$, that is, $R'(T') = \frac{n-\ell+1}{2}$ and u is a local maximum vertex in T'. By induction, $T' \in \mathcal{T}_{n-1}^{\ell-1}$ and u is a local maximum vertex in T', that is, $T \in \mathcal{T}_n^{\ell}$.

From the theorem we can infer that the smaller the value of ℓ is, the larger the minimum value of R' becomes. Since $2 \leq \ell \leq n - 1$ and $\mathcal{T}_n^{2} = \{P_n\}$ and $\mathcal{T}_n^{n-1} = \{S_n\}$, we have:

Corollary 3.2. *For a tree T of n ($n \geq 3$) vertices,*

$$\frac{n-1}{2} \geq R'(T) \geq 1,$$

where the upper bound holds if and only if $T \cong P_n$ and the lower bound holds if and only if $T \cong S_n$.

Note that Corollary 3.2 have been proved by Andova et al.[2] by a different approach.

4. Graphs with a Given Girth

Recall that the *girth* of a graph is the length of a shortest cycle contained in the graph. If the graph is acyclic, its girth is defined to be infinity. In this section, we deal with the minimum value of R' for connected cyclic graphs with girth at least g. We define a class of graphs as follows.

Definition. If $g \neq 4$. Take a cycle C_g on g vertices, and let X be any maximum independent set in C_g. Introduce $n-g$ independent vertices to the graph, and for each of them connect it to an arbitrarily chosen vertex of X. If $g = 4$. Take a cycle C_4 on 4 vertices, and let X be any maximum independent set in C_4. Introduce $n-4$ independent vertices to the graph, and for each of them connect it to an arbitrarily chosen vertex of X or to both two vertices of X. The class $\mathcal{G}_n^g$ comprises all the graphs that can be constructed in this manner.

For example, the graph C_n^g formed by attaching each $n-g$ isolated vertices with an edge to a unique vertex of C_g belongs to $\mathcal{G}_n^g$. Note that only two kinds of graphs in $\mathcal{G}_n^g$ are 2-edge connected, i.e., cycles and complete bipartite graph $K_{2,n-2}$ for $n \geq 5$.

Theorem 4.1. *For an $n-$vertex connected cyclic graph G with girth at least g ($g \geq 3$), we have*

$$R'(G) \geq \frac{g}{2},$$

where the equality holds if and only if $G \in \mathcal{G}_n^g$.

Proof. We will prove this result using induction on $n+m$, where m is the number of edges of G.

It is easy to verify that the result is true for $n+m \leq 6$. Thus, we assume $n+m \geq 7$ and the result is true for smaller $n+m$ in the following.

We divide the proof into two cases according to the minimum degree $\delta(G)$ of G, i.e., **Case** 1. $\delta(G) = 1$; **Case** 2. $\delta(G) \geq 2$.

Case 1. $\delta(G) = 1$.

Let $uv \in E(G)$ and $d_v = 1$, then the girth of the graph $G - v$ is at least g. By Lemma 2.1 and induction we have

$$\begin{aligned} R'(G) &= R'(G-v) + \frac{d_u - \ell_{uv}^u - 1}{d_u(d_u-1)} \\ &\geq \frac{g}{2} + \frac{d_u - \ell_{uv}^u - 1}{d_u(d_u-1)} \\ &\geq \frac{g}{2}, \end{aligned}$$

where the equality holds if and only if $G - v \in \mathcal{G}_{n-1}^g$ and $\ell_{uv}^u = d_u - 1$, that is, $G \in \mathcal{G}_n^g$.

Case 2. $\delta(G) \geq 2$.

Subcase 2.1. If G is 2-edge connected.

If $G \cong C_n$, we have $R'(G) = \frac{n}{2} = \frac{g}{2}$ and the result follows. If $G \neq C_n$, then G contains some cycle even after removing any of its edges. Let uv be an edge incident with a local minimum vertex v of G. Then by Lemma 2.1 and by induction we have, $R'(G) \geq R'(G - uv) \geq \frac{g}{2}$. The two equalities hold if and only if $G - uv \in \mathcal{G}_n^g$ and $d_u > d_w$ for every $w \in N(u)\backslash\{v\}$. If $\delta(G - uv) = 1$. Denote by V_1 the vertex set of leaves in $G - uv$. We can see that $v \in V_1$. If $|V_1| \geq 3$, then $\delta(G) = 1$, which contradicts the assumption that G is $2-$edge connected. If $|V_1| = 2$, then $u \in V_1$ and $d_u = d_v = 2$ in G. We have $d_w \geq 2$ in G for the vertex $w \in N(u)\backslash\{v\}$. Thus, $\ell_{uv}^u = 0 \neq d_u - 1$. Therefore, $R'(G) > \frac{g}{2}$. If $|V_1| = 1$ and $G - uv \in \mathcal{G}_n^g$. If $g \neq 4$, then $G - uv$ arises from connecting an isolated vertex v to a vertex of C_g. And G arises from connecting an isolated vertex v to two vertices of C_g. Therefore, we have $d_u = 3$ and $\ell_{uv}^u = 1 < d_u - 1$ in G if $g = 3$. Thus $R'(G) > \frac{g}{2}$. And $g(G) < g(G - uv) = g$ if $g \geq 5$, which contradicts our assumption. If $g = 4$, then $G - uv$ arises from connecting an isolated vertex v to a vertex in partite set of two vertices in $K_{2,n-3}$ ($n \geq 5$). Then $G \cong K_{2,n-2} \in \mathcal{G}_n^g$ is the only graph meets the two equalities' conditions.

Subcase 2.2. If G is not 2-edge connected.
Let uv be an edge-cut of G and $d_u \geq d_v$. Let $G' = G - uv + uu' + vv'$, where u' and v' are new added vertices. Let G_1 be a component of G' containing u and G_2 the other component. If G_1 or G_2 was a tree, then G would need to contain a vertex of degree one, which contradicts the assumption that $\delta(G) \geq 2$. Hence both girths of G_1 and G_2 are at least g.

Thus, by induction we have

$$\begin{aligned} R'(G) &= R'(G') - \frac{1}{d_v} \\ &\geq R'(G_1) + R'(G_2) - \frac{1}{d_v} \\ &\geq g - \frac{1}{d_v} \\ &> \frac{g}{2}. \end{aligned}$$

Acknowledgements

The author is very grateful to the referees for their valuable comments and corrections.

References

[1] M. Aouchiche, P. Hansen, M. Zheng, Variable neighborhood search for extremal graphs. 19. Further conjectures and results about the Randić index, MATCH Commun. Math. Comput. Chem. 58 (2007) 83–102.
[2] V. Andova, M. Knor, P. Potoćnik, R. Škrekovski, On a variation of Randić index, Australisian Journal of Combinatorics 56(2013) 61–75.
[3] B. Bollobás, P. Erdös, Graphs of extremal weights, Ars Combin. 50 (1998) 225–233.
[4] J.A. Bondy, U.S.R. Murty, Graph Theory, Springer, Berlin, 2008.
[5] G. Caporossi, P. Hansen, Variable neighbourhood search for extremal graphs 6, Analyzing Bounds for the Connectivity Index, J. Chem. Inf. Comput. Sci. 43 (2003) 1–14.
[6] G. Caporossi, P. Hansen, Variable neighbourhood search for extremal graphs 1, The AutographiX system, Discrete Math. 212 (2000) 29–44.
[7] M. Cygan, M. Pilipczuk, R. Škrekovski, On the inequality between radius and Randić index for graphs, MATCH Commun. Math. Comput. Chem. 67(2) (2012) 451–466.
[8] Z. Dvořák, B. Lidický, R. Škrekovski, Randić index and the diameter of a graph, European J. Combin. 32 (2011) 434–442.
[9] S. Fajtlowicz, On conjectures of Graffiti, Discrete Math. 72 (1988) 113–118.
[10] L.B. Kier, L.H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.
[11] L.B. Kier, L.H. Hall, Molecular Connectivity in Structure-Activity Analysis, Research Studies Press-Wiley, Chichester(UK), 1986.
[12] X. Li, I. Gutman, Mathematical Aspects of Randić-Type Molecular Structure Descriptors, Mathematical Chemistry Monographs No.1, Kragujevac, 2006.
[13] X. Li, Y. Shi, A survey on the Randić index, MATCH Commun. Math. Comput. Chem. 59(1) (2008) 127–156.
[14] M. Randić, On characterization of molecular branching, J. Amer. Chem. Soc. 97 (1975) 6609–6615.
[15] W. Rudin, Real and Complex Analysis, (3rd edition), McGraw-Hill, New York, 1986.
[16] J. A. Goguen, L-fuzzy sets, Journal of Mathematical Analysis and Applications 18 (1967) 145–174.
[17] P. Erdös, S. Shelah, Separability properties of almost-disjoint families of sets, Israel Journal of Mathematics 12 (1972) 207–214.