On R' index of a graph*

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Abstract

Randić index R is an important topological index in chemistry. In order to attack some conjectures concerning Randić index, a modification R' of this index was introduced by Dvořák et al. [6]. The R' index of a graph G is defined as the sum of the weights $\frac{1}{\max\{d(u),d(v)\}}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. We first give a best possible lower bound of R' for a graph with minimum degree at least two and characterize the corresponding extremal graphs, and then we establish some relations between R' and the chromatic number, the girth of a graph.

AMS classification: 05C07, 05C15
Keywords: R' index, the minimum degree, the chromatic number, the girth.

1 Introduction

In chemical graph theory topological indices belong to the set of molecular descriptors that are calculated based on the molecular graph of a chemical compound. In 1975 Milan Randić [8] introduced the topological connectivity index $R(G)$ of a graph G defined as the sum of weights $\frac{1}{\sqrt{d(u)d(v)}}$ over all edges uv of G, i.e., $R(G) = \sum\limits_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$, where $d(v)$ is the degree of a vertex v. 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, surface areas and others. For the last two decades researchers are investigating extremal values and relations between topological indices. Very recently, Dvořák et al.

*Project supported by Hunan Provincial Natural Science Foundation of China (13JJ3053).
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[6] and Cygan et al. [4] have shown that for every graph $R(G) \geq D(G)/2$. This immediately implies that $R(G) \geq r(G)/2$, which is the closest result to the well-known Graffiti conjecture $R(G) \geq r(G) - 1$ of Fajtlowicz [7]. Asymptotically, it approaches the bound $\frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}$ conjectured by Aouchiche, Hansen and Zheng [2], where $D(G)$ and $r(G)$ are the diameter and the radius of G, respectively. Their main idea was introducing a modification R' of Randić index defined as:

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

It is easy to see that for every graph G we have $R(G) \geq R'(G)$. However, $R'(G)$ proves to be very useful as it is much easier to follow during graph modifications than $R(G)$. Also, we have $H(G) \geq R'(G)$, where $H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}$ is the harmonic index. Recently, Andova et al. [1] gave some of the basic properties of R' and 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. Motivated by some already known results concerning Randić index and the harmonic index, in this paper we will present some new results of the index R'.

2 The minimum value of R' with respect to the minimum degree

In the following, we will establish a best possible lower bound of R' for a graph with the minimum degree at least two and characterize the corresponding extremal graph. 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.

Let $K_{2,n-2}$ be the complete bipartite graph with partite sets X and Y, where $|X| = 2$ and $|Y| = n-2$. $K^*_{2,n-2}$ is the graph obtained from $K_{2,n-2}$ by adding an edge in X. $\mathbf{K}^*$ denotes the set of all graphs with the minimum degree $\delta = 2$ obtained from $K^*_{2,n-2}$ by adding i edges in Y, where no multiple edges are allowed and $0 \leq i \leq \frac{(n-3)(n-4)}{2}$.

Lemma 1. *Let $G = (V, E)$ be a graph of order n with the minimum degree $\delta(G) = 2$. $v_0 \in V$ is a vertex with degree $d(v_0) = 2$ and its neighbors is $N(v_0) = \{v_1, v_2\}$, $v_1v_2 \in E$. If $d(v_1) \geq d(v_2) \geq 3$, then $R'(G) - R'(G - v_0) \geq \frac{1}{(n-1)(n-2)}$ with equality if and only if $G \in \mathbf{K}^*$.*

Proof. Let m_1 be the number of vertices in $N(v_1) - \{v_0, v_2\}$ with degree less than $d(v_1)$, and m_2 be the number of vertices in $N(v_2)-\{v_0,v_1\}$ with degree less than $d(v_2)$. Then, $0\le m_1\le d(v_1)-2$, $0\le m_2\le d(v_2)-2$. And

$$\begin{aligned}
& R'(G)-R'(G-v_0)\\
= & \tfrac{1}{d(v_1)}+\tfrac{1}{d(v_2)}+(\tfrac{1}{d(v_1)}-\tfrac{1}{d(v_1)-1})\\
& +m_1(\tfrac{1}{d(v_1)}-\tfrac{1}{d(v_1)-1})+m_2(\tfrac{1}{d(v_2)}-\tfrac{1}{d(v_2)-1})\\
= & \tfrac{1}{d(v_1)}+\tfrac{1}{d(v_2)}-\tfrac{m_1+1}{d(v_1)(d(v_1)-1)}-\tfrac{m_2}{d(v_2)(d(v_2)-1)}\\
\geq & \tfrac{1}{d(v_1)}+\tfrac{1}{d(v_2)}-\tfrac{d(v_1)-1}{d(v_1)(d(v_1)-1)}-\tfrac{d(v_2)-2}{d(v_2)(d(v_2)-1)}\\
= & \tfrac{1}{d(v_2)(d(v_2)-1)}\geq\tfrac{1}{(n-1)(n-2)}.
\end{aligned}$$

with equality if and only if $d(v_1)=m_1+2\ge d(v_2)=m_2+2=n-1$, i.e., $G\in\mathbf{K}^*$. □

Lemma 2. *If $G\in\mathbf{K}^*$ and $v_0\in V(G)$ such that $d(v_0)=2$. Then $R'(G-v_0)\ge R'(K^*_{2,n-3})$ with equality if and only if $G=K^*_{2,n-2}$.*

Proof. Let $E'=E(G)-E(K^*_{2,n-2})$. Since $G\in\mathbf{K}^*$ and $d(v_0)=2$, $G-v_0$ is exactly the graph obtained from $K^*_{2,n-3}$ by adding all edges in E'. So, we have

$$\begin{aligned}
R'(G-v_0)= & R'(K^*_{2,n-3})+\sum_{uv\in E'}\tfrac{1}{max\{d(u),d(v)\}}\\
\geq & R'(K^*_{2,n-3})
\end{aligned}$$

with equality if and only if $E'=\emptyset$, i.e., $G=K^*_{2,n-2}$. □

For an edge $e=uv$ of a graph G, its weight is defined to be $\frac{1}{max\{d(u),d(v)\}}$. The index $R'(G)$ is the sum of weights over all edges of G.

Lemma 3. *There is an edge e with the maximal weight in G such that $R'(G-e)\le R'(G)$.*

Proof. If there is an edge uv with the maximal weight in G such that $d(u)<d(v)$, then $d(w)\ge d(v)$ for $w\in N(u)$. Let m be the number of vertices in $N(v)-\{u\}$ with degree less than $d(v)$, where $0\le m\le d(v)-1$.

$$\begin{aligned}
R'(G)-R'(G-uv)= & \tfrac{1}{d(v)}+m(\tfrac{1}{d(v)}-\tfrac{1}{d(v)-1})\\
= & \tfrac{d(v)-1-m}{d(v)(d(v)-1)}\geq 0.
\end{aligned}$$

Otherwise, $d(u)=d(v)$ for any edge uv with the maximal weight in G. Then $d(w)\ge d(u)$ for $w\in N(u)$ and $d(w)\ge d(v)$ for $w\in N(v)$. We have

$$R'(G)-R'(G-uv)=\frac{1}{d(v)}>0.$$

□

In the following, we will give the minimum value of R' and the corresponding extremal graph among all graphs with the minimum degree $\delta(G) \geq 2$.

Theorem 4. *Let G be a graph with $n \geq 3$ vertices and the minimum degree $\delta(G) \geq 2$. Then $R'(G) \geq 2 - \frac{1}{n-1}$ with equality if and only if $G = K^*_{2,n-2}$.*

Proof. It is easy to check that the assertion is true for $n = 3$. Suppose it holds for $3 \leq k < n$; we next show that it also holds for n.

Let G be a graph with $n \geq 4$ vertices. If $\delta(G) \geq 3$, then, by Lemma 3, there is an edge e with the maximal weight such that $R'(G-e) \leq R'(G)$ and $\delta(G) - 1 \leq \delta(G-e) \leq \delta(G)$. So, we only need to prove the result is true for G with $\delta(G) = 2$.

Case 1. Every pair of adjacent vertices of degree two has a common neighbor.

Let u_1 and u_2 be a pair of adjacent vertices with degree two in G which has a common neighbor u_3. Obviously, $2 \leq d(u_3) \leq n-1$.

Subcase 1.1. If $d(u_3) = 2$, let $G_1 = G - \{u_1, u_2, u_3\}$, then $R'(G_1) \geq 2 - \frac{1}{n-4}$ by the induction hypothesis, and $R'(G) = R'(G_1) + \frac{3}{2} \geq 2 - \frac{1}{n-4} + \frac{3}{2} > 2 - \frac{1}{n-1}$.

Subcase 1.2. If $d(u_3) \geq 4$, let $G_2 = G - \{u_1, u_2\}$, then $R'(G_2) \geq 2 - \frac{1}{n-3}$ by the induction hypothesis. Let r, t be the number of vertices in $N(u_3) - \{u_1, u_2\}$ with degree $d(u_3) - 1$ and at most $d(u_3) - 2$, respectively, where $r + t \leq d(u_3) - 2$.

$$\begin{aligned}
R'(G) = {} & R'(G_2) + \tfrac{1}{2} + \tfrac{2}{d(u_3)} \\
& + \sum_{v \in N(u_3) \setminus \{u_1,u_2\}} \left(\tfrac{1}{max\{d(u_3),d(v)\}} - \tfrac{1}{max\{d(u_3)-2,d(v)\}}\right) \\
\geq {} & R'(G_2) + \tfrac{1}{2} + \tfrac{2}{d(u_3)} + r\left(\tfrac{1}{d(u_3)} - \tfrac{1}{d(u_3)-1}\right) + t\left(\tfrac{1}{d(u_3)} - \tfrac{1}{d(u_3)-2}\right) \\
\geq {} & R'(G_2) + \tfrac{1}{2} + \tfrac{2}{d(u_3)} + (r+t)\left(\tfrac{1}{d(u_3)} - \tfrac{1}{d(u_3)-2}\right) \\
\geq {} & R'(G_2) + \tfrac{1}{2} + \tfrac{2}{d(u_3)} + (d(u_3)-2)\left(\tfrac{1}{d(u_3)} - \tfrac{1}{d(u_3)-2}\right) \\
= {} & R'(G_2) + \tfrac{1}{2} \geq 2 - \tfrac{1}{n-3} + \tfrac{1}{2} > 2 - \tfrac{1}{n-1}.
\end{aligned}$$

Subcase 1.3. If $d(u_3) = 3$, let u_4 be the neighbor of u_3 in G different from u_1 and u_2, where $2 \leq d(u_4) \leq n-3$.

(i) Suppose that $d(u_4) = 2$. Denote by u_5 the neighbor of u_4 in G different from u_3, where $2 \leq d(u_5) \leq n-4$. Let $G_3 = G - u_4 + u_3u_5$, then $R'(G_3) \geq 2 - \frac{1}{n-2}$ by the induction hypothesis. Note that $d(u_5) \geq 2$ and $\frac{1}{max\{d(u_5),2\}} - \frac{1}{max\{d(u_5),3\}} \geq 0$.

$$\begin{aligned}
R'(G) = {} & R'(G_3) + \tfrac{1}{3} + \tfrac{1}{max\{d(u_5),2\}} - \tfrac{1}{max\{d(u_5),3\}} \\
\geq {} & R'(G_3) + \tfrac{1}{3} \\
\geq {} & 2 - \tfrac{1}{n-2} + \tfrac{1}{3} > 2 - \tfrac{1}{n-1}.
\end{aligned}$$

(ii) Suppose that $3 \leq d(u_4) \leq n-4$. Let $G_4 = G - u_1 - u_2 - u_3$, then $R'(G_4) \geq 2 - \frac{1}{n-4}$ by the induction hypothesis.

$$\begin{aligned}
R'(G) = \; & R'(G_4) + \tfrac{1}{2} + \tfrac{2}{3} + \tfrac{1}{d(u_4)} \\
& + \sum_{v \in N(u_4)\setminus\{u_3\}} \left(\tfrac{1}{max\{d(u_4),d(v)\}} - \tfrac{1}{max\{d(u_4)-1,d(v)\}}\right) \\
\geq \; & R'(G_4) + \tfrac{7}{6} + \tfrac{1}{d(u_4)} + (d(u_4)-1)\left(\tfrac{1}{d(u_4)} - \tfrac{1}{d(u_4)-1}\right) \\
= \; & R'(G_4) + \tfrac{7}{6} \geq 2 - \tfrac{1}{n-4} + \tfrac{7}{6} > 2 - \tfrac{1}{n-1}.
\end{aligned}$$

Case 2. There is a pair of adjacent vertices of degree two without common neighbor.

Let u_1 and u_2 be a pair of adjacent vertices with degree two in G which has no common neighbor. Denote by u_3 the neighbor of u_1 in G different from u_2. Let $G_5 = G - u_1 + u_2u_3$, then $R'(G_5) \geq 2 - \frac{1}{n-2}$ by the induction hypothesis, and $R'(G) = R'(G_5) + \frac{1}{2} \geq 2 - \frac{1}{n-2} + \frac{1}{2} > 2 - \frac{1}{n-1}$.

Case 3. There is no pair of adjacent vertices of degree two.

Let u be a vertex of degree two with neighbors v and w in G. Then $3 \leq d(v) \leq n-2$ and $3 \leq d(w) \leq n-2$. By Lemma 1, $R'(G) \geq R'(G-u) + \frac{1}{(n-1)(n-2)}$ with equality if and only if $G \in \mathbf{K}^*$. By the induction hypothesis, $R'(G-u) \geq 2 - \frac{1}{n-2}$ with equality if and only if $G-u = K^*_{2,n-3}$. So, $R'(G) \geq 2 - \frac{1}{n-2} + \frac{1}{(n-1)(n-2)} = 2 - \frac{1}{n-1}$ with equality if and only if $G = K^*_{2,n-2}$ by Lemma 2.

Hence, the assertion is true for all $n \geq 3$. □

3 A relation between R' index and the chromatic number

In this section, we discuss the relation between R' index and the chromatic number.

Lemma 5. *Let G be a graph with the minimum degree $\delta \geq 1$. If $v_0 \in V(G)$ such that $d(v_0) = \delta$, then $R'(G) \geq R'(G - v_0)$.*

Proof. Let $N(v_0) = \{v_1, v_2, \cdots, v_\delta\}$ and d_i the degree of vertex v_i. m_i is the number of vertices in $N(v_i) - \{v_0\}$ with degree less than d_i, where $0 \leq m_i \leq d_i - 1$. We have

$$\begin{aligned}
R'(G) - R'(G - v_0) = \; & \sum_{i=1}^{\delta} \tfrac{1}{d_i} + \sum_{i=1}^{\delta}\left(\tfrac{m_i}{d_i} - \tfrac{m_i}{d_i - 1}\right) \\
= \; & \sum_{i=1}^{\delta}\left(\tfrac{m_i+1}{d_i} - \tfrac{m_i}{d_i-1}\right) = \sum_{i=1}^{\delta} \tfrac{d_i - m_i - 1}{d_i(d_i-1)} \geq 0
\end{aligned}$$

□

Theorem 6. *Let G be a graph with the chromatic number $\chi(G)$. Then $R'(G) \geq \frac{\chi(G)}{2}$ with equality if and only if G is a complete graph possibly with some additional isolated vertices.*

Proof. If G is a complete graph possibly with some additional isolated vertices, then it is easily to get $R'(G) = \frac{\chi(G)}{2}$.

Suppose there is a graph G such that $R'(G) < \frac{\chi(G)}{2}$, then we can choose a graph G with the property $R' < \frac{\chi}{2}$ such that

1) there is no graph H such that $R'(H) < \frac{\chi(H)}{2}$ and $\chi(H) < \chi(G)$, i.e., G is a graph with the minimum chromatic number among all graphs with the property $R' < \frac{\chi}{2}$;

2) there is no proper subgraph F of G such that $R'(F) < \frac{\chi(F)}{2}$, i.e., G is minimal among all graphs with the property $R' < \frac{\chi}{2}$.

Note that $\delta(G) \geq 1$ and $\chi(G) \geq 2$ by the choice of G.

Claim. The minimum degree $\delta(G) \geq \chi(G) - 1$.

Proof. Suppose that $\delta(G) < \chi(G) - 1$. Let v be a vertex with the minimum degree $d_v = \delta$. Note that $\chi(G-v) < \chi(G)$, otherwise $\chi(G-v) = \chi(G)$, and using Lemma 5, $R'(G-v) \leq R'(G) < \frac{\chi(G)}{2} = \frac{\chi(G-v)}{2}$, which contradicts the choice of G. Hence, all vertices of $G - v$ can be regularly colored with $\chi(G) - 1$ colors. Now, $d_v < \chi(G) - 1$ implies that G can also be regularly colored with $\chi(G) - 1$ colors, which is a contradiction.

We continue to prove Theorem 6. Let v_0 be a vertex with the maximum degree in G and d'_u the degree of u in $G - v_0$. By the choice of G, we have

$$R'(G - v_0) \geq \frac{\chi(G - v_0)}{2} \geq \frac{\chi(G) - 1}{2}$$

Note that $d'_u \geq d_u - 1$ and $\frac{max\{d'_u,d'_v\}}{max\{d_u,d_v\}} \geq 1 - \frac{1}{max\{d_u,d_v\}} \geq 1 - \frac{1}{\delta(G)}$, it follows that

$$\begin{aligned}
R'(G) &= \sum_{uv\in E(G)} \frac{1}{max\{d_u, d_v\}} = 1 + \sum_{uv\in E(G-v_0)} \frac{1}{max\{d_u, d_v\}} \\
&= 1 + \sum_{uv\in E(G-v_0)} \frac{1}{max\{d'_u, d'_v\}} \cdot \frac{max\{d'_u, d'_v\}}{max\{d_u, d_v\}} \\
&\geq 1 + \sum_{uv\in E(G-v_0)} \frac{1}{max\{d'_u, d'_v\}} \cdot (1 - \frac{1}{\delta(G)}) \\
&= 1 + (1 - \frac{1}{\delta(G)})R'(G - v_0) \geq 1 + \frac{\chi(G) - 2}{\chi(G) - 1} R'(G - v_0) \quad (\textit{by } \textbf{Claim}) \\
&\geq 1 + \frac{\chi(G) - 2}{\chi(G) - 1} \cdot \frac{\chi(G) - 1}{2} = \frac{\chi(G)}{2}
\end{aligned}$$

a contradiction.

So, there is no graph G such that $R'(G) < \frac{\chi(G)}{2}$. □

Since $\frac{2}{d_u+d_v} \geq \frac{1}{max\{d_u,d_v\}}$ for an edge $uv \in E(G)$, we have $H(G) \geq R'(G)$. Theorem 6 strengthens a result in [5].

Corollary 7. *[5] Let G be a graph with the chromatic number $\chi(G)$ and the harmonic index $H(G)$, then $H(G) \geq \frac{\chi(G)}{2}$ with equality if and only if G is a complete graph possibly with some additional isolated vertices.*

4 A relation between R' index and the girth

In this section, we discuss the relation between R' index and the girth of a graph.

Lemma 8. *[1] For a graph G on n vertices, $R'(G) \leq \frac{n}{2}$ with equality if and only if G is regular.*

Theorem 9. *Let G be a graph with $n \geq 3$ vertices and girth g. Then*

(i) $R' + g \leq \frac{3n}{2}$ and $R' \cdot g \leq \frac{n^2}{2}$ with equality if and only if $G = C_n$ is the cycle on n vertices;

(ii) $\frac{R'}{g} \geq \frac{1}{2}$;

(iii) $R' - g \geq -\frac{n}{2}$;

(iv) $R' - g \leq \frac{n}{2} - 3$ and $\frac{R'}{g} \leq \frac{n}{6}$ with equality if and only if G is a regular graph with a triangle.

Proof. (i) follows from Lemma 8 and $g(G) \leq n$, $R' + g \leq \frac{3n}{2}$ and $R' \cdot g \leq \frac{n^2}{2}$ with equality if and only if G is a regular graph and $g(G) = n$, i.e., $G = C_n$ is the cycle on n vertices.

(ii) We will show that $\frac{R'}{g} \geq \frac{1}{2}$, i.e., $g \leq 2R'$, by the induction on $n + m$, where m is the number of edges of G. It is obvious that the assertion holds for $n + m = 6$. Now, we assume that $n + m \geq 7$ and the result holds for smaller value of $n + m$. If G is a cycle, then it is easy to check that $g(G) = 2R'(G)$. If G has a pendant vertex v, then $g(G) = g(G - v)$ and $R'(G - v) \leq R'(G)$ from Lemma 5. By the inductive assumption, $g(G - v) \leq 2R'(G - v)$. So, $g(G) \leq 2R'(G)$. If G is not a cycle and has no pendant vertex, then, from Lemma 3, there is an edge e with maximal weight in G such that $R'(G - e) \leq R'(G)$, and $g(G) \leq g(G - e)$. By the inductive assumption, $g(G - e) \leq 2R'(G - e)$. So, $g(G) \leq 2R'(G)$.

(iii) From (ii), $R' - g \geq \frac{1}{2}g - g = -\frac{1}{2}g \geq -\frac{1}{2}n$.

(iv) follows from Lemma 8 and $g(G) \geq 3$, $R' - g \leq \frac{n}{2} - 3$ and $\frac{R'}{g} \leq \frac{n}{6}$ with equality if and only if G is a regular graph and $g(G) = 3$, i.e., a regular graph with a triangle. □

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