

ON A CONJECTURE ON RANDIĆ INDICES

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Abstract

The Randić index of a graph G is defined as $R(G) = \sum_{u \sim v} (d(u)d(v))^{-\frac{1}{2}}$, where $d(u)$ is the degree of the vertex u , and the summation goes over all pairs of adjacent vertices u, v . In this paper, we investigate a conjecture on $R(G)$ for a connected graph G as follows: $R(G) \geq r(G) - 1$, where $r(G)$ denotes the radius of G . We prove that the conjecture is true for unicyclic graphs, bicyclic graphs and chemical graphs with cyclomatic number $c(G) \leq 5$.

1. INTRODUCTION

In 1975 the Croatian scientist Milan Randić was aiming at constructing a mathematical model suitable for describing the extent of branching of organic molecules, especially of the carbon-atom skeleton of alkanes. For this purpose Randić conceived a so-called “branching index” [1], that nowadays is referred to as the Randić index and is denoted by $R(G)$. Here G stands for a molecular graph, that is a graph representation of the carbon-atom skeleton of the underlying hydrocarbon.

Let $G = (V, E)$ be a simple graph, where V is vertex set, E is edge set. If $|V| = n$, $|E| = m$, we call G an (n, m) -graph.

For $v \in V(G)$, $d(v)$ (or d_v) denotes the degree of vertex v . The minimum and maximum degree of G is denoted by $\delta(G)$ and $\Delta(G)$, respectively. If $\delta(G) = \Delta(G) = k$, then G is said to be k -regular. If $\Delta(G) \leq 4$, then G is called a chemical graph. For terminology and notation not defined here, we refer the readers to [2].

The Randić index is a graph invariant defined as

$$R = R(G) = \sum_{u \sim v} \frac{1}{\sqrt{d(u)d(v)}}$$

where $u \sim v$ denotes adjacent vertices u, v .

Recently many researches on extremal aspects of the theory of Randić index have been reported (see [3]). But some open problems that are interesting and challenging from a mathematical point of view still exist. In [4], Fajtlowicz proposed the following:

Conjecture. [4] For all connected graphs G ,

$$R(G) \geq r(G) - 1$$

where $r(G)$ denotes the radius of G .

In [5], Caporossi and Hansen proved the following:

Theorem A. [5]

- (1) For all trees T , $R(T) \geq r(T) + \sqrt{2} - \frac{3}{2} \geq r(T) - 0.086$.
- (2) For all trees T except even paths, $R(T) \geq r(T)$.

Recently in [3], X. Li and I. Gutman pointed out that "It does not seem to be easy to extend these results to general graphs."

In this paper, we prove the conjecture for some (n, m) -graphs and chemical graphs.

2. RANDIĆ INDEX OF (n, m) -GRAPHS

The general Randić index of a (molecular) graph G is

$$R_\alpha = R_\alpha(G) = \sum_{u \sim v} (d(u)d(v))^\alpha$$

where α is a real number. Evidently, the Randić index is a special case of the general Randić index for $\alpha = -1/2$. Sometimes we denote

$$Q_\alpha = Q_\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha.$$

Q_1 and R_1 are called Zagreb indices.

For $R(G)$, Bollobás and Erdős ([6]) have given the following lower bound:

Lemma 2.1. *Let G be an (n, m) -graph. Then*

$$R(G) \geq \frac{\sqrt{8m+1} + 1}{4} .$$

The equality holds if and only if G consists of a complete graph and some isolated vertices.

Thus we immediately obtain the following:

Theorem 2.1. *Let G be an (n, m) -graph with $r(G) \leq \sqrt{m/2}$, then*

$$R(G) > r(G) > r(G) - 1 .$$

Proof. Since $r(G) \leq \sqrt{m/2}$, by Lemma 2.1,

$$R(G) \geq \frac{\sqrt{8m+1} + 1}{4} \geq \frac{\sqrt{8 \cdot 2r^2 + 1} + 1}{4} > \frac{4r}{4} > r - 1 . \quad \blacksquare$$

In fact in [7, 8, 9], the next results were established.

Lemma 2.2 [7] *Let G be an (n, m) -graph,*

$$R_\alpha(G)R_{-\alpha}(G) \geq m^2 .$$

Lemma 2.3. [8, 9] *Let G be a connected (n, m) -graph. Then*

$$Q_2(G) \leq m(m+1) .$$

The equality holds if and only if $G \cong K_3$ or $K_{1,n-1}$.

Lemma 2.4. [9] *Let G be a connected (n, m) -graph with girth $g(G) \geq 4$. Then*

$$Q_2(G) \leq m^2$$

where the equality holds if and only if $G \cong C_4$ (a cycle of order 4).

Thus we have:

Theorem 2.2. *Let G be a connected (n, m) -graph with $r(G) \leq \frac{2m}{m+1} + 1$. Then*

$$R(G) \geq r(G) - 1 .$$

Proof. By Lemma 2.2,

$$R(G) \geq \frac{m^2}{\sum_{i \sim j} \sqrt{d_i d_j}} \geq \frac{m^2}{\frac{1}{2} \sum_{i \sim j} (d_i + d_j)} = \frac{2m^2}{Q_2(G)} . \tag{1}$$

By Lemma 2.3,

$$R(G) \geq \frac{2m^2}{m(m+1)} \geq \frac{2m}{m+1} \geq r(G) - 1 . \quad \blacksquare$$

Using formula (1) and Lemma 2.4 we arrive at:

Corollary 2.1 *If G is a connected (n, m) -graph with girth $g(G) \geq 4$ and $r(G) \leq 3$, then*

$$R(G) \geq r(G) - 1 .$$

Comparing Theorem 2.2 with Theorem 2.1, we know that when $m < 18$, $\sqrt{\frac{m}{2}} \leq 2$.

We can use Theorem 2.2 while when $m \geq 18$, $\sqrt{\frac{m}{2}} \geq 3$, we should use Theorem 2.1.

From graph theory (see [2]), we know the following:

Lemma 2.5. *Let G be an (n, m) -graph with spanning tree T . Then the radius of G satisfies $r(G) \leq \frac{n}{2}$ and $r(T) \geq r(G)$.*

In [10], the following bound was obtained:

Lemma 2.6. [10] *Let G be a graph of order n with $\delta(G) \geq 2$. Then*

$$R(G) \geq f(n)$$

$$\text{where } f(n) = \sqrt{2(n-1)} + \frac{1}{n-1} - \sqrt{2/(n-1)} .$$

Thus we have

Theorem 2.3. *Let G be a graph of order n with $\delta(G) \geq 2$. If $n \leq 9$, then*

$$R(G) \geq r(G) - 1 .$$

Proof. If $n \leq 9$, it is easy to prove that

$$f(n) \geq \frac{n}{2} - 1.$$

By Lemmas 2.5 and 2.6,

$$R(G) \geq f(n) \geq \frac{n}{2} - 1 \geq r(G) - 1. \quad \blacksquare$$

In Theorem A, the conjecture for trees was proved. Now we investigate the conjecture for unicyclic and bicyclic graphs.

Theorem 2.4. *Let G be a unicyclic (n, m) -graph ($n \geq 3$). Then*

$$R(G) \geq r(G) - 1.$$

Proof. Let v_1v_2 be an edge in a cycle of G with $d(v_1) = d_1$, $d(v_2) = d_2$. By definition of Randić index, it is not difficult to obtain the following result by counting

$$\begin{aligned} R(G) - R(G - v_1v_2) &= \sum_{v_1 \sim v_x \neq v_2} \frac{1}{\sqrt{d_x}} \left(\frac{1}{\sqrt{d_1}} - \frac{1}{\sqrt{d_1 - 1}} \right) \\ &+ \sum_{v_2 \sim v_y \neq v_1} \frac{1}{\sqrt{d_y}} \left(\frac{1}{\sqrt{d_2}} - \frac{1}{\sqrt{d_2 - 1}} \right) + \frac{1}{\sqrt{d_1 d_2}}. \end{aligned} \quad (2)$$

Since v_1v_2 is an edge in a cycle, there exists at least one vertex $v_x \neq v_2$, $v_y \neq v_1$ for which $d_x, d_y \geq 2$, because v_x and v_y have to be connected by a path, different from $\{v_1, v_2\}$ (or $d_x = d_y$).

Hence from expression (2)

$$\begin{aligned} R(G) - R(G - v_1v_2) &\geq \left(d_1 - 2 + \frac{1}{\sqrt{2}} \right) \left(\frac{1}{\sqrt{d_1}} - \frac{1}{\sqrt{d_1 - 1}} \right) \\ &+ \left(d_2 - 2 + \frac{1}{\sqrt{2}} \right) \left(\frac{1}{\sqrt{d_2}} - \frac{1}{\sqrt{d_2 - 1}} \right) + \frac{1}{\sqrt{d_1 d_2}}. \end{aligned}$$

Since G is a unicyclic (n, m) -graph, ($n \geq 3$), the minimum value for the difference $R(G) - R(G - v_1v_2)$ is reached when $d_1 = d_2 = \frac{n+1}{2}$, and is equal to

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

Note that $\sqrt{\frac{1}{n+1}} - \sqrt{\frac{1}{n-1}} < 0$ and

$$\begin{aligned}
 & 2 \left(\frac{n+1}{2} - 2 + \frac{1}{\sqrt{2}} \right) \left(\sqrt{\frac{2}{n+1}} - \sqrt{\frac{2}{n-1}} \right) + \frac{2}{n+1} \\
 = & 2 \left(\frac{n+1}{\sqrt{2}} - 2\sqrt{2} + 1 \right) \left(\sqrt{\frac{1}{n+1}} - \sqrt{\frac{1}{n-1}} \right) + \frac{2}{n+1} \\
 > & 2 \left(\frac{n+1}{\sqrt{2}} - 2 + 1 \right) \left(\sqrt{\frac{1}{n+1}} - \sqrt{\frac{1}{n-1}} \right) + \frac{2}{n+1} \\
 = & \left[\sqrt{2}(n+1) - 2 \right] \left(\sqrt{\frac{1}{n+1}} - \sqrt{\frac{1}{n-1}} \right) + \frac{2}{n+1} \\
 > & \left[\sqrt{2}(n+1) - \sqrt{2} \right] \left(\sqrt{\frac{1}{n+1}} - \sqrt{\frac{1}{n-1}} \right) + \frac{2}{n+1} \\
 = & \sqrt{2} \cdot n \cdot \left(\sqrt{\frac{1}{n+1}} - \sqrt{\frac{1}{n-1}} \right) + \frac{2}{n+1} := f(n).
 \end{aligned}$$

Let $g(x) = \frac{1}{\sqrt{2}} f(x) = x \left(\sqrt{\frac{1}{x+1}} - \sqrt{\frac{1}{x-1}} \right) + \frac{\sqrt{2}}{x+1} \quad (x \geq 3).$

It is sufficient to show that $f(x)$ is monotonously increasing in x , i. e., $g'(x) > 0$ for $x \geq 3$.

$$\begin{aligned}
 g'(x) &= \sqrt{\frac{1}{x+1}} - \sqrt{\frac{1}{x-1}} + x \left(-\frac{1}{2\sqrt{x+1}(x+1)} \right. \\
 &\quad \left. + \frac{1}{2\sqrt{x-1}(x-1)} \right) - \frac{\sqrt{2}}{(x+1)^2} \\
 &= \frac{x+2}{2\sqrt{x+1}(x+1)} + \frac{2-x}{2\sqrt{x-1}(x-1)} - \frac{\sqrt{2}}{(x+1)^2}.
 \end{aligned}$$

Thus,

$$\begin{aligned}
 & 2(x+1)^2(x-1)^2 g'(x) \\
 = & (x+2)\sqrt{x+1}(x-1)^2 + (2-x)(x+1)^2\sqrt{x-1} - \sqrt{2}(x-1)^2 \\
 = & (x+1)\sqrt{x+1}(x-1)^2 + (2-x)(x+1)^2\sqrt{x-1} + \sqrt{x+1}(x-1)^2 \\
 & - \sqrt{2}(x-1)^2 \\
 = & (x+1)[\sqrt{x+1}(x-1)^2 + (2-x)(x+1)\sqrt{x-1}] + \sqrt{x+1}(x-1)^2 \\
 & - \sqrt{2}(x-1)^2.
 \end{aligned} \tag{3}$$

Claim 1: $\sqrt{x+1}(x-1)^2 + (2-x)(x+1)\sqrt{x-1} > 0$ for $x \geq 3$.

It is sufficient to prove that $\sqrt{x+1}(x-1)^2 > (x-2)(x+1)\sqrt{x-1}$.

Note that $\sqrt{x+1}(x-1)^2 > 0$ and $(x-2)(x+1)\sqrt{x-1} > 0$ for $x \geq 3$.

It is sufficient to prove that $(x+1)(x^2-2x+1)^2 > (x-1)(x^2-x-2)^2$, i. e., that $x^5-3x^4+2x^3+2x^2-3x+1 > x^5-3x^4-x^3+7x^2-4$, namely, $3x^3-5x^2-3x+5 > 0$ ($x \geq 3$). In fact,

$$\begin{aligned} 3x^3 - 5x^2 - 3x + 5 &= 3x^2 \left(x - \frac{5}{3} \right) - 3x + 5 \\ &\geq 4x^2 - 3x + 5 \\ &= 4 \left(x - \frac{3}{8} \right)^2 + \frac{71}{16} > 0 \quad \text{for } x \geq 3. \end{aligned}$$

Claim 2: $\sqrt{x+1}(x-1)^2 - \sqrt{2}(x-1)^2 = (\sqrt{x+1} - \sqrt{2})(x-1)^2 > 0$ for $x \geq 3$.

Thus from (3), $2(x+1)^2(x-1)^2g'(x) > 0$ for $x \geq 3$.

We have $g'(x) > 0$ for $x \geq 3$.

Note that $g(x) = \frac{1}{\sqrt{2}}f(x)$. Then $f(x)$ monotonically increases in x for $x \geq 3$.

Thus $f(x) \geq f(3) = \sqrt{2} \cdot 3 \cdot \left(\sqrt{\frac{1}{3+1}} - \sqrt{\frac{1}{3-1}} \right) + \frac{2}{3+1} \approx -0.37868$.

Hence

$$2 \left(\frac{n+1}{2} - 2 + \frac{1}{\sqrt{2}} \right) \left(\sqrt{\frac{2}{n+1}} - \sqrt{\frac{2}{n-1}} \right) + \frac{2}{n+1} > -0.4. \quad (4)$$

Note that $G - v_1v_2$ is a spanning tree of G and $r(G - v_1v_2) \geq r(G)$. Thus by inequality (4) and Theorem A, we have

$$\begin{aligned} R(G) &\geq R(G - v_1v_2) - 0.4 \\ &\geq r(G - v_1v_2) - 0.086 - 0.4 \\ &\geq r(G - v_1v_2) - 1 \\ &\geq r(G) - 1. \end{aligned}$$

By this Theorem 2.4 has been proven. \blacksquare

Note that the conclusion of Theorem 2.4 can be improved as follows: $R(G) \geq r(G) - 0.4$. Because if n is odd, then $R(G - v_1v_2) \geq r(G - v_1v_2)$ by proposition (2) in Theorem A. If n is even, then for an even cycle C_n , $R(C_n) = \frac{n}{2} = r(C_n)$. For

$G \not\cong C_n$, we must find an edge v_1v_2 such that $G - v_1v_2$ is not an even path. Then by Theorem A, $R(G - v_1v_2) \geq r(G - v_1v_2)$.

Theorem 2.5. *Let G be a bicyclic (n, m) -graph $(n \geq 3)$, then*

$$R(G) \geq r(G) - 1 .$$

Proof. Let v_1v_2, v_3v_4 be two edges in cycle of G with $d(v_i) = d_i$ for $i = 1, 2, 3, 4$, such that $G - v_1v_2 - v_3v_4$ is a spanning tree of G . Using the method similar to Theorem 2.4, we also have expression (2) and inequality (4), i. e.,

$$R(G) \geq R(G - v_1v_2) - 0.4 .$$

Similarly,

$$\begin{aligned} R(G) &\geq R(G - v_1v_2 - v_3v_4) - 0.8 \\ &\geq r(G - v_1v_2 - v_3v_4) - 0.086 - 0.8 \quad (\text{Theorem A}) \\ &\geq r(G - v_1v_2 - v_3v_4) - 1 \\ &\geq r(G) - 1 . \end{aligned} \quad \blacksquare$$

We define an edge v_1v_2 as a simple edge if $d_1 = d_2 = 2$. The following general conclusion can be established:

Theorem 2.6. *Let G be an (n, m) -graph with at least a simple edge in each cycle (or each cycle has a simple edge to can be deleted step-by-step). Then*

$$R(G) > r(G) - 1 .$$

Proof. Let v_1v_2 be a simple edge of a cycle in G . Then

$$\begin{aligned} &R(G) - R(G - v_1v_2) \\ &= \sum_{v_1 \sim v_x \neq v_2} \frac{1}{\sqrt{d_x}} \left(\frac{1}{\sqrt{d_1}} - \frac{1}{\sqrt{d_1 - 1}} \right) + \sum_{v_2 \sim v_y \neq v_1} \frac{1}{\sqrt{d_y}} \left(\frac{1}{\sqrt{d_2}} - \frac{1}{\sqrt{d_2 - 1}} \right) \\ &+ \frac{1}{\sqrt{d_1 d_2}} \geq \left(d_1 - 2 + \frac{1}{\sqrt{2}} \right) \left(\frac{1}{\sqrt{d_1}} - \frac{1}{\sqrt{d_1 - 1}} \right) \\ &+ \left(d_2 - 2 + \frac{1}{\sqrt{2}} \right) \left(\frac{1}{\sqrt{d_2}} - \frac{1}{\sqrt{d_2 - 1}} \right) + \frac{1}{\sqrt{d_1 d_2}} . \end{aligned}$$

Since $d_1 = d_2 = 2$,

$$R(G) - R(G - v_1v_2) \geq \sqrt{2} \left(\frac{1}{\sqrt{2}} - 1 \right) + \frac{1}{2} = 1.5 - \sqrt{2} > 0 .$$

Thus

$$R(G) > R(G - v_1v_2) \tag{5}$$

where v_1v_2 is a simple edge in a cycle of G .

Let cyclomatic number of G be $c(G) = k \geq 1$ (For tree, one can see Theorem A). Then using inequality (5) k times, we have

$$R(G) > R(T)$$

where T is a spanning tree of G .

Hence $R(G) > R(T) \geq r(T) - 1 \geq r(G) - 1$. ■

3. RANDIĆ INDEX OF CHEMICAL GRAPHS

In expression (2) (Section 2) note that $d_1 \leq 4$ and $d_2 \leq 4$ for a chemical graph G . Then it is easy to obtain:

Lemma 3.1. (see [3]) *Let G be a chemical graph with cyclomatic number $c(G) \geq 1$. Let v_1v_2 be an edge in a cycle of G . Then*

$$R(G) \geq R(G - v_1v_2) - 0.169 .$$

Thus we obtain the following:

Theorem 3.1. *Let G be a chemical graph with cyclomatic number $1 \leq c(G) \leq 5$. Then*

$$R(G) \geq r(G) - 1 .$$

Proof. Without loss of generality, let $c(G) = 5$ and let $v_1^{(i)}v_2^{(i)}$, $i = 1, 2, 3, 4, 5$ be an edge in a cycle of G such that $G - \sum_{i=1}^5 v_1^{(i)}v_2^{(i)}$ is a spanning tree of G . Thus by

Lemma 3.1 and Theorem A,

$$\begin{aligned} R(G) &\geq R(G - v_1^{(1)}v_2^{(1)}) - 0.169 \\ &\geq R(G - v_1^{(1)}v_2^{(1)} - v_1^{(2)}v_2^{(2)}) - 2 \times 0.169 \\ &\dots \\ &\geq R\left(G - \sum_{i=1}^5 v_1^{(i)}v_2^{(i)}\right) - 5 \times 0.169 \\ &\geq r\left(G - \sum_{i=1}^5 v_1^{(i)}v_2^{(i)}\right) - 0.086 - 5 \times 0.169 \\ &\geq r\left(G - \sum_{i=1}^5 v_1^{(i)}v_2^{(i)}\right) - 1 \\ &\geq r(G) - 1. \quad \blacksquare \end{aligned}$$

NOTE ADDED IN PROOF.

Since the completion of this paper significant progress in the theory of the Randić index has been achieved. This is best seen from the three new reviews [11–13], Milan Randić’s extensive historical article [14], the recent book [15], and the recent papers [16–20]. In the book [15] a list of works on Randić index is found [21], quoting those articles that appeared between January 2006 and February 2008. This list contains 59 bibliographic units, and in the book [15] there are additional 20 articles.

Of these numerous recently produced results on Randić index the following needs to be mentioned. In [22] it is shown that the conjecture studied in the present paper is true for biregular graphs, tricyclic graphs, tetracyclic graphs, and all connected graphs of order less than 11.

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