A proof of a conjecture on the Randić index of graphs with given girth*

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Abstract

The Randić index $R(G)$ of a graph G is defined by $R(G) = \sum\limits_{uv} \frac{1}{\sqrt{d(u)d(v)}}$, where $d(u)$ is the degree of a vertex u in G and the summation extends over all edges uv of G. Aouchiche, Hansen and Zheng proposed the following conjecture: For any connected graph on $n \geq 3$ vertices with Randić index R and girth g,

$$R + g \geq \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{7}{2} \quad \text{and} \quad R \cdot g \geq \frac{3n-9+3\sqrt{2}}{\sqrt{n-1}} + \frac{3}{2}$$

with equalities if and only if $G = S_n^+$. This paper is devoted to giving a confirmative proof to this conjecture.

Key words: Randić index; conjecture; girth

AMS Subject Classification 2000: 05C07, 05C35, 92E10

1 Introduction

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

$$R = R(G) = \sum_{u,v} \frac{1}{\sqrt{d(u)d(v)}}, \tag{1.1}$$

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 [13] in 1975, suitable for measuring

*Supported by NSFC No.10831001, PCSIRT, and the "973" program.

the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Randić himself demonstrated [13] that his index is well correlated with a variety of physico-chemical properties of alkanes. The index R became one of the most popular molecular descriptors to which three books are devoted [7, 8, 9].

In this paper, we only consider finite, undirected and simple graphs. A simple connected graph G is called unicyclic if it contains exactly one cycle. Bicyclic graphs are connected graphs in which the number of edges equals to the number of vertices plus one. A pendant vertex is a vertex of degree one. For undefined terminology and notations we refer to [3].

There are many results concerning the Randić index. In [2], Bollobás and Erdős gave a sharp lower bound of $R(G) \geq \sqrt{n-1}$ for G of order n without isolated vertices. Gao and Lu [6] gave sharp lower and upper bounds on the Randić index of unicyclic graphs of order n. For more references, see [10, 12].

Let $n \geq 3$ be an integer. Let S_n^+ be a unicyclic graph obtained from the star $K_{1,n-1}$ by joining two pendant vertices of $K_{1,n-1}$ by a new edge (see Figure 1.1).

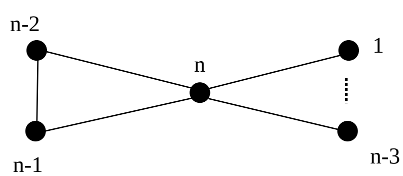

Figure 1.1 The graph S_n^+

In [1], Aouchiche, Hansen and Zheng proposed the following conjecture:

Conjecture 1.1 *For any connected graph on $n \geq 3$ vertices with Randić index R and girth g,*

$$R + g \geq \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{7}{2} \quad \text{and} \quad R \cdot g \geq \frac{3n-9+3\sqrt{2}}{\sqrt{n-1}} + \frac{3}{2}$$

with equalities if and only if $G = S_n^+$.

Liu, Zhu and Cai [11] showed that the above conjecture is true for unicyclic graphs. Wang, Zhu and Liu [14] showed it is true for bicyclic graphs. In this paper, we prove that Conjecture 1.1 is true in general, completely solving the conjecture.

2 Some Lemmas

This section gives some lemmas which will be used in the sequel.

Lemma 2.1 *Let* $f(d,\ell) := \frac{1}{\sqrt{\ell d}} - \frac{1}{\sqrt{\ell+d-1}} + (d-1)(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d+\ell-1}})$*, where* $d \geq 4, \ell \geq 2$*. Then* $f(d,\ell) \geq 0$*.*

Proof. Since $\ell d > \ell + d - 1$, we have $\frac{\partial f(d,\ell)}{\partial \ell} = -\frac{d}{2(\ell d)^{3/2}} + \frac{d}{2(d+\ell-1)^{3/2}} > 0$. We want $\frac{\partial f(d,2)}{\partial d} < 0$, that is, $\frac{\partial f(d,2)}{\partial d} = -\frac{1}{2\sqrt{2}d^{3/2}} - \frac{-1+d}{2d^{3/2}} + \frac{1}{\sqrt{d}} + \frac{d}{2(1+d)^{3/2}} - \frac{1}{\sqrt{1+d}} = \frac{1}{2}\left(\frac{d+1-\frac{1}{\sqrt{2}}}{d^{3/2}} - \frac{d+2}{(1+d)^{3/2}}\right) < 0$ or $(d+1-\frac{1}{\sqrt{2}})(d+1)^{3/2} < d^{3/2}(d+2)$, that is to say $(\frac{d+1}{d})^3 < (\frac{d+2}{d+1-1/\sqrt{2}})^2$ or $(1+\frac{1}{d})^3 < (1+\frac{1+1/\sqrt{2}}{d+1-1/\sqrt{2}})^2$. To prove this it suffices to prove $(1+\frac{1}{d})^3 < (1+\frac{1+1/\sqrt{2}}{d})^2$. But, if $d \geq 5$ we have $\frac{1+1/\sqrt{2}}{d+1-1/\sqrt{2}} > \frac{1.6}{d}$. Thus it suffices to prove $1 + \frac{3}{d} + \frac{3}{d^2} + \frac{1}{d^3} < 1 + \frac{3.2}{d} + \frac{2.56}{d^2}$, that is to say $3.2d^2 + 2.56d > 3d^2 + 3d + 1$ or $0.2d^2 - 0.44d - 1 > 0$. Since the positive root of this polynomial is less than 4, we have proven the inequality. By direct calculation we know that the result is also valid for $d = 4$. We have thus proven that $f(d,\ell) \geq f(d,2) \geq f(+\infty,2) = 0$. ∎

Lemma 2.2 *[4]. For any connected graph* G *of order* n *with minimum degree* $\delta \geq 2$*, we have*

$$R(G) \geq \frac{2n-4}{\sqrt{2n-2}} + \frac{1}{n-1} \tag{2.2}$$

and the bound is tight if and only if $G = K^{\star}_{2,n-2}$ *which arises from complete bipartite graph* $K_{2,n-2}$ *by joining the vertices in the partite set with two vertices by a new edge.*

Corollary 2.3 *Conjecture 1.1 is true for any connected graph* G *of order* n *with minimum degree* $\delta \geq 2$*.*

Proof. It is easy to see that G contains at least one cycle since the minimum degree δ is at least 2. Thus, we have $R + g \geq \frac{2n-4}{\sqrt{2n-2}} + \frac{1}{n-1} + 3 > \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{7}{2}$ and $R \cdot g \geq \frac{6(n-2)}{\sqrt{2n-2}} + \frac{3}{n-1} > \frac{3n-9+3\sqrt{2}}{\sqrt{n-1}} + \frac{3}{2}$ by Lemma 2.2 and some manipulations. ∎

Lemma 2.4 *[5]. For any triangle-free graph* G *with size* m*, we have* $R(G) \geq \sqrt{m}$*.*

Corollary 2.5 *Conjecture 1.1 is true for any connected triangle-free graph* G *of order* n *with girth* g*.*

Proof. It is easy to see that the size of G is not less than n, since G is connected and with $g \geq 4$. Thus, by Lemma 2.4,

$$R+g \geq \sqrt{n}+4 > \sqrt{n-1}+4 > \sqrt{n-1}+\frac{\sqrt{2}-2}{\sqrt{n-1}}-\frac{1}{2}+4 = \frac{n-3+\sqrt{2}}{\sqrt{n-1}}+\frac{7}{2},$$
$$R \cdot g \geq 4\sqrt{n} > \frac{3n-9+3\sqrt{2}}{\sqrt{n-1}}+\frac{3}{2},$$

because

$$4\sqrt{n}-\frac{3n-9+3\sqrt{2}}{\sqrt{n-1}}-\frac{3}{2} = \frac{\sqrt{n}\Big(6(\sqrt{n-1}-\sqrt{n})+\sqrt{n-1}\Big)+\sqrt{n-1}(\sqrt{n}-3)+18-6\sqrt{2}}{2\sqrt{n-1}} > 0.$$

∎

3 Main result

In this section we give a confirmative proof to Conjecture 1.1.

Theorem 3.1 *For any connected graph on $n \geq 3$ vertices with Randić index R and girth g,*

$$R+g \geq \frac{n-3+\sqrt{2}}{\sqrt{n-1}}+\frac{7}{2} \quad \text{and} \quad R \cdot g \geq \frac{3n-9+3\sqrt{2}}{\sqrt{n-1}}+\frac{3}{2}$$

with equalities if and only if $G = S_n^+$.

Proof. Let $\mathcal{C}$ be the class of connected graphs with minimum degree $\delta = 1$ and girth $g = 3$ on at least 3 vertices. We only need to show the theorem for graphs in $\mathcal{C}$ is true by Corollary 2.3 and 2.5. Consequently, it is sufficient to show that $R(G) \geq \frac{n-3+\sqrt{2}}{\sqrt{n-1}}+\frac{1}{2}$ for any graph $G \in \mathcal{C}$.

We apply induction on n. For $n = 3$, no graph belongs to $\mathcal{C}$. For $n = 4$ and $n = 5$, it is easy to check that the theorem is true (see Figure 3.1).

Thus, assume the theorem is true for graphs of order less than n (≥ 6). Let G be a graph of order n with minimum Randić index in $\mathcal{C}$. Set $V_1 = \{u \in V(G) | d(u) = 1\}$ and let $u \in V_1$ and $uv \in E(G)$. Then $d(v) \geq 2$. Denote $d(v) = d$ and $N(v) = \{u, u_1, u_2, \cdots, u_{d-1}\}$. Let $N_2 = \{u_i | d(u_i) \geq 2, u_i \in N(v)\}$. Then we have $|N_2| \geq 1$ since G is a connected graph with cycle(s). Let $G' = G - \{u\}$. Then G' is connected and $g(G') = 3$. If $\delta(G') \geq 2$, then

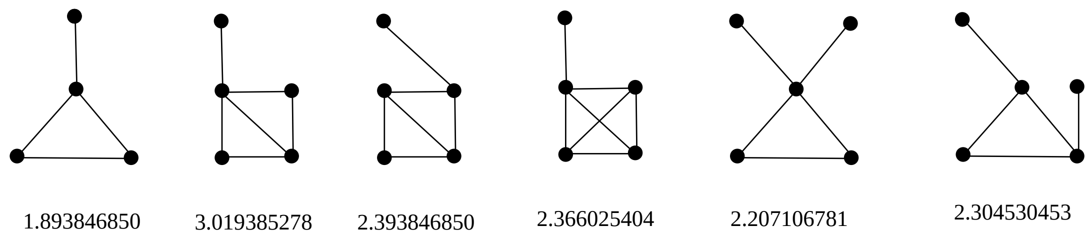

Figure 3.1 Graphs on four and five vertices in $\mathcal{C}$ and their approximate Randić indices

$R(G') \geq \frac{2(n-3)}{\sqrt{2(n-2)}} + \frac{1}{n-2} \geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2}$ by Corollary 2.3. If $\delta(G') = 1$, then $R(G') \geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2}$ by induction assumption. And we have

$$R(G) - R(G') = \frac{1}{\sqrt{d}} + \sum_{i=1}^{d-1} \frac{1}{\sqrt{d(u_i)}} \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right) \tag{3.3}$$

Since $\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}$ is negative, the latter expression is minimum when all $d(u_i), i = 1, \cdots, d-1$ are minimum, i.e., $d(u_i) = 1, i = 1, \cdots, d-1$. Thus

$$R(G) - R(G') \geq \sqrt{d} - \sqrt{d-1} \tag{3.4}$$

Case 1. $d \leq 3$.

Then by (3.4), we have $R(G) \geq R(G') + \sqrt{d} - \sqrt{d-1}$. Since $\sqrt{d} - \sqrt{d-1}$ is monotonically decreasing in d, we get $R(G) \geq R(G') + \sqrt{3} - \sqrt{2}$. By induction hypothesis we have $R(G) \geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} + \sqrt{3} - \sqrt{2}$. Since $n \geq 6$ and both $\sqrt{n-1} - \sqrt{n-2}$ and $\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}$ are monotonically decreasing in n, we have that $\sqrt{n-1} - \sqrt{n-2} + (2-\sqrt{2})(\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}) \leq \sqrt{5} - \sqrt{4} + (2-\sqrt{2})(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{5}}) \approx 0.2669895369 < \sqrt{3} - \sqrt{2}$. Therefore, $\frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \sqrt{3} - \sqrt{2} \geq \frac{n-3+\sqrt{2}}{\sqrt{n-1}}$. Hence, $R(G) \geq \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{1}{2}$, for $n \geq 6$.

Case 2. $d \geq 4$.

We first claim that $|N_2| \geq 2$. Otherwise, assume $|N_2| = 1$ and $w \in N_2$. Denote $d(w) = \ell$ and $N(w) = \{w_1, w_2, \cdots, w_{\ell-1}, v\}$. Let $G'' = G - \{ww_1, \cdots, ww_{\ell-1}\} + \{vw_1, \cdots, vw_{\ell-1}\}$ (see Figure 3.2). Then G'' is a graph in $\mathcal{C}$ of order n.

By Lemma 2.1,

$$\begin{aligned} R(G) - R(G'') &= \frac{1}{\sqrt{\ell d}} - \frac{1}{\sqrt{\ell+d-1}} + (d-1)\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d+\ell-1}}\right) + \sum_{i=1}^{\ell-1} \frac{1}{\sqrt{d(w_i)}}\left(\frac{1}{\sqrt{\ell}} - \frac{1}{\sqrt{d+\ell-1}}\right) \\ &> \frac{1}{\sqrt{\ell d}} - \frac{1}{\sqrt{\ell+d-1}} + (d-1)\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d+\ell-1}}\right) \geq 0, \end{aligned}$$

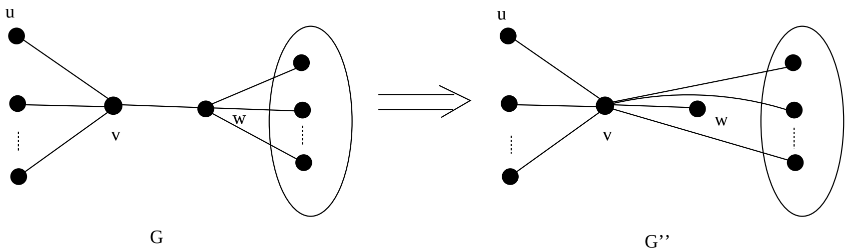

Figure 3.2 Graphs G and G''

contradicting to the assumption that G is the graph with minimum Randić index of order n in $\mathcal{C}$.

Therefore, $|N_2| \geq 2$. Noticing again that $\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}$ is negative, the latter expression of (3.3) is minimum when $d(u_i), i = 1, \cdots, d-1$ is as small as possible, i.e., $d(u_i) = 1, i = 1, \cdots, d-3$ and, without loss of generality, $d(u_{d-2}) = d(u_{d-1}) = 2$. We then have

$$\begin{aligned}
R(G) &\geq R(G') + \frac{1}{\sqrt{d}} + 2 \times \frac{1}{\sqrt{2}}(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}) + (d-3) \times \frac{1}{\sqrt{1}}(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}) \\
&= R(G') + \sqrt{d} - \sqrt{d-1} + (2-\sqrt{2})(\frac{1}{\sqrt{d-1}} - \frac{1}{\sqrt{d}}) \\
&\geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} + \sqrt{n-1} - \sqrt{n-2} + (2-\sqrt{2})(\frac{1}{\sqrt{n-2}} - \frac{1}{\sqrt{n-1}}) \\
&= \sqrt{n-1} - (2-\sqrt{2})\frac{1}{\sqrt{n-1}} + \frac{1}{2} \\
&= \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{1}{2},
\end{aligned}$$

where the equalities hold if and only if $d(v) = d = n-1, d(u) = d(u_1) = d(u_2) = \cdots = d(u_{n-4}) = 1, d(u_{n-3}) = d(u_{n-2}) = 2$, i.e., $G = S_n^+$, completing the proof. ∎

Acknowledgement. The authors are very grateful to the referees for helpful comments and suggestions, one of which helped to improve the proof of Lemma 2.1.

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