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On the Randić index and girth of graphs☆

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ABSTRACT

The Randić index $R(G)$ of a graph G is defined by $R(G) = \sum_{uv} \frac{1}{\sqrt{d(u)d(v)}}$, where $d(u)$ is the degree of a vertex u in G and the summation extends over all edges uv of G. In this work, we give a sharp upper bound and a lower bound of the Randić index among connected n-vertex graphs with girth $g \geq k (k \geq 3)$.

1. Introduction

All the graphs considered in this paper are simple undirected ones. The *girth* of a graph G, denoted by $g(G)$, is the minimum length of its cycles. A *leaf* is a vertex of degree one. The set of vertices adjacent to a vertex u of G, the *neighborhood* of u, is denoted by $N(u)$. We will use $G - \{u\}$ or $G - \{e\}$ to denote the graph obtained from G by deleting the vertex u or the edge e of G. By deleting a vertex, we mean deleting vertex together with its incident edges. For undefined terminology and notations we refer the reader to [3].

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

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

where $d(u)$ denotes the degree of a vertex u and $E(G)$ is the set of edges. This index is also known as connectivity index or branching index. Randić [13] in 1975 proposed this index for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. There is also a good correlation between the Randić index and several physicochemical properties of alkanes: boiling points, surface areas, energy levels, etc. In 1998, Bollobás and Erdős [2] generalized this index by replacing the square-root by power of any real number, which is called the general Randić index. For a comprehensive survey of its mathematical properties, see the book of Li and Gutman [8], or a survey of Li and Shi [10]. See also the books of Kier and Hall [6,7] for chemical properties of this index.

There are many results concerning the relations between the Randić index and other graph invariants such as diameter, minimum degree, radius, average distance, girth, and chromatic number; see [5]. Regarding the girth, Aouchiche et al. [1] showed the following.

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Theorem 1.1 ([1]). *For any connected graph G on $n \geq 3$ vertices with Randić index R and girth g,*

$$R + g \leq \frac{3n}{2}, \qquad R \cdot g \leq \frac{n^2}{2}, \qquad R - g \geq -\frac{n}{2}, \qquad \frac{R}{g} \geq \frac{1}{2},$$

with equalities if and only if G is C_n, the cycle on n vertices.

$$R - g \leq \frac{n}{2} - 3, \qquad \frac{R}{g} \leq \frac{n}{6},$$

with equalities if and only if G is a regular graph with a triangle.

They also conjectured the following.

Conjecture 1.2 ([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 is the graph obtained by adding an edge in an n-vertex star.

Liu et al. [11] showed that the conjecture is true for unicyclic graphs. Wang et al. [14] showed that it is true for bicyclic graphs. It is proved to be true in general by Li and Liu [9].

Note that all the above results are dealing with the relationship between the Randić index and girth, which can be proved immediately if we can characterize the minimum Randić index and the maximum Randić index with the given general lower bound of the girth.

In this work, we give the sharp lower and upper bounds of R with the girth $g \geq k (k \geq 3)$.

The rest of the paper is organized as follows. In Section 2 we list some lemmas which will be used in the proofs of the main results. In Section 3 we give the main results of this work.

2. Some lemmas

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

For an edge uv of a graph G, the *weight* of the edge $e = uv$ is denoted by $w(e) = \frac{1}{\sqrt{d(u) \cdot d(v)}}$. In 1998, Bollobás and Erdős [2] showed the following.

Lemma 2.1 ([2]). *Let uv be an edge of maximum weight in a graph G. Then*

$$R(G) > R(G - \{uv\}).$$

In 2009, Li and Liu [9] gave the following inequality.

Lemma 2.2 ([9]). *Let $f(d, \ell) := \frac{1}{\sqrt{\ell d}} - \frac{1}{\sqrt{\ell + d - 1}} + (d-1)\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d + \ell - 1}}\right)$. Then $f(d, \ell) \geq 0$, where d, ℓ are integers and $d \geq 2, \ell \geq 2$.*

Caporossi et al. [4] and Pavlović et al. [12] showed the following.

Lemma 2.3. *For any connected graph G on n vertices,*

$$R(G) \leq \frac{n}{2}$$

with equality if and only if G is regular.

3. Main results

Denote by C_k^n the graph obtained by linking each $(n - k)$ isolated vertices an edge to the same vertex of cycle C_k; see Fig. 3.1 for example.

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

$$R(G) \geq \sqrt{n - k + 2} - \frac{2 - \sqrt{2}}{\sqrt{n - k + 2}} + \frac{k - 2}{2}$$

with equality if and only if $G \cong C_k^n$.

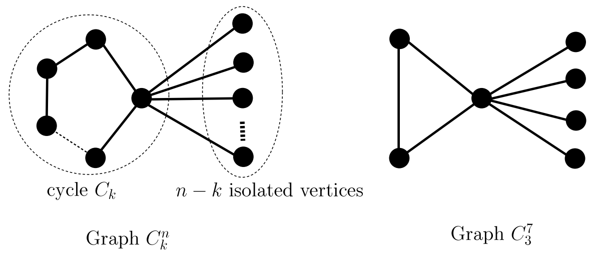

Fig. 3.1. Graphs C_k^n and C_3^7.

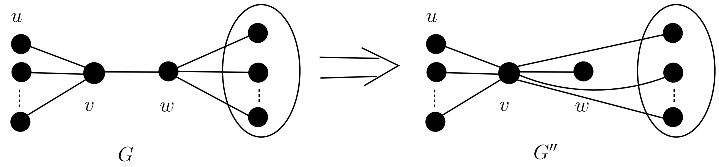

Fig. 3.2. Graphs G and G''.

Proof. To prove the assertion of the theorem we apply induction on $n+m$, where m is the number of edges of the considered graph. It is elementary to check that the assertion holds for $n+m \le 6$; so we assume that $n+m \ge 7$ and the result holds for smaller value of $n+m$. Furthermore, we assume that G is the graph with the minimum Randić index with n vertices, m edges and girth $g(G)(\ge k)$. The proof is divided into two cases: Case 1, $\delta(G) = 1$; Case 2, $\delta(G) \ge 2$.

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

Let V_1 be the set of all leaves of G and let $u \in V_1$ and $uv \in E(G)$, then $d(v) \ge 2$. Denote $d(v) = d$ and $N(v) = \{u, u_1, u_2, \ldots, u_{d-1}\}$. Note that $d \le \Delta(G) \le n-k+2$ since $g(G) \ge k$.

Let $N_2 = \{u_i | d(u_i) \ge 2, u_i \in N(v)\}$. Then we have $|N_2| \ge 1$ since G is a connected graph with cycle(s). Let $G' = G - \{u\}$. Then G' is a connected graph with the same girth as G and $R(G') \ge \sqrt{n-k+1} - \frac{2-\sqrt{2}}{\sqrt{n-k+1}} + \frac{k-2}{2}$ by induction. We also have

$$R(G) - R(G') = \frac{1}{\sqrt{d}} + \sum_{i=1}^{d-1} \frac{1}{\sqrt{d(u_i)}} \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}} \right) \tag{3.2}$$

Now, we have the following claim.

Claim. $|N_2| \ge 2$.

For otherwise, assume $|N_2| = 1$ and $w \in N_2$. Denote $d(w) = \ell$ and $N(w) = \{w_1, w_2, \ldots, w_{\ell-1}, v\}$. Let $G'' = G - \{ww_1, \ldots, ww_{\ell-1}\} + \{vw_1, \ldots, vw_{\ell-1}\}$ (see Fig. 3.2). Then G'' is a graph which satisfies the conditions in this case.

By Lemma 2.2,

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

contradicting to the assumption that G is the graph with the minimum Randić index.

Therefore, $|N_2| \ge 2$. Noticing that $\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}$ is negative, the latter expression of (3.2) is minimum when $d(u_i), i = 1, \ldots, d-1$ is as small as possible, i.e., $d(u_i) = 1, i = 1, \ldots, d-3$ and, without loss of generality, $d(u_{d-2}) = d(u_{d-1}) = 2$. We then have

$$\begin{aligned} R(G) &\ge R(G') + \frac{1}{\sqrt{d}} + 2 \times \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}} \right) + (d-3) \times \frac{1}{\sqrt{1}} \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}} \right) \\ &= R(G') + \sqrt{d} - \sqrt{d-1} + \left(2 - \sqrt{2}\right) \left(\frac{1}{\sqrt{d-1}} - \frac{1}{\sqrt{d}} \right) \\ &\ge \sqrt{n-k+1} - \frac{2-\sqrt{2}}{\sqrt{n-k+1}} + \frac{k-2}{2} \end{aligned}$$

$$+\sqrt{n-k+2}-\sqrt{n-k+1}+\left(2-\sqrt{2}\right)\left(\frac{1}{\sqrt{n-k+1}}-\frac{1}{\sqrt{n-k+2}}\right)$$
$$=\sqrt{n-k+2}-\frac{2-\sqrt{2}}{\sqrt{n-k+2}}+\frac{k-2}{2},$$

where the equalities hold if and only if $d(v)=d=n-k+2$, $d(u)=d(u_1)=d(u_2)=\cdots=d(u_{n-k})=1$, $d(u_{n-k+1})=d(u_{n-k+2})=2$, i.e., $G\cong C_k^n$.

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

Case 2.1. $m=n$. In this case, it is easy to see that C_n is the unique graph which satisfies the conditions. Thus, $R(G)=\frac{n}{2}$ and the result holds obviously.

Case 2.2. $m\geq n+1$. Let $e_m=uv$ be the edge with maximum weight in G. We divide Case 2.2 into two subcases.

Subcase 2.2.1. $e_m=uv$ is a cut-edge. Denote $G'=G-\{e_m\}$ and $G'=G_1\bigcup G_2$, where G_1 is the connected component containing u and G_2 is the connected component containing v. Let n_i be the number of vertices of $G_i (i=1,2)$ and assume that $n_1\geq n_2$, then $n=n_1+n_2$. Bearing in mind that $\delta(G)\geq 2$, $g(G)\geq k$ and $e_m=uv$ is a cut-edge of G, we conclude that G_i contains cycle(s) with girth at least k and $n_i\geq k (i=1,2)$. By induction, we have $R(G_i)\geq\sqrt{n_i-k+2}-\frac{2-\sqrt{2}}{\sqrt{n_i-k+2}}+\frac{k-2}{2}$ $(k=1,2)$. Therefore,

$$\begin{aligned}R(G) &> R(G-\{e_m\})=R(G_1)+R(G_2)\\ &\geq\sum_{i=1}^{2}\left[\sqrt{n_i-k+2}-\frac{2-\sqrt{2}}{\sqrt{n_i-k+2}}+\frac{k-2}{2}\right]\\ &> \sqrt{n_1-k+2}+\sqrt{n-n_1-k+2}+\sqrt{2}-4+k\\ &> \sqrt{n-k+2}+\frac{\sqrt{2}-2}{\sqrt{n-k+2}}+\frac{k-2}{2},\end{aligned}$$

because

$$\begin{aligned}&\sqrt{n_1-k+2}+\sqrt{n-n_1-k+2}+\sqrt{2}-4+k-\left(\sqrt{n-k+2}+\frac{\sqrt{2}-2}{\sqrt{n-k+2}}+\frac{k-2}{2}\right)\\ &=\sqrt{n_1-k+2}+\sqrt{n_2-k+2}-\sqrt{n-k+2}+\frac{k}{2}+\frac{2-\sqrt{2}}{\sqrt{n-k+2}}\\ &>\sqrt{n_1-k+2}+\sqrt{n-n_1-k+2}-\sqrt{n-k+2}+\frac{k}{2}:=f(n,n_1,k) \qquad (3.3)\\ &\geq f(n,n_1,3)=\sqrt{n_1-1}+\sqrt{n-n_1-1}-\sqrt{n-1}+\sqrt{2}-\frac{3}{2}\\ &\geq 2\sqrt{\frac{n}{2}-1}-\sqrt{n-1}+\sqrt{2}-\frac{3}{2} \qquad (3.4)\\ &=\sqrt{2n-4}-\sqrt{n-1}+\sqrt{2}-\frac{3}{2}\\ &>0. \qquad (3.5)\end{aligned}$$

Inequality (3.3) holds because $\frac{\partial f(n,n_1,k)}{\partial k}=-\frac{1}{2\sqrt{n_1-k+2}}-\frac{1}{2\sqrt{n-n_1-k+2}}+\frac{1}{\sqrt{n-k+2}}+\frac{1}{2}>-\frac{1}{2\sqrt{4}}+\frac{1}{2}=0$ for $n_1-k\geq 2$, $n-n_1-k\geq 2$. For $n_1-k\leq 1$, then $n-n_1-k\leq n_1-k\leq 1$, it is easy to verify that $f(n,n_1,k)>0$.

Inequality (3.4) holds because $\frac{\partial f(n,n_1,3)}{\partial n_1}=-\frac{1}{2\sqrt{n_1-k+2}}+\frac{1}{2\sqrt{n-n_1-k+2}}\geq 0$ for $n_1\geq n-n_1$.

Inequality (3.5) holds because $n\geq 4$, which means $n+4\sqrt{n-2}-3\sqrt{n-1}>\frac{13}{4}$, i.e., $2n-4+2+4\sqrt{n-2}>n-1+\frac{9}{4}+3\sqrt{n-1}$, that is $\sqrt{2n-4}+\sqrt{2}>\sqrt{n-1}+\frac{3}{2}$.

Subcase 2.2.2. e_m is not a cut-edge. Then by Lemma 2.1 and induction, $R(G)>R(G-\{e_m\})\geq\sqrt{n-k+2}+\frac{\sqrt{2}-2}{\sqrt{n-k+2}}+\frac{k-2}{2}$. The proof is complete. □

Since

$$\begin{aligned}\left(\sqrt{n-k+2}-\frac{2-\sqrt{2}}{\sqrt{n-k+2}}+\frac{k-2}{2}\right)' &= -\frac{1}{2\sqrt{n-k+2}}-\frac{2-\sqrt{2}}{2(n-k+2)^{3/2}}+\frac{1}{2}\\ &\geq -\frac{1}{2\sqrt{2}}-\frac{2-\sqrt{2}}{2\cdot 2^{3/2}}+\frac{1}{2}\\ &= \frac{3\sqrt{2}-4}{4\sqrt{2}}\\ &> 0,\end{aligned}$$

which means that $\sqrt{n-k+2}-\frac{2-\sqrt{2}}{\sqrt{n-k+2}}+\frac{k-2}{2}$ is increasing on k. Combining with Theorem 3.1, we can get the following result.

Theorem 3.2. *For any connected graph on $n \geq 3$ vertices with Randić index R and girth $g \geq k$,*

$$R+g \geq \sqrt{n-k+2}-\frac{2-\sqrt{2}}{\sqrt{n-k+2}}+\frac{3k-2}{2} \quad \text{and} \quad R\cdot g \geq \left(\sqrt{n-k+2}-\frac{2-\sqrt{2}}{\sqrt{n-k+2}}+\frac{k-2}{2}\right)\cdot k$$

with equalities if and only if $G \cong C_k^n$.

In fact, this result generalizes the result of Li and Liu [9] which proved Conjecture 1.2.

For the upper bound of the Randić index of connected graphs with girth g, using Lemma 2.3 we have the following theorem.

Theorem 3.3. *For any connected graph G on n vertices with Randić index R and girth $g \geq k(k \geq 3)$,*

$$R(G) \leq \frac{n}{2}$$

with equality if and only if G is regular.

Thus, combining with Theorem 3.3, we generalize Theorem 1.1 of Aouchiche et al. [1] as follows.

Theorem 3.4. *For any connected graph G on n vertices with Randić index R and girth $g \geq k$,*

$$R+g \leq \frac{3n}{2}, \qquad R\cdot g \leq \frac{n^2}{2}, \qquad R-g \geq -\frac{n}{2}, \qquad \frac{R}{g} \geq \frac{1}{2},$$

with equalities if and only if G is C_n.

$$R-g \leq \frac{n}{2}-k, \qquad \frac{R}{g} \leq \frac{n}{2k},$$

with equalities if and only if G is a regular graph with girth $g = k$.

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