Sharp bounds for the Randić index of graphs with given minimum and maximum degree

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Abstract

The Randić index of a graph G, written $R(G)$, is the sum of $\frac{1}{\sqrt{d(u)d(v)}}$ over all edges uv in $E(G)$. Let d and D be positive integers $d < D$. In this paper, we prove that if G is a graph with minimum degree d and maximum degree D, then $R(G) \geq \frac{\sqrt{dD}}{d+D}n$; equality holds only when G is an n-vertex (d, D)-biregular. Furthermore, we show that if G is an n-vertex connected graph with minimum degree d and maximum degree D, then $R(G) \leq \frac{n}{2} - \sum_{i=d}^{D-1} \frac{1}{2}\left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i+1}}\right)^2$; it is sharp for infinitely many n, and we characterize when equality holds in the bound.

1 Introduction

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

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

where for a vertex $v \in V(G)$, $d(v)$ is the degree of v. The concept was introduced by Milan Randić under the name "*branching index*" or "*connectivity index*" in 1975 [19], which has a good correlation with several physicochemical properties of alkanes. In 1998 Bollobás and Erdös [5] generalized this index by replacing $-\frac{1}{2}$ with any real number α, which is called the general Randić index. There are also many other variants of Randić index [10, 12, 18]. For more results on Randić index, see the survey papers [13, 17].

Many important mathematical properties of Randić index have been established. Especially, the relations between Randić index and other graph parameters have been widely

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studied, such as the minimum degree [5], the chromatic index [15], the diameter [10, 20], the radius [8], the average distance [8], the eigenvalues [4, 2], and the matching number [2].

In 1988, Shearer proved if G has no isolated vertices then $R(G) \geq \sqrt{|V(G)|}/2$ (see [11]). A few months later Alon improved this bound to $\sqrt{|V(G)|} - 8$ (see [11]). In 1998, Bollobás and Erdös [5] proved that the Randić index of an n-vertex graph G without isolated vertices is at least $\sqrt{n-1}$, with equality if and only if G is a star. In [11], Fajtlowicz mentioned that Bollobás and Erdös asked the minimum value for the Randić index in a graph with given minimum degree. Then the question was answered in various ways [1, 9, 16, 14].

For a graph G, we denote its complement by $\overline{G}$, which is a graph with the same vertex set of G such that two distinct vertices of $\overline{G}$ are adjacent if and only if they are not adjacent in G. We also denote by K_n the complete graph with n vertices and by $K_n - e$ the graph obtained from the complete graph K_n by deleting an edge. A graph is (a, b)-biregular if it is bipartite with the vertices of one part all having degree a and the others all having degree b.

Aouchiche et al. [3] studied the relations between Randić index and the minimum degree, the maximum degree, and the average degree, respectively. They proved that for any connected graph G on n vertices with minimum degree d and maximum degree D, then $R(G) \geq \frac{d}{d+D}n$.

In this paper, we prove that if G is an n-vertex graph with minimum degree d and maximum degree D, then $R(G) \geq \frac{\sqrt{dD}}{d+D}n$, which improves the result of Aouchiche et al. in [3]; equality holds only when G is an n-vertex (d, D)-biregular. Furthermore, we show that if G is an n-vertex connected graph with minimum degree d and maximum degree D, then $R(G) \leq \frac{n}{2} - \sum_{i=d}^{D-1} \frac{1}{2}\left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i+1}}\right)^2$; it is sharp for infinitely many n.

2 Main Results

In this section, we first give a sharp lower bound for $R(G)$ in an n-vertex graph with givien minimum and maximum degree, improving the one that Aouchiche et al. [3] proved.

Theorem 2.1. *If G is an n-vertex graph with minimum degree d and maximum degree D, then $R(G) \geq \frac{\sqrt{dD}}{d+D}n$. Equality holds only when G is an n-vertex (d, D)-biregular.*

Proof. For each $i \in \{d, \ldots, D\}$, let V_i be the set of vertices with degree i, and let $n_i = |V_i|$. Note that

$$\sum_{i=d}^{D} n_i = n. \tag{1}$$

Let $m_{ij} = |[V_i, V_j]|$ for all $i, j \in \{d, \ldots, D\}$, where $[A, B]$ is the set of edges with one end-vertex in A and the other in B. Since G has minimum degree d and maximum degree D, we have

$$R(G) = \sum_{d \leq i \leq j \leq D} \frac{m_{ij}}{\sqrt{ij}}. \tag{2}$$

For fixed i, the degree sum over all vertices in V_i can be computed by counting the edges between V_i and V_j over all $j \in \{d, \ldots, D\}$;

$$in_i = m_{ii} + \sum_{j=d}^{D} m_{ij}. \tag{3}$$

Note that m_{ii} must be counted twice.

By manipulating equation (3), we have the followings:

$$dn_d = (m_{dd} + \sum_{j=1}^{D} m_{dj}) \quad \Rightarrow \quad n_d - \frac{m_{dD}}{d} = \frac{1}{d}(m_{dd} + \sum_{j=d}^{D-1} m_{dj}) \tag{4}$$

$$Dn_D = (m_{DD} + \sum_{j=1}^{D} m_{Dj}) \quad \Rightarrow \quad n_D - \frac{m_{dD}}{D} = \frac{1}{D}(m_{DD} + \sum_{j=d+1}^{D} m_{jD}) \tag{5}$$

$$n_i = \frac{1}{i}(m_{ii} + \sum_{j=d}^{D} m_{ij}) \tag{6}$$

By equations (1) and (6), we have

$$n_d + n_D = n - \sum_{i=d+1}^{D-1} n_i = n - \sum_{i=d+1}^{D-1} \frac{1}{i}(m_{ii} + \sum_{j=d}^{D} m_{ij}). \tag{7}$$

By combining equations (4), (5), and (7), we have

$$n_d - \frac{m_{dD}}{d} + n_D - \frac{m_{dD}}{D} = n - \sum_{i=d+1}^{D-1} \frac{1}{i}(m_{ii} + \sum_{j=d}^{D} m_{ij}) - \left(\frac{d+D}{dD}\right) m_{dD}$$

$$= \frac{1}{d}(m_{dd} + \sum_{j=d}^{D-1} m_{dj}) + \frac{1}{D}(m_{DD} + \sum_{j=d+1}^{D} m_{jD}) \quad \Rightarrow$$

$$\left(\frac{d+D}{dD}\right) m_{dD} = n - \sum_{i=d+1}^{D-1} \frac{1}{i}(m_{ii} + \sum_{j=d}^{D} m_{ij}) - \frac{1}{d}(m_{dd} + \sum_{j=d}^{D-1} m_{dj}) - \frac{1}{D}(m_{DD} + \sum_{j=d+1}^{D} m_{jD})$$

$$\Rightarrow \quad m_{dD} = \frac{dD}{d+D} n - \frac{dD}{d+D} \left[-(\frac{1}{d} + \frac{1}{D}) m_{dD} + \sum_{d \le i \le j \le D} \left(\frac{1}{i} + \frac{1}{j}\right) m_{ij} \right] \tag{8}$$

which implies

$$\frac{\sqrt{dD}}{d+D} n - \frac{\sqrt{dD}}{d+D} \sum_{d \le i \le j \le D} \left[\left(\frac{1}{i} + \frac{1}{j}\right) \right] m_{ij} = 0.$$

Then we have

$$\sum_{d\le i\le j\le D}\frac{m_{ij}}{\sqrt{ij}}=\frac{\sqrt{dD}}{d+D}n+\sum_{d\le i\le j\le D}\left[\frac{1}{\sqrt{ij}}-\frac{\sqrt{dD}}{d+D}\left(\frac{1}{i}+\frac{1}{j}\right)\right]m_{ij}. \tag{9}$$

Note that except when $i=d$ and $j=D$, we have $\frac{1}{\sqrt{ij}}-\frac{\sqrt{dD}}{d+D}\left(\frac{1}{i}+\frac{1}{j}\right)>0$, since $\frac{d+D}{\sqrt{dD}}>\frac{i+j}{\sqrt{ij}}$ and $d\le i\le j\le D$. Since m_{ij} is non-negative, we have

$$R(G)\ge\frac{\sqrt{dD}}{d+D}n.$$

If there are vertices u and v such that $d(u)\neq d$ or $d(v)\neq D$, then $m_{d(u)d(v)}>0$. Thus the equality holds only when G is (d,D)-biregular. $\square$

From now, we first construct the class of graphs with mimimum degree d and maximum degree D that we will show are those achieving equality in Theorem 2.7.

Construction 2.2. Let d and D be positive integers with $d<D$, and let H be a graph with minimum degree d and maximum degree D. Suppose that for $i\in[d,D]$, $V_i(H)$ is the set of vertices with degree i in $V(H)$. Let $\mathcal{F}$ be the family of graphs H such that for $i\in[d,D-1]$, there exists only one vertex in $V_i(H)$ having exactly one neighbor in $V_{i+1}(H)$.

In Example 2.3, we show that this family is nonempty.

Example 2.3. Let d and D be odd positive integers $1\le d<D$. Suppose that

$$H_i=\begin{cases}K_1 \text{ if } d=1 \text{ and } i=1\\ \overline{P_3+\frac{i-1}{2}K_2} \text{ if } d\ge 3 \text{ and } i=d \text{ or } D\\ K_{i+1}-e \text{ if } i\in[d+1,D-1].\end{cases}$$

Note that for $i\in[d,D]$, each vertex in H_i has degree i, except for one vertex when $i=d$ or D, or two vertices when $i\in[d+1,D-1]$. For $d\le i\le D-1$, add an edge joining H_i and H_{i+1} so that for $j\in[d,D]$, every vertex in H_j in the resulting graph $F_{d,D}$ has degree j.

Recall that Caporossi et al. [7] gave another description of the Randić index by using linear programming.

Theorem 2.4. *If G is an n-vertex graph without isolated vertices, then*

$$R(G)=\frac{n}{2}-\sum_{uv\in E(G)}\frac{1}{2}\left(\frac{1}{\sqrt{d(u)}}-\frac{1}{\sqrt{d(v)}}\right)^2.$$

Lemma 2.5 shows that the graph $F_{d,D}$ is included in the family $\mathcal{F}$.

Lemma 2.5. *If the graph $F_{d,D}$ in Example 2.3 has n vertices, then*

$$R(F_{d,D}) = \frac{n}{2} - \sum_{i=d}^{D-1} \frac{1}{2} \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i+1}} \right)^2.$$

Proof. Note that there are exactly $D-d$ edges uv such that $d(u)$ and $d(v)$ are different. In fact, for such an edge uv, we have $d(v) = d(u)+1$ if $d(v) > d(u)$. By Theorem 2.4, we have the desired result. □

Observation 2.6 is used in Theorem 2.7.

Observation 2.6. *For $1 \leq x < y < z$, we have*

$$\left(\frac{1}{\sqrt{x}} - \frac{1}{\sqrt{z}} \right)^2 > \left(\frac{1}{\sqrt{x}} - \frac{1}{\sqrt{y}} \right)^2 + \left(\frac{1}{\sqrt{y}} - \frac{1}{\sqrt{z}} \right)^2.$$

Proof.

$$\left(\frac{1}{\sqrt{x}} - \frac{1}{\sqrt{z}} \right)^2 - \left(\frac{1}{\sqrt{x}} - \frac{1}{\sqrt{y}} \right)^2 - \left(\frac{1}{\sqrt{y}} - \frac{1}{\sqrt{z}} \right)^2 = 2 \left(\frac{1}{\sqrt{x}} - \frac{1}{\sqrt{y}} \right) \left(\frac{1}{\sqrt{y}} - \frac{1}{\sqrt{z}} \right) > 0.$$

□

Now, we give a sharp upper bound for $R(G)$ in an n-vertex connected graph G with given minimum and maximum degree. Note that for a regular graph G, $R(G) = \frac{|V(G)|}{2}$. Thus we assume that $d < D$ in Theorem 2.7.

Theorem 2.7. *If G is an n-vertex connected graph with minimum degree d and maximum degree D, then*

$$R(G) \leq \frac{n}{2} - \sum_{i=d}^{D-1} \frac{1}{2} \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i+1}} \right)^2.$$

Equality holds only for $G \in \mathcal{F}$.

Proof. Let V_d and V_D be the sets of vertices with degree d and D, respectively. Among paths whose one end-vertex is in V_d and the other is in V_D, consider a shortest path $P = x_0 ... x_l$, where $x_0 \in V_d$ and $x_l \in V_D$. For $i \in [0, l-1]$, if $|d(x_i) - d(x_{i+1})| \geq 2$ (say $d(x_i) < d(x_{i+1})$), then by Observation 2.6,

$$\left(\frac{1}{\sqrt{d(x_i)}} - \frac{1}{\sqrt{d(x_{i+1})}} \right)^2 > \left(\frac{1}{\sqrt{d(x_i)}} - \frac{1}{\sqrt{d(x_i)+1}} \right)^2 + \left(\frac{1}{\sqrt{d(x_i)+1}} - \frac{1}{\sqrt{d(x_{i+1})}} \right)^2$$
$$> \sum_{j=d(x_i)}^{d(x_{i+1})-1} \left(\frac{1}{\sqrt{j}} - \frac{1}{\sqrt{j+1}} \right)^2.$$

Note that for any positive integer k between d and D, there exists $i \in [0, l-1]$ such that $k \in [d(x_i), d(x_{i+1})]$, since P has end-vertices with degree d and D and is clearly connected. Thus, by Theorem 2.4, we have

$$R(G) = \frac{n}{2} - \sum_{uv \in E(G)} \frac{1}{2}\left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}}\right)^2 \leq \frac{n}{2} - \sum_{uv \in E(P)} \frac{1}{2}\left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}}\right)^2$$
$$\leq \frac{n}{2} - \sum_{i=d}^{D-1} \frac{1}{2}\left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i+1}}\right)^2.$$

Equality holds in this bound if and only if edges uv with $d(u) \neq d(v)$ are only on the path P and $d(x_{i+1}) - d(x_i) = 0$ or 1. Note that $d(x_0) = d, d(x_1) = d+1, \ldots, d(x_{l-1}) = D-1, d(x_l) = D$. Thus G must be in $\mathcal{F}$. $\square$

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