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

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May 18, 2017

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 $R(G) \geq \sqrt{dD}/d + D/n$; 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 [18], which has a good correlation with several physicochemical properties of alkanes. In 1998 Bollobás and Erdős [5] generalized this index by replacing $-\frac{1}{2}$ with any real number $\alpha$, which is called the general Randić index. There are also many other variants of Randić index [10, 12, 17]. For more results on Randić index, see the survey paper [13].

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 \([10, 19]\), 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 Erdős \([5]\) 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 Erdős 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 \(\overline{G}\). 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 \(R(G) \leq \frac{n}{2} - \sum_{i=d}^{D-1} \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{i+1}}\right)^2\); 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 given 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 $j \in \{d, \ldots, D\}$;

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

Note that $m_{ii}$ must be counted twice.

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

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

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

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

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

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

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

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

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

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

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

By plugging equation (8) into (2), we have

$$\sum_{d \leq i \leq j \leq D} \frac{m_{ij}}{\sqrt{ij}} = \frac{\sqrt{dD}}{d + D}n + \sum_{d \leq i \leq j \leq D} \left[\frac{1}{\sqrt{ij}} - \frac{\sqrt{dD}}{d + D} \left(\frac{1}{i} + \frac{1}{j}\right)\right] m_{ij}. \quad (9)$$
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 \( m_{ij} \) is non-negative, we have

\[
R(G) \geq \frac{\sqrt{dD}}{d+D} n.
\]

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.

From now, we first construct the class of graphs with minimum 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 \( 1 \leq d < D \). Suppose that

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

Note that for \( i \in [d, D] \), each vertex in \( V_i \) has degree \( i \), except for one vertex when \( i = d \) or \( D \), or two vertices when \( i \in [d+1, D-1] \). For \( d \leq i \leq D-1 \), add an edge joining \( V_i \) and \( V_{i+1} \) so that for \( j \in [d, D] \), every vertex in \( V_j \) 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.

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Observation 2.6 is used in Theorem 2.7.

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

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

**Proof.**

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

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 $P = x_0 \ldots x_l$, 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

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

$$> \frac{d(x_{i+1}) - 1}{\sqrt{d(x_i)} - \sqrt{d(x_{i+1})}}.$$

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 $\mathcal{F}$. \hfill \Box
Acknowledgements

Suil O would like to thank the Chern Institute of Mathematics, Nankai University, for their generous hospitality. He was able to carry out part of this research during his visit there. Yongtang Shi is partially supported by the Natural Science Foundation of Tianjin (No. 17JCQNJC00300) and the National Natural Science Foundation of China. The authors would like to thank Shenwei Huang for his discussion.

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