On the Randić index

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Abstract

The Randić index $R(G)$ of a graph $G = (V,E)$ is the sum of $(d(u)d(v))^{-1/2}$ over all edges $uv \in E$ of $G$. Bollobás and Erdős (Ars Combin. 50 (1998) 225) proved that the Randić index of a graph of order $n$ without isolated vertices is at least $\sqrt{n-1}$. They asked for the minimum value of $R(G)$ for graphs $G$ with given minimum degree $\delta(G)$. We answer their question for $\delta(G) = 2$ and propose a related conjecture. Furthermore, we prove a best-possible lower bound on the Randić index of a triangle-free graph $G$ with given minimum degree $\delta(G)$.

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1. Introduction

All graphs $G = (V,E)$ will be finite, undirected and simple. The degree and the neighbourhood of a vertex $u \in V$ will be denoted by $d(u)$ and $N(u)$, respectively. The minimum degree of a graph $G$ is denoted by $\delta(G)$. The graph that arises from $G$ by deleting the vertex $u \in V$ or the edge $uv \in E$ will be denoted by $G-u$ or $G-uv$, respectively. Finally, the graph $G+uv$ arises from $G$ by adding an edge $uv \notin E$ between the endpoints $u,v \in V$.

The Randić index $R(G)$ of a graph $G = (V,E)$ was introduced by the chemist Milan Randić under the name of “branching index” in 1975 [12] as the sum of $1/\sqrt{d(u)d(v)}$
over all edges $uv \in E$, i.e.

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

The term $1/\sqrt{d(u)d(v)}$ will be called the weight of the edge $uv \in E$. The Randić index is sometimes also called “Randić connectivity index” or “connectivity index” (see e.g. [13]).

Randić proposed this index in order to “quantitatively characterize the degree of molecular branching”. According to him, “the degree of branching of the molecular skeleton is a critical factor” for some molecular properties such as “boiling points of hydrocarbons and the retention volumes and the retention times obtained from chromatographic studies” (all citations are taken from [12]).

Already in 1947 Wiener [14,15] proposed the average distance of a graph for the same purpose. This parameter is somehow easier to handle theoretically and it received far more attention than the Randić index. For results and further references the reader may refer to [7,10,11] or to the recent survey article [6].

The Randić index of a graph $G$ and its average distance $\mu(G)$ are probably not independent of each other. It is conjectured [8, Conjecture 3] that they satisfy the inequality $R(G) \geq \mu(G)$ for every graph. This conjecture has been refined to $R(G) \geq \mu(G) + \sqrt{n-1} + (2/n) - 2$ in [2] where also other results and conjectures related to the Randić index can be found.

In [1] Bollobás and Erdős proved that the Randić index of a graph $G$ of order $n$ with $\delta(G) \geq 1$ is at least $\sqrt{n-1}$ with equality if and only if $G$ is a star. This statement was claimed without proof by Randić in his original paper [12]. Earlier, James Shearer and Noga Alon already gave weaker lower bounds on the Randić index (see [8]). In [8] Fajtlowicz mentions that Bollobás and Erdős asked for the minimum value of the Randić index for graphs $G$ with given minimum degree $\delta(G)$. We will answer this question for $\delta(G) = 2$ and present a conjecture about the general case.

Furthermore, we prove a best-possible lower bound on the Randić index of a triangle-free graph $G$ with arbitrary minimum degree $\delta(G)$.

**Remark.** In an earlier version of this paper [5] we proved that the Randić index of a tree is maximum for paths which was also claimed without proof by Randić in [12]. Only recently we learned from [4] that a proof of this result was already published in [16]. The reader who is interested in alternative proofs may refer to [3] and [5].

### 2. Results

Our first lemma investigates the effect of the deletion of a vertex of degree two and corresponds to Lemma 1 in [1] which did the same for a vertex of degree one.
The unique graph which arises from a complete bipartite graph $K_{\delta,n-\delta}$ by joining each pair of vertices in the part with $\delta$ vertices by a new edge will be denoted by $K^*_{\delta,n-\delta}$.

**Lemma 1.** Let $G = (V,E)$ be a graph of order $n$ with $\delta(G) = 2$ and let $v_0, v_1, v_2 \in V$ with $N(v_0) = \{v_1, v_2\}$, $v_1v_2 \in E$ and $d_1 = d(v_1)$, $d_2 = d(v_2) \geq 3$. Then

$$R(G) - R(G - v_0) \geq f(d_1, d_2)$$

for

$$f(d_1, d_2) = \frac{1}{\sqrt{2}}(\sqrt{d_1} - \sqrt{d_1 - 1}) + \frac{1}{\sqrt{2}}(\sqrt{d_2} - \sqrt{d_2 - 1})$$

$$+ \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_1}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_2}}\right)$$

$$- \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_1 - 1}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_2 - 1}}\right)$$

and we have

$$f(d_1, d_2) \geq f(n-1, n-1)$$

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

Moreover, $R(G) - R(G - v_0) = f(n-1, n-1)$ if and only if $G = K^*_2,n-2$.

**Proof.** For $i = 1,2$ let $S_i$ be the weight of the edges of $G$ incident with $v_i$ different from $v_0v_i$ and $v_iv_{3-i}$. Clearly, $S_i \leq (d_i - 2)/\sqrt{2d_i}$ for $i = 1, 2$. We will now consider the graph $G - v_0$. In this graph all edges incident with $v_i$ different from $v_iv_{3-i}$ for $i = 1, 2$ will change their weight by the factor $\sqrt{d_i/(d_i - 1)}$. Hence the total weight of these edges will be $S_i\sqrt{d_i/(d_i - 1)}$ and we have

$$R(G) - R(G - v_0)$$

$$= \frac{1}{\sqrt{2d_1}} + \frac{1}{\sqrt{2d_2}} + \frac{1}{\sqrt{d_1d_2}} + S_1 + S_2$$

$$- \frac{1}{\sqrt{(d_1 - 1)(d_2 - 1)}} - S_1\sqrt{\frac{d_1}{d_1 - 1}} - S_2\sqrt{\frac{d_2}{d_2 - 1}}$$

$$\geq \frac{1}{\sqrt{2d_1}} + \frac{1}{\sqrt{2d_2}} + \frac{1}{\sqrt{d_1d_2}} - \frac{1}{\sqrt{(d_1 - 1)(d_2 - 1)}}$$

$$+ d_1 - 2 \sqrt{\frac{d_1}{d_1 - 1}} + d_2 - 2 \sqrt{\frac{d_2}{d_2 - 1}}$$

$$+ \frac{1}{\sqrt{2d_1}} \left(1 - \sqrt{\frac{d_1}{d_1 - 1}}\right) + \frac{1}{\sqrt{2d_2}} \left(1 - \sqrt{\frac{d_2}{d_2 - 1}}\right).$$
\[
\begin{align*}
&= \frac{1}{\sqrt{2}} (\sqrt{d_1} - \sqrt{d_1 - 1}) + \frac{1}{\sqrt{2}} (\sqrt{d_2} - \sqrt{d_2 - 1}) \\
&\quad + \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_1}} \right) \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_2}} \right) - \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_1 - 1}} \right) \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_2 - 1}} \right).
\end{align*}
\]

Now, to show that \( f(d_1, d_2) \) for \( d_1, d_2 \in [3, n - 1] \) attains its minimum value for \( d_1 = d_2 = n - 1 \), we consider some partial derivatives.

\[
\frac{\partial}{\partial d_1} f(d_1, d_2) = \frac{1}{\sqrt{2}} \left( \frac{1}{2\sqrt{d_1}} - \frac{1}{2\sqrt{d_1 - 1}} \right) + \frac{1}{2\sqrt{d_1^3}} \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_2}} \right)
\]
\[
- \frac{1}{2\sqrt{(d_1 - 1)^3}} \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_2 - 1}} \right),
\]

\[
\frac{\partial}{\partial d_2} \frac{\partial}{\partial d_1} f(d_1, d_2) = \frac{1}{4} \left( \frac{1}{\sqrt{(d_1d_2)^3}} - \frac{1}{\sqrt{(d_1 - 1)(d_2 - 1))^3}} \right).
\]

Since \( (\partial/\partial d_2)(\partial/\partial d_1) f(d_1, d_2) < 0 \) for \( d_1, d_2 \geq 3 \), we have

\[
\frac{\partial}{\partial d_1} f(d_1, d_2) < \frac{\partial}{\partial d_1} f(d_1, 3) = \frac{1}{\sqrt{2}} \left( \frac{1}{2\sqrt{d_1}} - \frac{1}{2\sqrt{d_1 - 1}} \right)
\]
\[
+ \frac{1}{2\sqrt{d_1^3}} \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right).
\]

We leave it to the reader to check that the last expression is negative for \( d_1 \geq 3 \) and hence, by symmetry, \( (\partial/\partial d_1)(\partial/\partial d_2) f(d_1, d_2) < 0 \) for \( d_1, d_2 \geq 3 \) which implies \( f(d_1, d_2) \geq f(n - 1, n - 1) \) and the proof is complete.

The equality \( R(G) - R(G - v_0) = f(n - 1, n - 1) \) holds if and only if equality holds throughout the above inequalities, that is if and only if \( S_i = (d_i - 2)/\sqrt{2d_i} \) and \( d_i = n - 1 \) for \( i = 1, 2 \). The graph \( G \) is then \( K^*_2, n-2 \). \( \square \)

We cite the next lemma from [1] as we need it in the proof of our main result.

**Lemma 2** (Bollobás and Erdős [1]). Let \( x_1, x_2 \) be an edge of maximal weight in a graph \( G \). Then

\[ R(G - x_1, x_2) < R(G). \]

For \( x \geq 3 \) we define the following function and make some observations about its behaviour.

\[ r(x) := \sqrt{2(x - 1)} + \frac{1}{x - 1} - \frac{\sqrt{2}}{\sqrt{x - 1}}. \]
**Theorem 1.** Let $G = (V, E)$ be a graph of order $n$ with $\delta(G) \geq 2$. Then

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

with equality if and only if $G = K_{2, n-2}^*$.

**Proof.** We assume that $G$ is a counterexample of minimal order for which $R(G)$ is minimal. It is easy to verify that $n \geq 6$ (see Fig. 1). If $\delta(G) > 2$, then, by Lemma 2, the deletion of an edge of maximal weight yields a graph $G'$ of minimum degree at least 2 and with $R(G') < R(G)$, thus contradicting the choice of $G$. Hence $\delta(G) = 2$.

**Claim 1.** There is no vertex $x \in V$ of degree 2 with $N(x) = \{y, z\}$ such that $yz \notin E$. 

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**Lemma 3.** (i) For $x \geq 3$ the function $r(x)$ is concave, i.e. $(d/dx)^2 r(x) < 0$.

(ii) For $x \geq 6$ the functions $r(x) - r(x-2)$ and $r(x) - r(x-3)$ are monotonously decreasing in $x$.

(iii) $\sqrt{2(x-2)} > r(x)$ for $x \geq 4$.

**Proof.** (i) We have

$$
\left(\frac{d}{dx}\right)^2 r(x) = -\frac{1}{2\sqrt{2}(\sqrt{x-1})^3} + \frac{2}{(x-1)^3} - \frac{3}{2\sqrt{2}(\sqrt{x-1})^5}
$$

$$
= \frac{1}{2\sqrt{2}(x-1)^3}(-1 + 3\sqrt{x-1} + 4\sqrt{2} - 3\sqrt{x-1}).
$$

For $x \geq 3$, $(x-1)\sqrt{x-1} + 3\sqrt{x-1} \geq 5\sqrt{2} > 4\sqrt{2}$ and hence $(d/dx)^2 r(x) < 0$.

(ii) Follows from (i).

(iii) The simple proof is left to the reader. \(\square\)
Proof. The graph $G' = G - x + yz$ is no counterexample and for $d_1 = d(y) \leq n - 2$ and $d_2 = d(z) \leq n - 2$ we have, by Lemma 3(iii),

$$R(G) = R(G') - \frac{1}{\sqrt{d_1d_2}} + \frac{1}{\sqrt{2d_1}} + \frac{1}{\sqrt{2d_2}}$$

$$\geq r(n-1) - \frac{1}{\sqrt{d_1d_2}} + \frac{1}{\sqrt{2d_1}} + \frac{1}{\sqrt{2d_2}}$$

$$\geq r(n-1) - \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_1}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_2}}\right) + \frac{1}{2}$$

$$\geq r(n-1) - \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{n-2}}\right)^2 + \frac{1}{2}$$

$$= \sqrt{2(n-2)} > r(n)$$

which is a contradiction.

Claim 2. There are no two adjacent vertices $x_1, x_2$ of degree 2 with a common neighbour $y$.

Proof. We have $2 \leq d = d(y) \leq n - 1$. If $d = 2$, then the graph $G' = G - x_1 - x_2 - y$ is no counterexample and we have

$$R(G) = R(G') + \frac{3}{2} \geq r(n-3) + \frac{3}{2} > r(n).$$

The last inequality follows by Lemma 3(ii), since $r(6) - r(3) < \frac{3}{2}$.

Next, we assume that $d \geq 4$. Let $S$ be the weight of the edges incident with $y$ different from $x_1y$ and $x_2y$. We have $S \leq (d - 2)/\sqrt{2d}$. The graph $G' = G - x_1 - x_2$ is no counterexample and we have

$$R(G) = R(G') + S - S\sqrt{\frac{d}{d-2}} + \frac{1}{2} + \frac{\sqrt{2}}{\sqrt{d}}$$

$$\geq r(n-2) + \frac{d-2}{\sqrt{2d}} \left(1 - \sqrt{\frac{d}{d-2}}\right) + \frac{1}{2} + \frac{\sqrt{2}}{\sqrt{d}}$$

$$= r(n-2) + \frac{d-2}{\sqrt{2d}} - \frac{\sqrt{d-2}}{\sqrt{2}} + \frac{1}{2} + \frac{\sqrt{2}}{\sqrt{d}}$$

$$= r(n-2) + \frac{\sqrt{d}}{\sqrt{2}} - \frac{\sqrt{d-2}}{\sqrt{2}} + \frac{1}{2}$$

$$\geq r(n-2) + \frac{\sqrt{n-1}}{\sqrt{2}} - \frac{\sqrt{n-3}}{\sqrt{2}} + \frac{1}{2} > r(n).$$
Since \( r(11) - r(9) < \frac{1}{2} \), the last inequality follows for \( n \geq 11 \) by Lemma 3(ii). For \( 6 \leq n \leq 10 \) it can be checked by evaluation.

Now, we assume that \( d = 3 \) and that \( z \) is the neighbour of \( y \) different from \( x_1 \) and \( x_2 \). If \( d' = d(z) \geq 3 \), then \( G' = G - x_1 - x_2 - y \) is no counterexample. Let \( S' \) be the weight of the edges incident with \( z \) different from \( yz \). We have \( S' \leq (d' - 1)/\sqrt{2d'} \) and

\[
R(G) = R(G') + S' - S'\sqrt{\frac{d'}{d' - 1}} + \frac{1}{2} + \frac{\sqrt{2}}{\sqrt{3}} + \frac{1}{\sqrt{3d'}}
\]

\[
\geq r(n - 3) + \frac{\sqrt{d'}}{\sqrt{2}} - \frac{\sqrt{d' - 1}}{\sqrt{2}} + \frac{1}{2} + \frac{\sqrt{2}}{\sqrt{3}} - \frac{1}{\sqrt{3d'}} \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)
\]

\[
\geq r(n - 3) + \frac{1}{2} + \frac{\sqrt{2}}{\sqrt{3}} - \frac{1}{\sqrt{3}} \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right) \geq r(n).
\]

The last inequality follows by Lemma 3(ii), since \( r(6) - r(3) < \frac{1}{2} + \frac{\sqrt{2}}{\sqrt{3}} - \frac{1}{\sqrt{3}} \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right) \).

Finally, if \( d' = 2 \), then let \( u \) be the neighbour of \( z \) different from \( y \). By Claim 1, \( d(u) \geq 3 \) and once again a similar reasoning as above for the graph \( G' = G - x_1 - x_2 - y - z \) yields \( R(G) > r(n) \). Hence, all cases lead to a contradiction and the proof of the claim is complete. \( \square \)

Now let \( v_0 \in V \) be a vertex of degree 2 with the adjacent neighbours \( v_1, v_2 \in V \). By Claim 2, we have \( d(v_1), d(v_2) \geq 3 \). The application of Lemma 1 yields now

\[
R(G) \geq R(G - v_0) + \sqrt{2(n - 1)} - \sqrt{2(n - 2)} - \frac{\sqrt{2}}{\sqrt{n - 1}} + \frac{1}{n - 1}
\]

\[
+ \frac{\sqrt{2}}{\sqrt{n - 2}} - \frac{1}{n - 2}
\]

\[
\geq r(n - 1) + \sqrt{2(n - 1)} - \sqrt{2(n - 2)} - \frac{\sqrt{2}}{\sqrt{n - 1}} + \frac{1}{n - 1}
\]

\[
+ \frac{\sqrt{2}}{\sqrt{n - 2}} - \frac{1}{n - 2}
\]

\[
= r(n).
\]

Equality \( R(G) = r(n) \) implies that equality holds in the inequality coming from Lemma 1, that is \( G \) is the complete split graph \( K_{2,n-2}^* \). Conversely, it is immediate to check that \( R(K_{2,n-2}^*) = r(n) \). \( \square \)

We believe that Theorem 1 generalizes to larger minimum degrees in the obvious way and pose the following conjecture.
Conjecture 1. Let $G = (V,E)$ be a graph of order $n$ with $\delta(G) \geq \delta$. Then

$$R(G) \geq \frac{\delta(n - \delta)}{\sqrt{\delta(n - 1)}} + \left( \frac{\delta}{2} \right) \frac{1}{n - 1}$$

with equality if and only if $G = K_{\delta,n-\delta}$. 

The main obstacle to prove this conjecture is the fact that the case analysis we made in the proofs of Claims 1 and 2 during the proof of Theorem 1 becomes more and more intricate for $\delta \geq 3$.

Nevertheless, if the graph $G$ is triangle-free, then the calculation becomes much simpler and we can get a bound on $R(G)$ in terms of $\delta$ by a similar method as in Theorem 1. First, Lemma 1 is replaced by the following one.

Lemma 4. Let $G$ be a triangle-free graph of order $n$ with $\delta(G) = \delta \geq 1$ and let $v_0$ be a vertex of degree $\delta$. Then

$$R(G) - R(G - v_0) \geq \frac{\sqrt{\delta(n - \delta)}}{\sqrt{\delta(n - 1)}} - \frac{\sqrt{\delta(n - \delta - 1)}}{\sqrt{\delta(n - 1)}}.$$

Proof. Let $N(v_0) = \{v_1, v_2, \ldots, v_\delta\}$. Since $G$ is triangle-free, no edge $v_iv_j$ belongs to $G$. Using the same notation as in Lemma 1, we have $S_i \leq (d_i - 1)/\sqrt{\delta d_i}$ for $1 \leq i \leq \delta$, since each of the $d_i - 1$ neighbours of $v_i$ different from $v_0$ has degree at least $\delta$. Therefore

$$R(G) - R(G - v_0) = \sum_{i=1}^{\delta} \left( \frac{1}{\sqrt{\delta d_i}} - S_i \left( \frac{d_i}{d_i - 1} - 1 \right) \right)$$

$$\geq \sum_{i=1}^{\delta} \left( \frac{1}{\sqrt{\delta d_i}} - \frac{d_i - 1}{\sqrt{\delta d_i}} \left( \frac{d_i}{d_i - 1} - 1 \right) \right)$$

$$\geq \sum_{i=1}^{\delta} \left( \frac{1}{\sqrt{\delta d_i}} - \sqrt{\frac{d_i - 1}{\delta}} + \sqrt{\frac{d_i}{\delta}} - \frac{1}{\sqrt{\delta d_i}} \right)$$

$$\geq \frac{1}{\sqrt{\delta}} \sum_{i=1}^{\delta} g(d_i)$$

with $g(x) = \sqrt{x} - \sqrt{x - 1}$. Since the function $g$ is decreasing for $x \geq 1$ and since $d_i \leq n - \delta$ for $1 \leq i \leq \delta$, this gives $R(G) - R(G - v_0) \geq \sqrt{\delta g(n - \delta)}$ and thus

$$R(G) - R(G - v_0) \geq \frac{\sqrt{\delta(n - \delta)}}{\sqrt{\delta(n - 1)}} - \frac{\sqrt{\delta(n - \delta - 1)}}{\sqrt{\delta(n - 1)}}.$$

The equality $R(G) - R(G - v_0) = \sqrt{\delta(n - \delta)} - \sqrt{\delta(n - \delta - 1)}$ holds if and only if $S_i = (d_i - 1)/\sqrt{\delta d_i}$ and $d_i = n - \delta$ for $1 \leq i \leq \delta$. In this case, all the vertices of $V \setminus \{v_0, v_1, \ldots, v_\delta\}$ are adjacent to every vertex $v_i$ for $1 \leq i \leq \delta$ and have degree $\delta$. Hence the graph $G$ is the complete bipartite graph $K_{\delta,n-\delta}$. \qed
Theorem 2. Let \( G = (V, E) \) be a triangle-free graph of order \( n \) with \( \delta(G) \geq \delta \geq 1 \). Then

\[
R(G) \geq \sqrt{\delta(n - \delta)}
\]

with equality if and only if \( G = K_{\delta, n - \delta} \).

Proof. As in the proof of Theorem 1, we assume that \( G \) is a counterexample of minimum order for which \( R(G) \) is minimum, which implies \( \delta(G) = \delta \). Let \( v_0 \in V \) be a vertex of degree \( \delta \) with mutually non-adjacent neighbours \( v_1, v_2, \ldots, v_\delta \). By Lemma 4, we have

\[
R(G) \geq R(G - v_0) + \sqrt{\delta(n - \delta - \sqrt{n - \delta - 1})}
\]

\[
\geq \sqrt{\delta(n - \delta - 1) + \sqrt{\delta(n - \delta - \sqrt{n - \delta - 1})}}
\]

\[
\geq \sqrt{\delta(n - \delta)}.
\]

If the equality \( R(G) = \sqrt{\delta(n - \delta)} \) holds, then the graph \( G \) satisfies the equality in Lemma 4 and thus \( G = K_{\delta, n - \delta} \). Conversely, it is obvious that \( R(K_{\delta, n - \delta}) = \sqrt{\delta(n - \delta)} \). \( \square \)

Note that another lower bound on the Randić index in triangle-free graphs was already known, namely \( R(G) \geq \sqrt{m} \) where \( m \) is the number of edges of \( G \) [9, Corollary 2.12]. The two bounds are not comparable.

References