

A proof for a conjecture on the Randić index of graphs with diameter[☆]

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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 . Aouchiche et al. proposed a conjecture on the relationship between the Randić index and the diameter: for any connected graph on $n \geq 3$ vertices with the Randić index $R(G)$ and the diameter $D(G)$, $R(G) - D(G) \geq \sqrt{2} - \frac{n+1}{2}$ and $\frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}$, with equalities if and only if G is a path. In this work, we show that this conjecture is true for trees. Furthermore, we prove that for any connected graph on $n \geq 3$ vertices with the Randić index $R(G)$ and the diameter $D(G)$, $R(G) - D(G) \geq \sqrt{2} - \frac{n+1}{2}$, with equality if and only if G is a path.

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1. Introduction

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

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

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 [1] in 1975, as suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. It is well correlated with a variety of physico-chemical properties of alkanes. And it is one of the most popular molecular descriptors, to which three books [2–4] are devoted.

In this work, we only consider finite, undirected and simple graphs. The degree $d(u)$ of a vertex u is the number of edges incident to it. The minimum degree of vertices in G is denoted by $\delta(G)$. A *pendant* vertex (or *leaf*) is a vertex of degree 1. An edge incident with a leaf is called a *pendant edge*. If $S \subseteq V(G)$, then $G - S = G[V - S]$ is the subgraph of G obtained by deleting the vertices in S and all edges incident with them. Similarly, if $E' \subseteq E(G)$, then $G - E' = (V(G), E(G) - E')$. If $|G| > 1$ and $G - E'$ is connected for every set $E' \subseteq E$ of fewer than ℓ edges, then G is called ℓ -*edge-connected*. The greatest integer ℓ such that G is ℓ -*edge-connected* is the *edge-connectivity* $\lambda(G)$ of G . The distance between two vertices u and v in graph G , denoted by $d_G(u, v)$ (or $d(u, v)$ for short), is the length of a shortest path connecting u and v in G . The diameter $D(G)$ of G is the maximum distance $d(u, v)$ over all pairs of vertices u and v of G . The weight of an edge $uv \in E(G)$ is defined as $\frac{1}{\sqrt{d(u)d(v)}}$. For undefined terminology and notation we refer the reader to [5].

There are many results on the relationships between the Randić index and some other graph invariants, such as the minimum degree [6–8], chromatic number [9,10], radius [11], girth [12,13] and so on [14]. In this work, we will consider the relationship between the Randić index and the diameter.

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In [15], Aouchiche, Hansen and Zheng proposed the following conjecture:

Conjecture 1.1 ([15]). For any connected graph on $n \geq 3$ vertices with the Randić index $R(G)$ and the diameter $D(G)$, we have

$$R(G) - D(G) \geq \sqrt{2} - \frac{n+1}{2} \quad \text{and} \quad \frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2},$$

with equalities if and only if G is a path, namely $G \cong P_n$.

Zhang and Liu [16] showed that the above conjecture is true for unicyclic graphs. Li and Shi [17] showed if the minimum degree $\delta(G) \geq 5$, then $R(G) - D(G) \geq \sqrt{2} - \frac{n+1}{2}$; if $\delta(G) \geq \frac{n}{5}$ and $n \geq 15$, $\frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}$. Furthermore, for any arbitrary real number ϵ ($0 < \epsilon < 1$), if $\delta(G) \geq \epsilon n$, then $\frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}$ holds for sufficiently large n .

In this work, we prove that for any connected n -vertex graph G with the Randić index $R(G)$ and the diameter $D(G)$, $R(G) - D(G) \geq \sqrt{2} - \frac{n+1}{2}$, with equality if and only if $G \cong P_n$.

2. Some lemmas

In this section, we give some lemmas which will be used in the sequel.

Lemma 2.1 ([18]). Let x_1x_2 be a pendent edge of a graph G with n vertices and $d(x_2) = 1$; then

$$R(G) - R(G - x_1x_2) \geq \sqrt{d(x_1)} - \sqrt{d(x_1) - 1} \geq \sqrt{n-1} - \sqrt{n-2} > 0.$$

Lemma 2.2 ([18]). Let x_1x_2 be an edge of maximum weight in a graph G . Then

$$R(G) - R(G - x_1x_2) > 0.$$

Remark 2.3. From Lemmas 2.1 and 2.2, on deleting pendent vertices or edges with maximum weight step by step, the Randić index of the resultant graph will get smaller and smaller.

Lemma 2.4 ([18]). Let G be a connected graph with n vertices. Then

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

Here, we generalize Lemma 2.2 to the following one:

Lemma 2.5. Let x_1x_2 be an edge of maximum weight in its neighborhood in a graph G , i.e., for any edge x_iy ($i = 1$ or 2), $\frac{1}{\sqrt{d(x_1)d(x_2)}} \geq \frac{1}{\sqrt{d(x_i)d(y)}}$. Then

$$R(G) - R(G - x_1x_2) > 0.$$

Proof. For $i = 1, 2$, set $d(x_i) = d_i$ and denote by S_i the sum of the weights of the edges incident to x_i , except for the edge x_1x_2 . If $\min\{d_1, d_2\} = 1$, then by Lemma 2.1 we are done. Otherwise, $S_i \leq (d_i - 1)/\sqrt{d_1d_2}$ and, therefore,

$$\begin{aligned} R(G) - R(G - x_1x_2) &= \frac{1}{\sqrt{d_1d_2}} + S_1 + S_2 - S_1\sqrt{\frac{d_1}{d_1-1}} - S_2\sqrt{\frac{d_2}{d_2-1}} \\ &\geq \frac{1}{\sqrt{d_1d_2}} \left[1 + (d_1 - 1) \left(1 - \sqrt{\frac{d_1}{d_1-1}} \right) + (d_2 - 1) \left(1 - \sqrt{\frac{d_2}{d_2-1}} \right) \right] \\ &= \frac{1}{\sqrt{d_1d_2}} \left[d_1 - \frac{1}{2} - \sqrt{d_1(d_1-1)} + d_2 - \frac{1}{2} - \sqrt{d_2(d_2-1)} \right] > 0. \quad \square \end{aligned}$$

Now, we consider graphs with pendent vertices.

Lemma 2.6. Let w be a pendent vertex of a connected graph G and uv be the edge of maximum weight in $G - w$; then

$$R(G) > R(G - uv).$$

Proof. First, we have $R(G) > R(G - w) > R(G - w - uv)$ by Lemmas 2.1 and 2.2. If $\min\{d(u), d(v)\} = 1$, we can get our result by Lemma 2.1. Now, suppose that $\min\{d(u), d(v)\} \geq 2$. Assume $wz \in E(G)$. If $z \notin \{u, v\}$, then uv has maximum weight in its neighborhood and $R(G) > R(G - uv)$ there, by Lemma 2.5. Thus, we assume that $z = u$ without loss of generality.

If $R(G) \leq R(G-uv)$, then $R(G-uv) \geq R(G) > R(G-w) > R(G-w-uv)$, i.e. $R(G-uv) - R(G-w-uv) > R(G) - R(G-w)$, which gives

$$\begin{aligned} & \frac{1}{\sqrt{d(u)-1}} + \sum_{x \sim u, x \neq \{v,w\}} \frac{1}{\sqrt{d(x)}} \left(\frac{1}{\sqrt{d(u)-1}} - \frac{1}{\sqrt{d(u)-2}} \right) \\ & > \frac{1}{\sqrt{d(u)}} + \frac{1}{\sqrt{d(v)}} \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(u)-1}} \right) + \sum_{x \sim u, x \neq \{v,w\}} \frac{1}{\sqrt{d(x)}} \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(u)-1}} \right), \end{aligned}$$

where $x \sim u$ means that x is incident to u in G . Thus

$$\left(\frac{1}{\sqrt{d(v)}} - 1 \right) \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(u)-1}} \right) + \sum_{x \sim u, x \neq \{v,w\}} \frac{1}{\sqrt{d(x)}} \left(\frac{1}{\sqrt{d(u)}} + \frac{1}{\sqrt{d(u)-2}} - \frac{2}{\sqrt{d(u)-1}} \right) < 0.$$

However, $\frac{1}{\sqrt{x}} + \frac{1}{\sqrt{x-2}} - \frac{2}{\sqrt{x-1}} > 0$ for $x \geq 3$ because $x(x-2)(x-1)^2 - (x^2-2x-1)^2 = 3(x-1)^2 - 4 > 0$ for $x \geq 3$, that is $x(x-2)(x-1)^2 > (x^2-2x-1)^2$, namely, $x^2-2x+1+(x-1)\sqrt{x(x-2)} > 2x^2-4x$; then $(x-1)[(x-1)+\sqrt{x(x-2)}] > 2x(x-2)$, that is to say $(x-1)[2(x-1)+2\sqrt{x(x-2)}] > 4x(x-2)$, and thus $\sqrt{x-1}[\sqrt{x}+\sqrt{x-2}] > 2\sqrt{x(x-2)}$, so we have $\frac{1}{\sqrt{x}} + \frac{1}{\sqrt{x-2}} - \frac{2}{\sqrt{x-1}} > 0$. And it is easy to see that $\left(\frac{1}{\sqrt{d(v)}} - 1 \right) \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(u)-1}} \right) > 0$.

Therefore, $\left(\frac{1}{\sqrt{d(v)}} - 1 \right) \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(u)-1}} \right) + \sum_{x \sim u, x \neq \{v,w\}} \frac{1}{\sqrt{d(x)}} \left(\frac{1}{\sqrt{d(u)}} + \frac{1}{\sqrt{d(u)-2}} - \frac{2}{\sqrt{d(u)-1}} \right) > 0$, which is a contradiction. Note that if $d(u) = 2$, the second summand on the left in the above inequality does not exist; hence we get $\left(\frac{1}{\sqrt{d(v)}} - 1 \right) \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(u)-1}} \right) > 0$, which again is a contradiction. The proof is complete. \square

Lemma 2.7. Let w, z be two pendent vertices in a connected graph G such that $d(w, z) \geq 4$ and uv is the edge with maximum weight in $G - w - z$; then

$$R(G) > R(G - uv).$$

Proof. First, we have $R(G) > R(G-w-z) > R(G-w-z-uv)$ by Lemmas 2.1 and 2.2. If $\min\{d(u), d(v)\} = 1$, we get our result by Lemma 2.1. Suppose now that $\min\{d(u), d(v)\} \geq 2$. Suppose $wx, zy \in E(G)$. If $x, y \notin \{u, v\}$, then $R(G) > R(G-uv)$ by Lemma 2.5. Otherwise, since $d(u, v) \geq 4$, we assume that $x = u$ and $v \notin \{x, y\}$ without loss of generality. Now, we can see that uv has maximum weight in its neighborhood in $G - w$; then $R(G-w) > R(G-w-uv)$ by Lemma 2.5.

If $R(G) \leq R(G-uv)$, then $R(G-uv) \geq R(G) > R(G-w) > R(G-w-uv)$, i.e. $R(G-uv) - R(G-w-uv) > R(G) - R(G-w)$; then $\left(\frac{1}{\sqrt{d(v)}} - 1 \right) \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(u)-1}} \right) + \sum_{x \sim u, x \neq \{v,w\}} \frac{1}{\sqrt{d(x)}} \left(\frac{1}{\sqrt{d(u)}} + \frac{1}{\sqrt{d(u)-2}} - \frac{2}{\sqrt{d(u)-1}} \right) < 0$. From the proof of Lemma 2.6, we also have $\left(\frac{1}{\sqrt{d(v)}} - 1 \right) \left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(u)-1}} \right) + \sum_{x \sim u, x \neq \{v,w\}} \frac{1}{\sqrt{d(x)}} \left(\frac{1}{\sqrt{d(u)}} + \frac{1}{\sqrt{d(u)-2}} - \frac{2}{\sqrt{d(u)-1}} \right) > 0$, which is a contradiction. The proof is finished. \square

3. Main results

In this section, we give our main results concerning Conjecture 1.1. First, we show that Conjecture 1.1 is true for trees.

Theorem 3.1. For any tree T on $n \geq 3$ vertices with the Randić index $R(T)$ and the diameter $D(T)$, we have

$$R(T) - D(T) \geq \sqrt{2} - \frac{n+1}{2} \quad \text{and} \quad \frac{R(T)}{D(T)} \geq \frac{n-3+2\sqrt{2}}{2n-2},$$

with equalities if and only if $T \cong P_n$.

Proof. If T is a path, we have $R(T) = \sqrt{2} + \frac{n-1}{2}$ and $D(T) = n - 1$. It is obvious that both equalities hold. Now we assume that T is not a path; then $D(T) \leq n - 2$ and there are at least three pendent vertices in T . Assume $P = u_0u_1 \cdots u_D$ to be the longest path in T . Then at least one pendent vertex, say v_1 , is not contained in P . Now we start an operation on T , i.e., we continually delete pendent vertices which are not contained in P until the resulting tree is P . Assume v_1, \dots, v_k are the vertices in the order they were deleted, we have $R(T) > R(T - v_1) > \cdots > R\left(T - \bigcup_{i=1}^k v_i\right) = R(P) = \sqrt{2} + \frac{D-2}{2}$ by Lemma 2.1 and $D(T) = D(T - v_1) = \cdots = D\left(T - \bigcup_{i=1}^k v_i\right) = D$. Thus, we have $R(T) - D(T) > R(P) - D(P) = \sqrt{2} - \frac{D+2}{2} \geq \sqrt{2} - \frac{n}{2} > \sqrt{2} - \frac{n+1}{2}$ and $\frac{R(T)}{D(T)} > \frac{R(P)}{D(P)} = \frac{\sqrt{2} - \frac{D+2}{2}}{D} = \frac{\sqrt{2}-1}{D} - \frac{1}{2} \geq \frac{\sqrt{2}-1}{n-2} - \frac{1}{2} > \frac{n-3+2\sqrt{2}}{2n-2}$. The proof is complete. \square

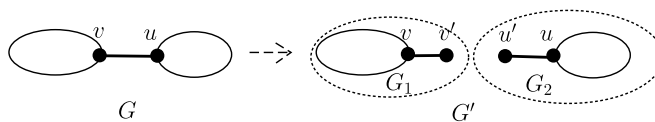


Fig. 3.1. Graphs G and G' in Case 1.

Now, we come to our main result:

Theorem 3.2. For any connected graph G on $n \geq 3$ vertices with the Randić index $R(G)$ and the diameter $D(G)$, we have

$$R(G) - D(G) \geq \sqrt{2} - \frac{n+1}{2}, \tag{3.2}$$

with equality if and only if $G \cong P_n$.

Proof. If G is a path, we have $R(G) = \sqrt{2} + \frac{n-1}{2}$ and $D(G) = n - 1$. It is obvious that the equality holds.

Now, we assume that G is a connected graph with cycle(s), since if G is a tree, the correctness of the result is given by Theorem 3.1. To prove the main assertion of the theorem we apply induction on $n + m$, where m is the number of edges of G and $m \geq n$. It is elementary to check that the assertion holds for $n = 2, 3, 4$, so let us assume that $n \geq 5$ and that the result holds for smaller values of $n + m$.

If $\lambda(G) \geq 2$, let $e = uv$ be the edge with maximum weight in G ; then $G - e$ is connected. It is easy to see that $R(G) > R(G - e)$ by Lemma 2.2 and $D(G) \leq D(G - e)$. Therefore, by induction we have $R(G) - D(G) > R(G - e) - D(G - e) \geq \sqrt{2} - \frac{n+1}{2}$.

If $\lambda(G) = 1$, we divide our proof into two cases, i.e., case 1: there is a cut-edge of G which is not a pendent edge; case 2: every cut-edge of G is a pendent edge.

Case 1: There exists a cut-edge which is not a pendent edge.

Assume $e = uv$ to be a cut-edge which is not a pendent edge of G . Let $G' = G - uv + vv' + uu'$, where v' and u' are new added vertices (see Fig. 3.1). Let G_1 be the component that contains v and G_2 the component that contains u in G' ; then $D(G_1) + D(G_2) \geq D(G) + 1$. Denote by n_i and m_i the number of vertices and edges of G_i for $i = 1, 2$, respectively. We have $n_1 + n_2 = n + 2$ and $n_i + m_i < n + m$ ($i = 1, 2$).

By induction, we have

$$\begin{aligned} R(G) - D(G) &= R(G') + \frac{1}{\sqrt{d(u)d(v)}} - \frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} - D(G) \\ &= R(G_1) + R(G_2) - D(G) + \frac{1}{\sqrt{d(u)d(v)}} - \frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} \\ &\geq R(G_1) + R(G_2) - (D(G_1) + D(G_2) - 1) + \frac{1}{\sqrt{d(u)d(v)}} - \frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} \\ &= R(G_1) - D(G_1) + R(G_2) - D(G_2) + 1 + \frac{1}{\sqrt{d(u)d(v)}} - \frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} \\ &> \sqrt{2} - \frac{n_1 + 1}{2} + \sqrt{2} - \frac{n_2 + 1}{2} + 1 + \frac{1}{\sqrt{d(u)d(v)}} - \frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} \end{aligned} \tag{3.3}$$

$$\begin{aligned} &= \sqrt{2} - \frac{n+1}{2} + \sqrt{2} - \frac{1}{2} + \frac{1}{\sqrt{d(u)d(v)}} - \frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} \\ &\geq \sqrt{2} - \frac{n+1}{2} + \sqrt{2} - \frac{1}{2} + \frac{1}{\sqrt{4}} - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \\ &= \sqrt{2} - \frac{n+1}{2}, \end{aligned} \tag{3.4}$$

where (3.3) holds because of induction and at least one of $\{G_1, G_2\}$ has cycle(s) since G has cycle(s). The reason why the last inequality (3.4) holds is as follows. Let $h(x, y) = \frac{1}{\sqrt{xy}} - \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{y}}$, $x \geq 2, y \geq 2$; then we have $\frac{\partial h(x, y)}{\partial x} = (\sqrt{y} - 1)/(2x\sqrt{xy}) > 0$, $\frac{\partial h(x, y)}{\partial y} = (\sqrt{x} - 1)/(2y\sqrt{xy}) > 0$. Therefore $h(x, y)$ is nondecreasing on x and y respectively. Thus, the proof is complete for Case 1.

Case 2. Every cut-edge of G is a pendent edge.

Let V_1 be the vertex set of pendent vertices. If $|V_1| \geq 3$, there exists a pendent vertex, namely, $v_0 \in V_1$, such that $D(G) = D(G - v_0)$. Then $R(G) - D(G) > R(G - v_0) - D(G - v_0) \geq \sqrt{2} - \frac{n}{2} > \sqrt{2} - \frac{n+1}{2}$ by induction and Lemma 2.1.

If $|V_1| = 1$, suppose $u \in V_1, uw \in E(G)$ and let $G' = G - u$ (see Fig. 3.2). It is easy to see that $\lambda(G') \geq 2$. Let xy be the edge with the maximum weight in G' ; then by Lemma 2.6, we have $R(G) > R(G - xy)$ and $D(G) \leq D(G - xy)$. By induction, we have $R(G) - D(G) > R(G - xy) - D(G - xy) \geq \sqrt{2} - \frac{n+1}{2}$.



Fig. 3.2. Graphs G and G' in the case when $|V_1| = 1$.

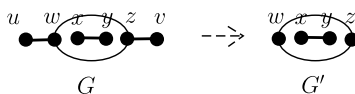


Fig. 3.3. Graphs G and G' in the case when $|V_1| = 2$.

If $|V_1| = 2$, suppose $u, v \in V_1$, $uw, vz \in E(G)$. If $w = z$, then $R(G) > R(G - u)$ and $D(G) = D(G - u)$. By induction, we have $R(G) - D(G) > R(G - u) - D(G - u) \geq \sqrt{2} - \frac{n}{2} > \sqrt{2} - \frac{n+1}{2}$.

Suppose now $w \neq z$. If $d(u, v) = 3$, then either $D(G) = 3$ or at least one of $\{u, v\}$, assumed to be u without loss of generality, is such that $D(G) = D(G - u)$. For $D(G) = 3$, by Lemma 2.4 we have $R(G) - D(G) \geq \sqrt{n-1} - 3 > \sqrt{2} - \frac{n+1}{2}$ for $n \geq 5$. For $D(G) = D(G - u)$, we again have $R(G) - D(G) > R(G - u) - D(G - u) \geq \sqrt{2} - \frac{n}{2} > \sqrt{2} - \frac{n+1}{2}$ by induction.

If $d(u, v) \geq 4$, define $G' = G - u - v$ (see Fig. 3.3). Then $\lambda(G') \geq 2$. Assume xy to be the edge with the maximum weight in G' ; then $R(G) > R(G - xy)$ by Lemma 2.7 and $D(G) \leq D(G - xy)$. By induction, we have $R(G) - D(G) > R(G - xy) - D(G - xy) \geq \sqrt{2} - \frac{n+1}{2}$. We now finish the proof. \square

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