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The Randić index and the diameter of graphs

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ABSTRACT

The *Randić index* $R(G)$ of a graph G is defined as the sum of $\frac{1}{\sqrt{d_u d_v}}$ over all edges uv of G, where d_u and d_v are the degrees of vertices u and v, respectively. Let $D(G)$ be the diameter of G when G is connected. Aouchiche et al. (2007) [1] conjectured that among all connected graphs G on n vertices the path P_n achieves the minimum values for both $R(G)/D(G)$ and $R(G) - D(G)$. We prove this conjecture completely. In fact, we prove a stronger theorem: If G is a connected graph, then $R(G) - \frac{1}{2}D(G) \geq \sqrt{2} - 1$, with equality if and only if G is a path with at least three vertices.

1. Introduction

In 1975, the chemist Milan Randić [13] proposed a topological index R under the name "branching index", suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The branching index was renamed the molecular connectivity index and is often referred to as the Randić index.

There is a good correlation between the Randić index and several physico-chemical properties of alkanes: boiling points, enthalpies of formation, chromatographic retention times, etc. [7–9].

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

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u d_v}}.$$

Here d_u and d_v are the degrees of vertices u and v, respectively.

From a mathematical point of view, the first question to be asked is what are the minimum and maximum values of the Randić index in various classes of graphs, and which graphs in these classes of graphs have an extremal (minimum or maximum) Randić index. Erdős and Bollobás [4] first considered such problems. They proved that the star minimizes the Randić index among all the graphs without isolated vertices on fixed number of vertices. After that a lot of extremal results on the Randić index were published.

It turns out that the Randić index is also related to some typical graph parameters such as: diameter, radius, average distance, girth, chromatic number, and eigenvalues of the adjacent matrices [2,3,12]. Some conjectures on them are still open [1,5,6,10].

Aouchiche et al. [1] posed the following conjecture on the diameter and the Randić index.

Conjecture 1. *If G is a connected graph of order $n \geq 3$, then the Randić index $R(G)$ and the diameter $D(G)$ satisfy*

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

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and

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

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

Li and Shi [11] proved this conjecture in some special cases. Namely, if G is a connected graph of order n with minimum degree at least 5, then

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

If $\delta(G) \geq \frac{n}{5}$, then

$$\frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}.$$

In this paper we settle the conjecture completely. In fact, we prove the following stronger theorem.

Theorem 1. *If G is a connected graph with at least three vertices, then we have*

$$R(G) - \frac{1}{2}D(G) \geq \sqrt{2} - 1.$$

Equality holds if and only if $G \cong P_n$ *for* $n \geq 3$.

Corollary 1. *If G is a connected graph of order $n \geq 3$, then the Randić index $R(G)$ and the diameter $D(G)$ satisfy*

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

and

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

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

Proof. Noticing that $D(G) \leq n-1$, we have

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

and

$$R(G) - \frac{D(G)}{2} \geq \sqrt{2} - 1 \Rightarrow \frac{R(G)}{D(G)} \geq \frac{1}{2} + \frac{\sqrt{2}-1}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}. \quad \square$$

The paper is organized as follows. In Section 2, we prove several useful lemmas. Our main idea is to capture the change of the Randić index when we simplify a graph. The proof of the main theorem is presented in Section 3.

2. Lemmas on vertex deletion and edge deletion

For any vertex v, let $\Gamma(v)$ denote the set of all neighbors of v and $\Gamma^*(v)$ denote the set of all non-leaf neighbors of v, i.e.,

$$\Gamma(v) = \{u : uv \in E(G)\} \quad \text{and} \quad \Gamma^*(v) = \{u : uv \in E(G) \text{ and } d_u \geq 2\}.$$

We also let $N(v) = \Gamma(v) \cup \{v\}$ and $N^*(v) = \Gamma^*(v) \cup \{v\}$. Throughout d_u will be the degree with respect to G, unless other graphs are considered.

We have the following Lemma.

Lemma 1. *If G is a connected graph on the vertex set $\{1, 2, \ldots, n\}$, then we have*

$$R(G) \geq \frac{\sum_{i=1}^{n} \sqrt{d_i}}{2\sqrt{\Delta}}.$$

Here $d_1, \ldots, d_n$ are degrees of G and Δ is the maximum degree.

Proof. We have

$$
\begin{aligned}
R(G) &= \sum_{ij\in E(G)} \frac{1}{\sqrt{d_i d_j}} \\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j\in\Gamma(i)} \frac{1}{\sqrt{d_i d_j}} \\
&\geq \frac{1}{2}\sum_{i=1}^{n}\sum_{j\in\Gamma(i)} \frac{1}{\sqrt{d_i \Delta}} \\
&\geq \frac{1}{2}\sum_{i=1}^{n} \frac{d_i}{\sqrt{d_i \Delta}} \\
&= \frac{\sum_{i=1}^{n}\sqrt{d_i}}{2\sqrt{\Delta}}.
\end{aligned}
$$

The proof of this lemma is finished. □

Let $G-v$ be the induced subgraph obtained by deleting the vertex v from G. Let $G-uv$ be the spanning subgraph obtained by deleting the edge uv from G.

If G is connected, then $D(G)$ is the diameter of G as defined earlier. We extend the function $D(G)$ to disconnected graphs as follows. If G is disconnected, then $D(G)$ is defined to be the maximum among diameters of all the connected components of G. A vertex v is said to be *essential* (to $D(G)$) if $D(G-v) < D(G)$; it is not essential otherwise. Thus a vertex v is essential if and only if every shortest path between any two vertices at distance $D(G)$ passes through v.

An edge is *essential* if its two endpoints are essential. A path is *essential* if all edges of this path are essential.

In general, $\Gamma(v)$ is not an independent set. Let $G|_{\Gamma(v)}$ be the induced subgraph of G on $\Gamma(v)$. We have the following lemma.

Lemma 2. *Given an orientation of the edges of $G|_{\Gamma(v)}$, for any two vertices u and x in G, we define*

$$
\epsilon_x^u = \begin{cases} 1, & \text{if } \overrightarrow{ux} \text{ is a directed edge of } G|_{\Gamma(v)}; \\ 0, & \text{otherwise}. \end{cases}
$$

If forany $u \in \Gamma^*(v)$,

$$
\frac{1}{d_u - 1}\sum_{x\in\Gamma(u)\setminus\{v\}} \frac{1}{\sqrt{d_x - \epsilon_x^u}} \leq \frac{2}{\sqrt{d_v}}, \tag{1}
$$

then we have

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

Proof. When the vertex v is deleted, all edges incident to v are also deleted. For any vertex u, if $u \in \Gamma(v)$, the degree of u decreases by one; if $u \notin N(v)$, the degree of u remains the same.

Let us consider $R(G) - R(G-v)$. For most edges xy in G, the contribution of $\frac{1}{\sqrt{d_x d_y}}$ to $R(G) - R(G-v)$ is canceled out unless one of x and y is in $N(v)$. There are three types of edges.

Type I: $x = v$ and $y = u \in \Gamma(v)$. The contribution of this type of edge to $R(G) - R(G-v)$ is

$$
\sum_{u\in\Gamma(v)} \frac{1}{\sqrt{d_v d_u}} \geq \sum_{u\in\Gamma^*(v)} \frac{1}{\sqrt{d_v d_u}}.
$$

Type II: $y = u \in \Gamma^*(v)$ and $x \in \Gamma(u) \setminus N(v)$. The contribution of this type of edge to $R(G) - R(G-v)$ is

$$
\sum_{u\in\Gamma^*(v)} \left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_u - 1}}\right) \sum_{x\in\Gamma(u)\setminus N(v)} \frac{1}{\sqrt{d_x}} = \sum_{u\in\Gamma^*(v)} \left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_u - 1}}\right) \sum_{x\in\Gamma(u)\setminus N(v)} \frac{1}{\sqrt{d_x - \epsilon_x^u}}
$$

since $\epsilon_x^u = 0$ in this case.

Type III: $y = u \in \Gamma^*(v)$, $x \in \Gamma^*(v)$, and $\overrightarrow{ux}$ is a directed edge of $G|_{\Gamma(v)}$. Note that

$$
\begin{aligned}
\frac{1}{\sqrt{d_u d_x}} - \frac{1}{\sqrt{(d_u - 1)(d_x - 1)}} &= \frac{1}{\sqrt{d_u}}\left(\frac{1}{\sqrt{d_x}} - \frac{1}{\sqrt{d_x - 1}}\right) + \frac{1}{\sqrt{d_x - 1}}\left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_u - 1}}\right) \\
&= \frac{1}{\sqrt{d_u - \epsilon_u^x}}\left(\frac{1}{\sqrt{d_x}} - \frac{1}{\sqrt{d_x - 1}}\right) + \frac{1}{\sqrt{d_x - \epsilon_x^u}}\left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_u - 1}}\right),
\end{aligned}
$$

since $\epsilon_u^x = 0$ and $\epsilon_x^u = 1$. The above expression is symmetric with respect to u and x. Thus, the contribution of this type of edge to $R(G) - R(G - v)$ is

$$\begin{aligned}
&\frac{1}{2} \sum_{u\in\Gamma^*(v), x\in\Gamma(u)\cap\Gamma(v)} \frac{1}{\sqrt{d_u - \epsilon_u^x}} \left(\frac{1}{\sqrt{d_x}} - \frac{1}{\sqrt{d_x - 1}}\right) + \frac{1}{\sqrt{d_x - \epsilon_x^u}} \left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_u - 1}}\right) \\
&\quad = \sum_{u\in\Gamma^*(v), x\in\Gamma(u)\cap\Gamma(v)} \frac{1}{\sqrt{d_x - \epsilon_x^u}} \left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_u - 1}}\right) \\
&\quad = \sum_{u\in\Gamma^*(v)} \left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_u - 1}}\right) \sum_{x\in\Gamma(u)\cap\Gamma(v)} \frac{1}{\sqrt{d_x - \epsilon_x^u}}.
\end{aligned}$$

Summing up the contribution of three types of edges, we have

$$\begin{aligned}
R(G) - R(G - v) &\geq \sum_{u\in\Gamma^*(v)} \frac{1}{\sqrt{d_v d_u}} + \sum_{u\in\Gamma^*(v)} \left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_u - 1}}\right) \sum_{x\in\Gamma(u)\setminus N(v)} \frac{1}{\sqrt{d_x - \epsilon_x^u}} \\
&\quad + \sum_{u\in\Gamma^*(v)} \left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_u - 1}}\right) \sum_{x\in\Gamma(u)\cap\Gamma(v)} \frac{1}{\sqrt{d_x - \epsilon_x^u}} \\
&= \sum_{u\in\Gamma^*(v)} \left[\frac{1}{\sqrt{d_v d_u}} - \left(\frac{1}{\sqrt{d_u - 1}} - \frac{1}{\sqrt{d_u}}\right) \sum_{x\in\Gamma(u)\setminus\{v\}} \frac{1}{\sqrt{d_x - \epsilon_x^u}}\right].
\end{aligned}$$

Now we apply the assumption (1).

$$\begin{aligned}
R(G) - R(G - v) &\geq \sum_{u\in\Gamma^*(v)} \left[\frac{1}{\sqrt{d_v d_u}} - \left(\frac{1}{\sqrt{d_u - 1}} - \frac{1}{\sqrt{d_u}}\right) \frac{2(d_u - 1)}{\sqrt{d_v}}\right] \\
&= \sum_{u\in\Gamma^*(v)} \frac{1}{\sqrt{d_v d_u}} \left(1 - \frac{2\sqrt{d_u - 1}}{\sqrt{d_u} + \sqrt{d_u - 1}}\right) \\
&= \sum_{u\in\Gamma^*(v)} \frac{(\sqrt{d_u} - \sqrt{d_u - 1})^2}{\sqrt{d_v d_u}} \\
&> 0. \quad \square
\end{aligned}$$

Inequality (1) is called the *deletion condition* for the vertex v. To check the deletion condition, we need to specify an orientation of the edges of $G|_{\Gamma(v)}$. We can relax this condition as follows.

Let $d_x^* = d_x - 1$ if $d_x \geq 2$ and $d_x^* = d_x$ if $d_x = 1$. Note for any orientation of the edges of $G|_{\Gamma(v)}$

$$d_x - \epsilon_x^u \geq d_x^*.$$

We have the following corollary.

Corollary 2. *If for any* $u \in \Gamma^*(v)$,

$$\frac{1}{d_u - 1} \sum_{x\in\Gamma(u)\setminus\{v\}} \frac{1}{\sqrt{d_x^*}} \leq \frac{2}{\sqrt{d_v}}, \tag{2}$$

then we have

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

Inequality (2) is called the *weak deletion condition* for the vertex v.

Corollary 3. *If* $d_v \leq 4$, *then we have*

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

Proof. It suffices to show that v satisfies the weak deletion condition. If $\Gamma^*(v) = \emptyset$, then the weak deletion condition is satisfied automatically. If $u \in \Gamma^*(v)$ and $x \in \Gamma(u) \setminus \{v\}$, then we have

$$d_x^* \geq 1.$$

Thus,

$$\frac{1}{d_u - 1} \sum_{x\in\Gamma^*(u)\setminus\{v\}} \frac{1}{\sqrt{d_x^*}} \leq \frac{1}{d_u - 1} \sum_{x\in\Gamma^*(u)\setminus\{v\}} 1 \leq 1 \leq \frac{2}{\sqrt{d_v}}.$$

Applying Corollary 2, we get

$$R(G) > R(G - v). \quad \square$$

Lemma 3. *If G is a connected graph, then there exists an induced connected subgraph G' satisfying the following conditions.*

1. $R(G) \geq R(G')$.
2. $D(G) \leq D(G')$.
3. *Every non-essential vertex in G' has degree at least* 9.
4. $R(G') = R(G)$ *holds if and only if* $G' = G$ *and every non-essential vertex in G has degree at least* 9.

Proof. Suppose that G contains a vertex v with $d_v \leq 4$. If v is not essential, then we can remove v from G and consider $G - v$ instead (by Corollary 3). Repeatedly find a non-essential vertex v with degree at most 4 and delete it until no such v is found.

From now on, we assume that every non-essential vertex has degree at least 5. Let v be a non-essential vertex with minimum degree $\delta \leq 8$. We claim

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

There are five cases.

Case I: The vertex v has one neighbor u_1 with degree 1, and u_1 is essential. Any path containing u_1 contains v. This contradicts with the assumption that v is not essential.

Case II: The vertex v has two neighbors u_1 and u_2 with degrees 2, and both u_1 and u_2 are essential vertices. Since v is not essential, there exists a shortest path P (of length $D(G)$) which does not contain v. The path P passes through u_1 and u_2. The degrees of u_1 and u_2 in P are at most 1. So u_1 and u_2 must be the two endpoints of P. In this case, we must have $D(G) = d(u_1, u_2) \leq 2$.

If $D(G) = 1$, then G is a complete graph. We have $R(G) = R(G - v) + \frac{1}{2} > R(G - v)$.

Now assume $D(G) = 2$. Since $d_v = \delta \geq 5$, $\Gamma(v)$ contains a vertex u which is not on the path P. We have $d(u, u_i) = 2$ for $i = 1, 2$. We can delete u_1 or u_2 without decreasing $D(G)$. Contradiction!

Case III: Every neighbor of v has degree at least 3, and no leaf lies within the distance 2 from v. For any $u \in \Gamma(v)$ with degree at least 3 and $x \in \Gamma(u) \setminus \{v\}$, we have

$$d_x^* \geq 2.$$

We have

$$\frac{1}{d_u - 1} \sum_{x \in \Gamma(u) \setminus \{v\}} \frac{1}{\sqrt{d_x^*}} \leq \frac{1}{\sqrt{2}} \leq \frac{2}{\sqrt{d_v}},$$

which holds for $d_v \leq 8$. The weak deletion condition (2) is satisfied. By Corollary 2, we have

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

Case IV: All neighbors of v except u_1 have degree at least 3 while u_1 has degree 2; no leaf lies within the distance 2 from v. In this case, we verify the deletion condition (1). Orient the edges of $G|_{\Gamma^*(v)}$ so that the edge incidents to u_1 leave u_1. For any $u \in \Gamma(v)$ and $x \in \Gamma^*(u) \setminus \{v\}$, it is clear that

$$d_x - \epsilon_x^u \geq 2.$$

Similarly, the condition (1) is satisfied. By Lemma 2, we have

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

Case V: There is a leaf x with $d(v, x) = 2$, and x is essential. Let u be the only neighbor of x. Clearly, $u \in \Gamma^*(v)$. Since x is essential, then u must be essential as well. We verify the weak deletion condition (2) for u.

If $d_u = 2$, then v is also essential. Contradiction! Suppose that u has a neighbor w with $d_w < \delta$ ($w \neq x$). The vertex w must be essential. Since $d_v = \delta > d_w$, there is a vertex $y \in \Gamma(v) \setminus \Gamma(w)$. Suppose that P is a shortest path of length $D(G)$ containing x, u, w. Replace the segment $x - u - w$ by the shortest path from y to w. Call this path P'. The path P' is also a shortest path with length at least $D(G)$, and P' does not contain x. This contradicts with the assumption that x is essential.

Suppose $d_u \geq 3$, and every neighbor w of u other than x satisfies $d_w \geq \delta$.

We have

$$
\begin{aligned}
\frac{1}{d_u-1}\sum_{x\in\Gamma^*(u)\setminus\{v\}}\frac{1}{\sqrt{d_x^*}} &\le \frac{1}{d_u-1}\left(1+(d_u-2)\frac{1}{\sqrt{\delta-1}}\right)\\
&= \frac{1}{\sqrt{\delta-1}}+\frac{1}{d_u-1}\left(1-\frac{1}{\sqrt{\delta-1}}\right)\\
&\le \frac{1}{\sqrt{\delta-1}}+\frac{1}{2}\left(1-\frac{1}{\sqrt{\delta-1}}\right)\\
&\le \frac{1}{2}\left(1+\frac{1}{\sqrt{\delta-1}}\right)\\
&< \frac{2}{\sqrt{\delta}}.
\end{aligned}
$$

The last inequality holds for $\delta \le 8$. Thus $R(G) \ge R(G-v)$.

For all five cases, we can delete a non-essential vertex v with $d_v \le 8$ such that

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

Repeat this process until every non-essential vertex has degree at least 9. □

A vertex v is a *local-minimum-vertex* if the following two conditions are satisfied.

1. The vertex v is not essential for G.
2. If u is a non-essential vertex with $d(u, v) \le 2$, then $d_u \ge d_v$.

Lemma 4. *Suppose v is a local-minimum-vertex with degree $d_v \ge 3$. If $R(G) \le R(G-v)$, then there exist two vertices w and y satisfying*

1. *vw and wy are edges of G.*
2. *$d_w < d_v$ and $d_y < d_v$. Consequently, wy is an essential edge of G.*

Proof. For any $u \in \Gamma(v)$ with $d_u \ge d_v$, we claim that $\Gamma(u)$ can contain at most two essential vertices.

Otherwise, say that $\Gamma(u)$ contains three essential vertices x, y, and z. Choose a shortest path P connecting two vertices of distance $D(G)$. By the definition of essential vertices, all x, y, and z are on the path P. Since $x, y, z \in \Gamma(u)$, x, y, and z must be adjacent on P. Without loss of generality, we assume $d(x, z) = 2$. We can replace y by u and obtain a new path P' from P. This contradicts with the assumption that y is also essential.

Since $R(G) \le R(G-v)$, the weak deletion condition (2) is violated for some u. There are three cases.

Case I: For any $x \in \Gamma(u) \setminus \{v\}$, $d_x \ge d_v$. In this case, we have

$$d_x^* = d_x - 1 \ge d_v - 1.$$

Thus,

$$
\begin{aligned}
\frac{1}{d_u-1}\sum_{x\in\Gamma(u)\setminus\{v\}}\frac{1}{\sqrt{d_x^*}} &\le \frac{1}{d_u-1}\sum_{x\in\Gamma(u)\setminus\{v\}}\frac{1}{\sqrt{d_v-1}}\\
&\le \frac{1}{\sqrt{d_v-1}}\\
&< \frac{2}{\sqrt{d_v}},
\end{aligned}
$$

where the lase step holds for $d_v \ge 2$. The weak deletion condition (2) is satisfied. Contradiction!

Case II: $d_u < d_v$. By Case I, we have a vertex $x \in \Gamma(u) \setminus \{v\}$, $d_x < d_v$. Choose $w = u$ and $y = x$. We are done.

Case III: $d_u \ge d_v$. Note that $\Gamma(u)$ can contain at most 2 essential vertices. Let y_1 and y_2 be the possible two essential vertices. If $x \in \Gamma(u) \setminus \{v, y_1, y_2\}$, then by the definition of local-minimum-vertex, we have

$$d_x^* = d_x - 1 \ge d_v - 1.$$

We bound $d_{y_1}^*$ and $d_{y_1}^*$ by 2. We get

$$\begin{aligned}\frac{1}{d_u-1}\sum_{x\in\Gamma(u)\setminus\{v\}}\frac{1}{\sqrt{d_x^*}} &\le \frac{1}{d_u-1}\left[2+\frac{d_u-3}{\sqrt{d_v-1}}\right]\\ &\le \frac{1}{\sqrt{d_v-1}}+\frac{2-\frac{2}{\sqrt{d_v-1}}}{d_u-1}\\ &\le \frac{1}{\sqrt{d_v-1}}+\frac{2-\frac{2}{\sqrt{d_v-1}}}{d_v-1}\\ &< \frac{2}{\sqrt{d_v}},\end{aligned}$$

where the last step holds for $d_v \ge 3$. Contradiction!

Only Case II is possible. There are two essential vertices y and w satisfying all the conditions. □

Lemma 5. *If uv is a non-leaf edge, then we have*

$$R(G) > R(G-uv) - \frac{1}{2}.$$

Proof. We have

$$\begin{aligned}R(G)-R(G-uv) &= \frac{1}{\sqrt{d_ud_v}} - \sum_{x\in\Gamma(u)\setminus\{v\}}\frac{1}{\sqrt{d_x}}\left(\frac{1}{\sqrt{d_u-1}}-\frac{1}{\sqrt{d_u}}\right) - \sum_{y\in\Gamma(v)\setminus\{u\}}\frac{1}{\sqrt{d_y}}\left(\frac{1}{\sqrt{d_v-1}}-\frac{1}{\sqrt{d_v}}\right)\\ &\ge \frac{1}{\sqrt{d_ud_v}} - (d_u-1)\left(\frac{1}{\sqrt{d_u-1}}-\frac{1}{\sqrt{d_u}}\right) - (d_v-1)\left(\frac{1}{\sqrt{d_v-1}}-\frac{1}{\sqrt{d_v}}\right)\\ &= \frac{1}{\sqrt{d_ud_v}} - \frac{\sqrt{d_u-1}}{\sqrt{d_u}(\sqrt{d_u}+\sqrt{d_u-1})} - \frac{\sqrt{d_v-1}}{\sqrt{d_v}(\sqrt{d_v}+\sqrt{d_v-1})}\\ &> \frac{1}{\sqrt{d_ud_v}} - \frac{1}{2\sqrt{d_u}} - \frac{1}{2\sqrt{d_v}}\\ &= \frac{1}{\sqrt{2d_ud_v}} + \frac{1}{2}\left(1-\frac{1}{\sqrt{d_u}}\right)\left(1-\frac{1}{\sqrt{d_v}}\right) - \frac{1}{2}\\ &> -\frac{1}{2}. \quad \square\end{aligned}$$

Corollary 4. *Suppose that uv is not a cut edge of G. If both u and v are essential, then*

$$R(G) - \frac{1}{2}D(G) > R(G-uv) - \frac{1}{2}D(G-uv).$$

Lemma 6. *Let u be a cut vertex of G. Suppose that G has a decomposition $G = G_1 \cup G_2$ satisfying $G_1 \cap G_2 = \{u\}$, $|G_2| \ge 8$, and $|\Gamma_u \cap V(G_1)| = 2$ (see Fig. 1). If u reaches the minimum degree in G_2, then we have*

$$R(G) > R(G_1).$$

Proof. Let u_1 and u_2 be the two adjacent vertices of u in G_1 and $v_1, \ldots, v_k$ be the adjacent vertices of u in G_2. Let $N(v_i)$ be the set of neighbors of v_i in G_2. We have

$$\begin{aligned}R(G) &\ge R(G_1)+R(G_2) - \left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{k+2}}\right)\left(\frac{1}{\sqrt{d_{u_1}}}+\frac{1}{\sqrt{d_{u_2}}}\right) - \sum_{i=1}^{k}\left(\frac{1}{\sqrt{d_{v_i}}}-\frac{1}{\sqrt{d_{v_i}+1}}\right)\sum_{x\in N(v_i)}\frac{1}{\sqrt{d_x}}\\ &\ge R(G_1)+R(G_2) - \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{d_{u_1}}}+\frac{1}{\sqrt{d_{u_2}}}\right) - \sum_{i=1}^{k}\frac{1}{(\sqrt{d_{v_i}}+\sqrt{d_{v_i}+1})\sqrt{d_{v_i}}\sqrt{d_{v_i}+1}}\cdot\frac{d_{v_i}}{\sqrt{k}}\\ &> R(G_1)+R(G_2) - \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{d_{u_1}}}+\frac{1}{\sqrt{d_{u_2}}}\right) - \sum_{i=1}^{k}\frac{1}{2\sqrt{k}\sqrt{d_{v_i}}}\\ &\ge R(G_1)+R(G_2) - \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{1}}+\frac{1}{\sqrt{1}}\right) - \frac{k}{2\sqrt{k}\sqrt{k}}\\ &\ge R(G_1)+R(G_2) - \sqrt{2} - \frac{1}{2} > R(G_1),\end{aligned}$$

where the last inequality hold for $R(G_2) \ge \sqrt{|G_2|-1} \ge \sqrt{7}$. □

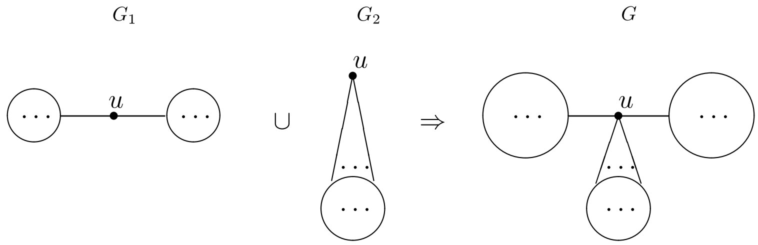

Fig. 1. $G = G_1 \cup G_2$.

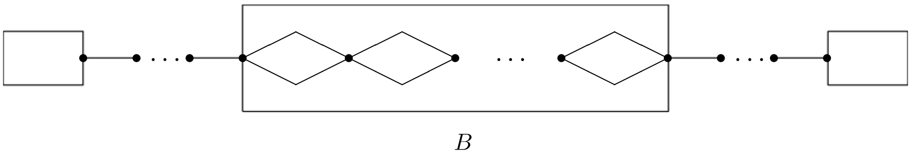

Fig. 2. The structure of G.

Lemma 7. *For any edge uv of G, let $G_{u\cdot v}$ be the graph obtained by subdividing the edge uv (i.e., by replacing the edge uv by a path of length 2). We have the following statements.*

1. *If $d_u = 2$ or $d_v = 2$, then $R(G_{u\cdot v}) = R(G) + \frac{1}{2}$.*
2. *If $d_u > 2$ and $d_v > 2$, then $R(G_{u\cdot v}) < R(G) + \frac{1}{2}$.*
3. *If $d_u = 1$ and $d_v > 2$, then $R(G_{u\cdot v}) > R(G) + \frac{1}{2}$.*
4. *If $d_u > 2$ and $d_v = 1$, then $R(G_{u\cdot v}) > R(G) + \frac{1}{2}$.*

Proof. We have

$$\begin{aligned} R(G_{u\cdot v}) - R(G) &= \frac{1}{\sqrt{2d_u}} + \frac{1}{\sqrt{2d_v}} - \frac{1}{\sqrt{d_u d_v}} \\ &= \frac{1}{2} - \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_u}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d_v}}\right). \end{aligned}$$

It is easy to verify all cases. □

3. Proof of main theorem

Proof of Theorem 1. For any graph G, we define $f(G) = R(G) - \frac{D(G)}{2}$. Note that $f(P_n) = \sqrt{2} - 1$ for $n \geq 3$. We need show that

$$f(G) > \sqrt{2} - 1 \tag{3}$$

for any connected graph $G \neq P_n$ ($n \geq 3$).

Suppose that there is such a graph G ($\neq P_n$) satisfying

$$f(G) \leq \sqrt{2} - 1.$$

Let G be such a graph with the smallest number of vertices. (If there are several such graphs with the same number of vertices, pick the one with minimum number of edges.) It is easy to check that G is connected and has at least 3 vertices.

By Lemma 3, every non-essential vertex of G has degree at least 9. By Corollary 4, every essential edge is an edge-cut of G. By Lemma 6, if there are two essential edges uv and vw, then $d_v = 2$. Therefore G is the graph consisting of several blocks which are linked by essential paths (see Fig. 2). A *block B* is an induced connected subgraph of G which contains no essential edges of G. By Lemma 7, the length of each essential path is either 1 or 2.

We classify G according to the number of blocks. If there is no block in G, then $G = P_n$. Contradiction!

Suppose that there are at least two blocks in G. In this case, take an essential path which links two blocks. If this essential path has length 1, we consider G' obtained by subdividing this essential edge. If this essential path has length 2, let $G' = G$. Let $u - v - w$ be this essential path. Let G_1 and G_2 be two induced subgraphs of G so that $G = G_1 \cup G_2$ and $G_1 \cap G_2 = v$. Note that each block contains at least one non-essential vertex, which has degree at least 9. We have

$$|G_1| \geq 9 \quad \text{and} \quad |G_2| \geq 9.$$

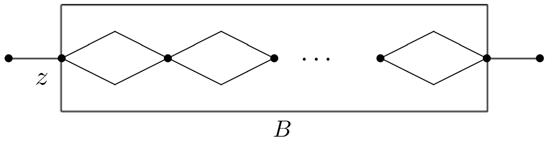

Fig. 3. G contains exactly one block with optional essential edges attached at the end.

Since $|G_1| + |G_2| = |G'| + 1 \le |G| + 2$, we have

$$|G_1| < |G| \quad \text{and} \quad |G_2| < |G|.$$

By the minimality of G, we have for $i = 1, 2$,

$$f(G_i) > \sqrt{2} - 1.$$

Note $D(G') \le D(G_1) + D(G_2)$.

$$\begin{aligned} R(G') - R(G_1) - R(G_2) &= \frac{1}{\sqrt{2d_u}} + \frac{1}{\sqrt{2d_w}} - \frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_w}} \\ &= -\left(1 - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{d_u}} + \frac{1}{\sqrt{d_w}}\right) \\ &> -\left(1 - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}}\right) \\ &= 1 - \sqrt{2}. \end{aligned}$$

By Lemma 7, we have

$$\begin{aligned} f(G) &\ge f(G') \\ &= R(G') - \frac{1}{2}D(G') \\ &= f(G_1) + f(G_2) + R(G') - R(G_1) - R(G_2) \\ &> f(G_1) + f(G_2) + 1 - \sqrt{2} \\ &> \sqrt{2} - 1 + \sqrt{2} - 1 + 1 - \sqrt{2} \\ &= \sqrt{2} - 1. \end{aligned}$$

Contradiction!

Now we consider the remaining case: there is exactly one block in G with possible essential edges attached at one or both ends. (See Fig. 3.)

Assume the maximum degree Δ is achieved at vertex v. Note that the neighborhood of v can contain at most two essential vertices. An essential vertex has degree at least 2 while a non-essiential vertex has degree at least 9. Applying Lemma 1, we have

$$\begin{aligned} R(G) &\ge \frac{\sum_{i=1}^{n} \sqrt{d_i}}{2\sqrt{\Delta}} \\ &\ge \frac{\sqrt{d_v} + \sum_{u \in \Gamma(v)} \sqrt{d_u}}{2\sqrt{\Delta}} \\ &\ge \frac{1}{2} + \frac{(\Delta - 2)\sqrt{9} + 2\sqrt{2}}{2\sqrt{\Delta}} \\ &= \frac{3}{2}\sqrt{\Delta} - \frac{3 - \sqrt{2}}{\sqrt{\Delta}} + \frac{1}{2}. \end{aligned}$$

Let $h(x) = \frac{3}{2}\sqrt{x} - \frac{3-\sqrt{2}}{\sqrt{x}} + \frac{1}{2}$. Note that $h(x)$ is an increasing function on $(0, \infty)$. Since G contains at least one non-essential vertex, we have $\Delta \ge 9$.

If $D(G) \le 8$, then we have

$$R(G) \ge h(9) = 4 + \frac{\sqrt{2}}{3} > \frac{D(G)}{2} + \sqrt{2} - 1.$$

It remains to show the case $D(G) \geq 9$. In fact, we show the maximum degree Δ grows exponentially as a function of $D(G)$.

Pick any path Q (in G) of length $D(G)$. Any optional essential edge(s) is located at the end(s) of Q. Let P be the remaining path after deleting essential edges from Q. Let k be the length of P, which is called the length of the block B. Since $D(G) \geq 9$, we have

$$k \geq D(G) - 2 \geq 7.$$

Let z be an end vertex of P. For $0 \leq i \leq k$, let A_i be the set of vertices in B of distance i to the vertex z (see Fig. 3). Let a_i be the minimum degree of nonessential vertices in A_i. If A_i is a single essential vertex, then define a_i to be infinite. We have the following two claims.

Claim A. *If* $3 \leq i \leq k-3$, *then we have*

$$a_i \geq 2.9(\min\{a_{i-2}, a_{i-1}, a_{i+1}, a_{i+2}\} - 1). \tag{4}$$

Claim B. *We have* $\Delta \geq 1.5 + 7.4 \cdot 2.9^{\lceil (k-6)/4 \rceil}$ *for* $k \geq 7$.

The proofs of these two claims are quite long. We leave these proofs to the end of this section. Now we use these claims to prove $f(G) > \sqrt{2} - 1$. For $k \geq 7$, we have

$$\begin{aligned} f(G) &= R(G) - \frac{D(G)}{2} \\ &\geq h(\Delta) - \frac{k+2}{2} \\ &\geq h(1.5 + 7.4 \cdot 2.9^{\lceil (k-6)/4 \rceil}) - \frac{k+2}{2} \\ &> \sqrt{2} - 1. \end{aligned}$$

The inequality in last step can be easily verified by Calculus. The proof of theorem is finished. □

It remains to prove the two claims.

Proof of Claim A. Obviously, (4) holds if a_i is infinite. Suppose there exists i such that

$$a_i < 2.9(\min\{a_{i-2}, a_{i-1}, a_{i+1}, a_{i+2}\} - 1).$$

Let v be the non-essential vertex with degree a_i in A_i. Let $\delta = \min\{a_{i-2}, a_{i-1}, a_{i+1}, a_{i+2}\}$. The above inequality implies

$$d_v < 2.9(\delta - 1). \tag{5}$$

We need show $R(G) > R(G - v)$ to derive the contradiction. It suffices to show that for any $u \in \Gamma^*(v)$ the weak deletion condition holds.

If u is essential, then u is not connected with any other essential vertex. We have

$$\begin{aligned} \frac{1}{d_u - 1} \sum_{x \in \Gamma(u) \setminus \{v\}} \frac{1}{\sqrt{d_x^*}} &\leq \frac{1}{d_u - 1} \sum_{x \in \Gamma(u) \setminus \{v\}} \frac{1}{\sqrt{\delta_v - 1}} \\ &= \frac{1}{\sqrt{\delta_v - 1}} \\ &< \frac{2}{\sqrt{d_v}}. \end{aligned}$$

At the last step, we applied inequality (5).

Otherwise, u can only be adjacent to at most two essential vertices. Since no two essential vertices are connected, each non-leaf essential vertex has a degree at least 3. Let y_1 and y_2 be two possible essential vertices. Noticing that essential vertices are not adjacent, we can orient the edges of $G|_{\Gamma(u)}$ such that directed edges always leave essential vertices. For $i \in \{1, 2\}$, we have

$$d_{y_i} - \epsilon_{y_i}^u = d_{y_i} \geq 3.$$

For $x \in \Gamma(u) \setminus \{v, y_1, y_2\}$, we apply the bound

$$d_x - \epsilon_x^u \geq d_x - 1 \geq \delta - 1.$$

We have

$$\frac{1}{d_u-1}\sum_{x\in\Gamma(u)\setminus\{v\}}\frac{1}{\sqrt{d_x-\epsilon_x^u}} \le \frac{1}{\sqrt{\delta-1}}+\frac{2}{\delta-1}\left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{\delta-1}}\right).$$

Let $f(x)=\frac{1}{\sqrt{x}}+\frac{2}{x}(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{x}})$. Note that $f(x)$ is decreasing on $(2.5,\infty)$. Since $d_v\ge 9$, we have $2.5<\frac{d_v}{2.9}<\delta-1$. Thus, $f(\delta-1)\le f(\frac{d_v}{2.9})$. We have

$$\begin{aligned}\frac{1}{d_u-1}\sum_{x\in\Gamma(u)\setminus\{v\}}\frac{1}{\sqrt{d_x-\epsilon_x^u}} &\le f(\delta-1)\\ &< f\left(\frac{d_v}{2.9}\right)\\ &< \frac{2}{\sqrt{d_v}}.\end{aligned}$$

The last step can be easily verified by Calculus. □

Proof of Claims B. Let $\{b_i\}$ be the sequence such that $b_i=2.9(b_{i-1}-1)$ and $b_0=9$. Solving the recurrence equation of the sequence $\{b_i\}$, we have

$$\begin{aligned}b_i &= \frac{29}{19}+\frac{142}{19}\cdot 2.9^i\\ &> 1.5+7.4\cdot 2.9^i.\end{aligned}$$

Since $a_i\ge 9=b_0$ for $0\le i\le k$, we get $a_i\ge b_1$ for $3\le i\le k-3$ by applying inequality (4). Applying inequality (4) again, we obtain $a_i\ge b_2$ for $5\le i\le k-5$. Repeatedly apply inequality (4). For each j in $\{1,2,\ldots,\lceil(k-6)/4\rceil\}$ and each i satisfying $2j+1\le i\le k-2j-1$, we have $a_i>b_j$. Let $j_0=\lceil(k-6)/4\rceil$. Note $k-4j_0-2\ge 1$. Thus, both a_{2j_0+1} and a_{2j_0+2} are greater than or equal to b_{j_0}. Note that there is no essential edge in the block B. We have

$$\Delta\ge\min\{a_{2j_0+1},a_{2j_0+2}\}\ge b_{j_0} > 1.5+7.4\cdot 2.9^{\lceil(k-6/)4\rceil}. \quad \square$$

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