The Randić index and signless Laplacian spectral radius of graphs

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Abstract

Given a connected graph G, the Randić index $R(G)$ is the sum of $(d(u)d(v))^{-1/2}$ over all edges $\{u, v\}$ of G, where $d(u)$ and $d(v)$ are the degree of vertices u and v respectively. Let $q(G)$ be the largest eigenvalue of the signless Laplacian matrix of G and $n = |V(G)|$. Hansen and Lucas (2010) made the following conjecture:

$$\frac{q(G)}{R(G)} \le \begin{cases} \frac{4n-4}{n} & 4 \le n \le 12 \\ \frac{n}{\sqrt{n-1}} & n \ge 13 \end{cases}$$

with equality if and only if $G = K_n$ for $4 \le n \le 12$ and $G = S_n$ for $n \ge 13$, respectively. Deng et al. verified this conjecture for $4 \le n \le 11$. In this paper, we prove the conjecture for $n \ge 12$.

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1 Introduction

For a connected graph $G = (V, E)$, the *Randić index* $R(G)$ is defined as

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

where $d(u)$ and $d(v)$ are the degree of vertices u and v respectively. This parameter was introduced by the chemist Milan Randić [22] in 1975 under the name 'branching index'. Originally, it was used to measure the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. It was noticed that there is a good correlation between the Randić index and several physico-chemical properties of alkanes: for example, boiling points, enthalpies of formation, chromatographic retention times, etc. [12, 16, 17].

From the view of extremal graph theory, one may ask what are the minimum and maximum values of the Randić index among a certain class of graphs and which graphs from the given class of graphs attain the extremal values. Bollobás and Erdős [3] first considered this kind of question. They proved that $R(G) \ge \sqrt{n-1}$ for each graph with n vertices and without isolated vertices. Moreover, the equality holds if and only G is the star. After that, there are a lot of references in this vein, for example, [2, 4, 6, 11]. Bollobás, Erdős, and Sarkar [4] studied generalizations of the Randić index.

Another direction of research is to ask the relationships between the Randić index and other parameters of graphs. Hansen and Vukicević [14] studied the connections between the Randić index and the chromatic number of graphs. Aouchiche, Hansen, and Zheng [1] made a conjecture on the minimum values of $\frac{R(G)}{D(G)}$ and $R(G) - D(G)$ over all connected graphs with the same number of vertices, where $D(G)$ is the diameter of G. Li and Shi [20] as well as Dvořák, Lidický, and Škrekovski [8] studied this conjecture before Yang and Lu [23] finally resolved it. Another result is $\lambda_1(G) \geq \frac{e(G)}{R(G)}$ which was proved by Favaron, Mahéo, and Saclé [9]. Here $\lambda_1(G)$ is the largest eigenvalue of the adjacency matrix of G. One may ask to prove similar results involving the Randić index and the spectral radius of other matrices associated with a graph.

For a graph G, the *signless Laplacian matrix* Q is defined as $D + A$, where D is the diagonal matrix of degrees in G and A is the adjacency matrix of G. Let $q(G)$ be the largest eigenvalue of Q. With the aid of AutoGraphiX system, Hansen and Lucas [13] proposed the following two conjectures. The first one is on the difference between $q(G)$ and $R(G)$. More precisely, they conjectured that if G is a connected graph on $n \geq 4$ vertices, then $q(G) - R(G) \leq \frac{3n}{2} - 2$ and equality holds for $G = K_n$. This conjecture was proved by Deng, Balachandran, and Ayyaswamy [7]. The second one concerns the ratio of $q(G)$ to $R(G)$.

Conjecture 1.1 (Hansen and Lucas [13])**.** *Let G be a connected graph on $n \geq 4$ vertices with the largest signless Laplacian eigenvalue $q(G)$ and Randić index $R(G)$. Then*

$$\frac{q(G)}{R(G)} \leq \begin{cases} \frac{4n-4}{n} & 4 \leq n \leq 12 \\ \frac{n}{\sqrt{n-1}} & n \geq 13 \end{cases}$$

with equality if and only if $G = K_n$ for $4 \leq n \leq 12$ and $G = S_n$ for $n \geq 13$, respectively.

Deng, Balachandran, and Ayyaswamy [7] were able to prove this conjecture for $4 \leq n \leq 11$ and established a nontrivial upper bound on $\frac{q(G)}{R(G)}$ which is larger than the conjectured one. We prove the conjecture for $n \geq 12$. Namely, we prove the following theorem.

Theorem 1.2. *For a connected graph G with n vertices, we have*

$$\frac{q(G)}{R(G)} \leq \begin{cases} \frac{11}{3} & n = 12; \\ \frac{n}{\sqrt{n-1}} & n \geq 13. \end{cases}$$

The equality holds if and only if $G = K_{12}$ for $n = 12$ and $G = S_n$ for $n \geq 13$.

For developments of the Randić index, we refer interested readers to excellent surveys, for instance, Li and Gutman [18], Li and Shi [19], as well as Li, Shi, and Wang [21].

We follow the standard notation throughout this paper. For those not defined here, we refer the reader to Bondy and Murty [5]. For a graph $G = (V, E)$, the *neighborhood* $N_G(v)$ of a vertex v is the set $\{u : u \in V(G) \text{ and } \{u, v\} \in E(G)\}$ and the *degree* $d_G(v)$ of a vertex v is $|N_G(v)|$. If the graph G is clear in the context, then we will drop the subscript G. We will use $e(G)$ to denote the number of edges in G.

The paper is organized as follows. In Section 2, we will collect several previous results which are needed in the proof of the main theorem. Also, we will prove a number of technical lemmas in Section 2. The proof of Theorem 1.2 will be given in Section 3.

2 Preliminaries

We first recall two theorems which provide upper bounds for the largest eigenvalue of the adjacency matrix and the signless Laplacian matrix of a graph respectively.

Theorem 2.1 (Hong [15]). *Let G be a graph with n vertices and m edges. Let λ_1 be the largest eigenvalue of its adjacency matrix. If the minimum degree $\delta(G) \geq 1$, then*

$$\lambda_1 \leq \sqrt{2m-n+1}.$$

Theorem 2.2 (Feng and Yu [10]). *Let G be a graph with n vertices and m edges. If $q(G)$ is the signless Laplacian spectral radius of G, then*

$$q(G) \leq \frac{2m}{n-1} + n - 2. \tag{1}$$

For a vertex v of a graph G, we define $m(v)$ as $\frac{1}{d(v)} \sum_{u \in N(v)} d(u)$. For a certain class of graphs, the following theorem gives a better upper bound on $q(G)$.

Theorem 2.3 (Feng and Yu [10]). *For a connected graph G, we have*

$$q(G) \leq \max\{d(v) + m(v) : v \in V(G)\}.$$

We will need the following lemma.

Lemma 2.4. *For a connected graph G with $n \geq 4$ vertices, if $m = e(G) \geq n$ and $R(G) > \sqrt{n-1} + \frac{2m-2n+2}{n\sqrt{n-1}}$, then $\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}$.*

Proof. Recall Theorem 2.2. We have

$$\frac{q(G)}{R(G)} < \frac{\frac{2m}{n-1} + n - 2}{\sqrt{n-1} + \frac{2m-2n+2}{n\sqrt{n-1}}}.$$

We note

$$\begin{aligned} \left(\sqrt{n-1} + \frac{2m-2n+2}{n\sqrt{n-1}}\right)\frac{n}{\sqrt{n-1}} &= \sqrt{n-1} \cdot \frac{n}{\sqrt{n-1}} + \frac{2m-2n+2}{n\sqrt{n-1}} \cdot \frac{n}{\sqrt{n-1}} \\ &= n + \frac{2m-2n+2}{n-1} \\ &= \frac{2m}{n-1} + n - 2. \end{aligned}$$

This lemma follows easily. □

We recall the following lower bound for $R(G)$.

Theorem 2.5 (Bollobás and Erdős [3]). *Let G be a graph with n vertices. If $\delta(G) \geq 1$, then $R(G) \geq \sqrt{n-1}$ and the equality holds if and only if $G = S_n$.*

If $\delta(G) \geq 2$, then we need the following better lower bound for $R(G)$.

Theorem 2.6 (Delorme, Favaron, and Rautenbach [6]). *Let G be a graph on n vertices. If $\delta(G) \geq 2$, then*

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

A consequence of the theorem above is the following lemma.

Lemma 2.7. *Let G be a connected graph with $n \geq 12$ vertices and $n+k$ edges, where $1 \leq k \leq 10$. If $\delta(G) \geq 2$, then*

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

Proof. Recall that $n \geq 12$ and $e(G) = n+k$, where $1 \leq k \leq 10$. By Theorem 2.6, we have

$$R(G) \geq \frac{2n-4}{\sqrt{2n-2}} + \frac{1}{n-1}.$$

When $n \geq 9$, we can verify

$$\frac{2n-4}{\sqrt{2n-2}} + \frac{1}{n-1} > \sqrt{n-1} + \frac{2(k+1)}{n\sqrt{n-1}}$$

easily. □

Among all unicyclic graphs, the minimum value of $R(G)$ is also known.

Theorem 2.8 (Gao and Lu [11]). *Let G be a unicyclic graph on n vertices. Then $R(G)$ attains its minimum value when G is S_n^*, where S_n^* is obtained from the star with n vertices by adding an edge between leaves.*

The following theorem allows us to compare the Randić index of a graph and that of a related graph obtained by deleting a minimum degree vertex.

Theorem 2.9 (Hansen and Vukicević [14]). *Let G be a graph with the Randić index R, minimum degree δ and maximum degree Δ. If v is a vertex of G with degree δ, then*

$$R(G) - R(G-v) \geq \frac{1}{2}\sqrt{\frac{\delta}{\Delta}}.$$

The following lemma will be useful for us later.

Lemma 2.10. *Let G be a connected graph with n vertices and $e(G) = n+k$, where $1 \leq k \leq 10$. Let v be a vertex with $d(v) = 1$. If*

$$R(G-v) > \sqrt{n-2} + \frac{2(k+1)}{(n-1)\sqrt{n-2}},$$

then we have

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

Proof. Let v_0 be a vertex with $d(v_0) = \Delta$. Recall v is a vertex with $d(v) = 1$ by the assumption. Let H be the subgraph induced by $V(G) - \{v_0, v\}$ and

$$L := \sum_{\{x,y\} \in E(H)} \frac{1}{\sqrt{d_G(x)d_G(y)}}.$$

If $\Delta = n-1$, then observe that

$$R(G-v) = \left(R(G) - \frac{1}{\sqrt{n-1}} - L\right) \cdot \frac{\sqrt{n-1}}{\sqrt{n-2}} + L.$$

Thus,

$$\begin{aligned}
R(G) &= L + \frac{1}{\sqrt{n-1}} + \frac{\sqrt{n-2}}{\sqrt{n-1}}(R(G-v)-L) \\
&= \frac{\sqrt{n-2}}{\sqrt{n-1}}R(G-v) + \frac{1}{\sqrt{n-1}} + \left(1 - \frac{\sqrt{n-2}}{\sqrt{n-1}}\right)L \\
&> \frac{\sqrt{n-2}}{\sqrt{n-1}}\left(\sqrt{n-2} + \frac{2(k+1)}{(n-1)\sqrt{n-2}}\right) + \frac{1}{\sqrt{n-1}} \\
&= \sqrt{n-1} + \frac{2(k+1)}{(n-1)\sqrt{n-1}} \\
&> \sqrt{n-1} + \frac{2(k+1)}{n\sqrt{n-1}}.
\end{aligned}$$

If $\Delta \leq n-2$, by Theorem 2.9, we have $R(G) \geq R(G-v) + \frac{1}{2}\sqrt{\frac{1}{n-2}}$. Thus

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

The proof is complete. □

We need the following proposition involving the vertex deletion.

Proposition 2.11. *For a connected graph G, assume $(v_1, \ldots, v_s)$ is an ordered set of vertices. Let $G_0 = G$ and $G_i = G_{i-1} - v_i$ for $1 \leq i \leq s$. If v_i has degree one in G_{i-1} for each $1 \leq i \leq s$, then we have*

$$R(G) \geq \sum_{i=0}^{s-1} \frac{1}{2\sqrt{\Delta(G_i)}} + R(G_s).$$

Proof. Since we assume for each $1 \leq i \leq s$, the vertex v_i has degree one in G_{i-1}. If we delete the vertex v_i from G_{i-1}, then we have $R(G_{i-1}) \geq \frac{1}{2\sqrt{\Delta(G_{i-1})}} + R(G_i)$ by Theorem 2.9. Since this observation holds for all $1 \leq i \leq s$, the proposition follows. □

Lastly, we need the following theorem.

Theorem 2.12 (Favaron, Mahéo, and Saclé [9]). *For any connected graph G with m edges. If R is the Randić index and λ_1 is the largest eigenvalue of its adjacency matrix, then $\lambda_1 \geq \frac{m}{R}$.*

3 Proof of the Main Theorem

The following lemma is the key ingredient in the course of proving the main theorem.

Lemma 3.1. *Let G be a connected graph with n vertices and m edges. If $n \geq 15$ and $n + 8 \leq m \leq \min\{2n^{3/2}, \binom{n}{2}\}$, then*

$$\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}.$$

Proof. We note $2n^{3/2} > \binom{n}{2}$ when $15 \leq n \leq 17$ and $2n^{3/2} < \binom{n}{2}$ when $n \geq 18$. We define a function

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

With the help of computer, one can check $f(m) > 0$ for $15 \leq n \leq 17$ and $n+8 \leq m \leq \binom{n}{2}$. We assume $n \geq 18$ for the rest of the proof and $\min\{2n^{3/2}, \binom{n}{2}\} = 2n^{3/2}$ in this case. We also consider a relevant function

$$g(m) = mn\sqrt{n-1} - n(n-1)\sqrt{2m-(n-1)} - (2m-2(n-1))\sqrt{2m-(n-1)}.$$

To show $f(m) > 0$, it suffices to show $g(m) > 0$ for $n+8 \leq m \leq 2n^{3/2}$ and $n \geq 18$ as $2m-(n-1) > 0$. Let $A = mn\sqrt{n-1}$ and $B = n(n-1)\sqrt{2m-(n-1)} + (2m-2(n-1))\sqrt{2m-(n-1)} = (2m+n^2-3n+2)\sqrt{2m-(n-1)}$. We define

$$h(m) = A^2 - B^2 = m^2n^2(n-1) - (2m+n^2-3n+2)^2(2m-(n-1)).$$

It is equivalent to prove $h(m) > 0$ for $n+8 \leq m \leq 2n^{3/2}$ and $n \geq 18$. We first show $h(n+8) > 0$ for $n \geq 18$. We note

$$h(n+8) = 45n^3 - 657n^2 + 288n - 5508.$$

We can show $45n^3 - 657n^2 + 288n - 5508 > 0$ when $n = 18$ directly. By taking the derivative, we can prove that $45n^3 - 657n^2 + 288n - 5508$ is increasing when $n \geq 18$, which completes the proof of $h(n+8) > 0$ for all $n \geq 18$.

We next show for fixed $n \geq 18$, the function $h(m)$ is increasing when $n+8 \leq m \leq 2n^{3/2}$. The derivative of $h(m)$ satisfies

$$h'(m) = 2mn^2(n-1) - 4(n^2+2m-3n+2)(2m-n+1) - 2(n^2+2m-3n+2)^2.$$

It is enough to show $h'(m) > 0$ for $n+8 \leq m \leq 2n^{3/2}$ and $n \geq 18$. Let $l(m) = h'(m)$. Taking derivative, we have

$$l'(m) = 2n^3 - 18n^2 - 48m + 56n - 40.$$

Also, the second derivative $l''(m) = -48$. Therefore, the function $l(m)$ is concave down. If we can show $l(n+8) > 0$ and $l(2n^{3/2}) > 0$ for $n \geq 18$, then we establish $l(m) > 0$ for all $n+8 \leq m \leq 2n^{3/2}$. We notice $l(n+8) = 14n^3 - 154n^2 + 68n - 1872 > 0$ when $n \geq 18$. We get

$$l(2n^{3/2}) = 4n^{9/2} - 2n^4 - 36n^{7/2} - 80n^3 + 112n^{5/2} - 42n^2 - 80n^{3/2} + 44n - 16.$$

One can confirm $l(2n^{3/2}) > 0$ for $n = 18$ and $l(2n^{3/2})$ is increasing when $n \geq 18$ easily by taking derivative. We already proved $l(m) = h'(m) > 0$ when $n+8 \leq m \leq 2n^{3/2}$ and $n \geq 18$. Combining with $h(n+8) > 0$, we get $h(m) > 0$ when $n+8 \leq m \leq 2n^{3/2}$ and $n \geq 18$. Thus, $f(m) > 0$ for $n \geq 15$ and $n+8 \leq m \leq \min\{2n^{3/2}, \binom{n}{2}\}$, that is,

$$\frac{m}{\sqrt{2m-(n-1)}} > \sqrt{n-1} - \frac{2m-2(n-1)}{n\sqrt{n-1}}.$$

By Theorems 2.12 and 2.1, we have

$$R(G) \geq \frac{m}{\lambda_1} \geq \frac{m}{\sqrt{2m-(n-1)}} > \sqrt{n-1} + \frac{2m-2(n-1)}{n\sqrt{n-1}}.$$

By Lemma 2.4, we get

$$\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}.$$

□

Similar to the lemma above, we can prove the following one.

Lemma 3.2. *Let G be a connected graph with n vertices and m edges. If $n = 13$ and $24 \le m \le 78 = \binom{13}{2}$, or $n = 14$ and $23 \le m \le 91 = \binom{14}{2}$, then*

$$\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}.$$

We can show $f(m) > 0$ using computer very easily, which is sufficient to prove the lemma by noticing Theorems 2.12, 2.1, and 2.4.

If a graph is relatively dense, then we can show the desired upper bound for $\frac{q(G)}{R(G)}$ easily by the following lemma.

Lemma 3.3. *Let G be a connected graph with n vertices and m edges. If $m \ge 2n^{3/2}$, then*

$$\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}.$$

Proof. If $m \ge 2n^{3/2}$, then by the definition of $R(G)$, we have

$$R(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{d(x)d(y)}} \ge \frac{m}{n-1} \ge \frac{2n^{3/2}}{n-1}. \tag{3}$$

Recall the well-known fact $q(G) \le 2\Delta \le 2(n-1)$. Thus, we have

$$\frac{q(G)}{R(G)} \le \frac{(n-1)^2}{n^{3/2}} < \frac{n}{\sqrt{n-1}}.$$

□

In the case of graphs with small maximum degree, the following lemma will prove the main theorem.

Lemma 3.4. *Let G be a connected graph with n vertices. If $\Delta(G) < n/2$, then we have*

$$\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}.$$

Proof. We note $q(G) \le 2\Delta < n$ and $R(G) \ge \sqrt{n-1}$ by Theorem 2.5. We get $\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}$. □

With strong assumptions on the maximum degree and the number of edges of a graph, we are able to establish the desired upper bound on $\frac{q(G)}{R(G)}$.

Lemma 3.5. *Let G be a connected graph with $n \ge 13$ vertices. If either of the following cases holds:*
(1) $n/2 \le \Delta \le n-4$ and $e(G) = n+k$ for $1 \le k \le 10$;
(2) $\Delta = n-3$ and $e(G) = n+k$ for $1 \le k \le 7$;
(3) $\Delta = n-2$ and $e(G) = n+k$ for $1 \le k \le 4$,
then

$$\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}.$$

Proof. We use Theorem 2.3 to show $q(G) \leq n$. For any vertex $v \in V(G)$, let $S_v = V(G) \setminus (\{v\} \cup N(v))$. We shall show

$$t(v) := d(v) + m(v) \leq n$$

for each $v \in V(G)$. We note $2(n+k) = \sum_{w \in V(G)} d(w) = d_v + \sum_{w \in N(v)} d_w + \sum_{w \in S_v} d_w$. Therefore, we have

$$\begin{aligned} t(v) &= d(v) + \frac{2(n+k) - d(v) - \sum_{u \in S_v} d(u)}{d(v)} \\ &\leq d(v) + \frac{2(n+k) - d(v) - (n-1-d(v))}{d(v)} \\ &= d(v) + \frac{n+2k+1}{d(v)}. \end{aligned}$$

Consider the function $f(x) = x + \frac{n+2k+1}{x}$. We know $f(x)$ is increasing when $x \in (\sqrt{n+2k+1}, \infty)$ and decreasing when $x \in (1, \sqrt{n+2k+1})$. Furthermore, for any vertex v with degree at least 4, we have

$$t(v) \leq \max\left\{\Delta + \frac{n+2k+1}{\Delta}, 4 + \frac{n+2k+1}{4}\right\} \leq \max\left\{\Delta + \frac{n+2k+1}{\Delta}, n\right\}.$$

Here we note $4 + \frac{n+2k+1}{4} \leq n$ when $1 \leq k \leq 10$ and $n \geq 13$. Suppose (1) holds. When $n \geq 13$ and $k \leq 10$, we have

$$(n-4) \geq \Delta \geq n/2 > \sqrt{n+21} \geq \sqrt{n+2k+1}.$$

Thus

$$\Delta + \frac{n+2k+1}{\Delta} \leq (n-4) + \frac{n+21}{n-4} < n$$

when $n \geq 13$. If (2) holds, then we get

$$\Delta + \frac{n+2k+1}{\Delta} \leq (n-3) + \frac{n+15}{n-3} < n$$

when $n \geq 13$. If (3) holds, then we obtain

$$\Delta + \frac{n+2k+1}{\Delta} \leq (n-2) + \frac{n+9}{n-2} \leq n$$

when $n \geq 13$.

Now we need only to consider the vertices with degree 1, or 2, or 3. If $d(v) = 1$, then $t(v) = d(v) + m(v) \leq 1 + \Delta \leq n$. If $d(v) = 2$, then $t(v) \leq 2 + \Delta \leq 2 + (n-2) = n$. If $d(v) = 3$ and $\Delta \leq n-3$, then $t(v) \leq 3 + (n-3) = n$. We are left with $d(v) = 3$ and $\Delta = n-2$, In this case, $k \leq 4$. Therefore, $t(v) \leq 3 + \frac{n+9}{3} \leq n$ when $n \geq 13$.

By Theorem 2.5, we have $R(G) > \sqrt{n-1}$ if G is connected and $e(G) \geq n$. Thus, $\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}$. □

We need the following lemma for the case of $n = 12$.

Lemma 3.6. *Let G be a connected graph with 12 vertices. If either of the following cases holds:*
(1) $6 \leq \Delta(G) \leq 8$ and $e(G) = 12 + k$ for $1 \leq k \leq 8$;

(2) $\Delta(G) = 9$ *and* $e(G) = 12 + k$ *for* $1 \le k \le 6$*;*
(3) $\Delta(G) = 10$ *and* $e(G) = 12 + k$ *for* $1 \le k \le 3$*,*
then

$$\frac{q(G)}{R(G)} < \frac{12}{\sqrt{11}}.$$

The proof of the lemma is exactly the same as the one for proving Lemma 3.5 and it is omitted here.

The next three lemmas will deal with those graphs with large maximum degree and small number of edges.

Lemma 3.7. *Let* G *be a connected graph with* 13 *vertices. If either of the following holds:*

1. $\Delta(G) = 12$ *and* $e(G) = 13 + k$ *for* $1 \le k \le 10$*;*
2. $\Delta(G) = 11$ *and* $e(G) = 13 + k$ *for* $5 \le k \le 10$*;*
3. $\Delta(G) = 10$*, and* $e(G) = 13 + k$ *for* $8 \le k \le 10$*,*

then we have

$$R(G) > \sqrt{12} + \frac{2(k+1)}{13\sqrt{12}}.$$

Proof. Since proofs of three cases are very similar, we will present the detailed proof of Case 1 and sketch proofs of others. For each case, we will assume v_0 is a vertex with the maximum degree and $N_G(v_0) = \{v_1, \ldots, v_\Delta\}$. If $\delta(G) \ge 2$, then Lemma 2.7 will complete the proof. Thus, we assume G has at least one vertex with degree one in each case.

Case 1: $\Delta(G) = 12$. We first consider the case of $k = 1$, i.e., $e(G) = 14$. Let H be the subgraph induced by $N_G(v_0)$. We have H is either a P_3 together with 9 isolated vertices or two disjoint edges together with 8 isolated vertices. For the former case, we have

$$R(G) = \frac{9}{\sqrt{12}} + \frac{2}{\sqrt{2 \cdot 12}} + \frac{1}{\sqrt{3 \cdot 12}} + \frac{2}{\sqrt{2 \cdot 3}} > \sqrt{12} + \frac{4}{13\sqrt{12}}.$$

For the latter case, we have

$$R(G) = \frac{8}{\sqrt{12}} + \frac{4}{\sqrt{2 \cdot 12}} + \frac{2}{\sqrt{2 \cdot 2}} > \sqrt{12} + \frac{4}{13\sqrt{12}}.$$

Next assume $2 \le k \le 10$. Recall that $d(v_0) = 12$ and $N_G(v_0) = \{v_1, \ldots, v_{12}\}$. Let $\{v_1, v_2, \ldots, v_s\}$ be the set of vertices with degree one in G.

When $k = 10$, we claim $1 \le s \le 6$. Otherwise, $s \ge 7$. Let G' be the subgraph induced by $\{v_{s+1}, \ldots, v_{12}\}$. We have $e(G') = e(G) - d(v_0) = 11$. Since $s \ge 7$, we have $|V(G')| \le 5$. However, G' can have at most $\binom{5}{2} = 10$ edges, which is a contradiction. Repeating the argument above, we can show $s \le 7$ when $6 \le k \le 9$. Similarly, we have $s \le 8$ when $3 \le k \le 5$. In the case of $k = 2$, we have $s \le 9$.

We next apply Proposition 2.11 to $(v_1, \ldots, v_s)$. We observe that $d_{G_i}(v_{i+1}) = 1$ and $\Delta(G_i) = 12 - i$ for $0 \le i \le s - 1$. Moreover, $|V(G_s)| = 13 - s$ and $\delta(G_s) \ge 2$. Recalling Theorem 2.6, we have

$$R(G) \ge \sum_{i=0}^{s-1} \frac{1}{2\sqrt{12 - i}} + \sqrt{2(12 - s)} + \frac{1}{12 - s} - \sqrt{\frac{2}{12 - s}}. \tag{4}$$

Since we have proved an upper bound on s depending on the value of k, the inequality

$$\sum_{i=0}^{s-1} \frac{1}{2\sqrt{12-i}} + \sqrt{2(12-s)} + \frac{1}{12-s} - \sqrt{\frac{2}{12-s}} > \sqrt{12} + \frac{2(k+1)}{13\sqrt{12}} \tag{5}$$

can be verified using the computer for each k.

Case 2: $\Delta(G) = 11$. Let $\{v_{12}\} = V(G) \setminus (\{v_0\} \cup N(v_0))$. We have two subcases depending on the degree of v_{12}.

Subcase 2.1: $d(v_{12}) = 1$. Let $G_1 = G - v_{12}$. If $\{v_1, \ldots, v_t\}$ is the set of vertices of degree one in G_1, then we can prove an upper bound on $s = t+1$ depending on the value of k by the same argument as Case 1. We apply Proposition 2.11 to $(v_{12}, v_1, \ldots, v_{s-1})$. We observe $\Delta(G_i) \le 12 - i$ for $0 \le i \le s-1$, $|V(G_s)| = 13 - s$, and $\delta(G_s) \ge 2$. Therefore, Inequalities (4) and (5) still hold for this case and we can prove the desired lower bound for $R(G)$ similarly.

Subcase 2.2: $d(v_{12}) \ge 2$. Let $\{v_1, \ldots, v_s\}$ be the set of vertices with degree one in G. Repeating the argument for Case 1, we can get the asserted lower bound on $R(G)$. Here, we note $\Delta(G_i) \le 12 - i$ for $0 \le i \le s-1$ still holds when we apply Proposition 2.11. We may have a smaller upper bound on s than the one in Case 1 for the same value of k, which does not affect the result.

Case 3: $\Delta(G) = 10$. Let $\{v_{11}, v_{12}\} = V(G) \setminus (\{v_0\} \cup N(v_0))$. We have two subcases.

Subcase 3.1: $d(v_{11}), d(v_{12}) \ge 2$. Let $\{v_1, \ldots, v_s\}$ be the set of vertices with degree one in G. We can repeat the argument in Subcase 2.2 to show the desired lower bound for $R(G)$.

Subcase 3.2: Either $d(v_{11}) = 1$ or $d(v_{12}) = 1$. We assume $d(v_{11}) = 1$. Let $G_1 = G - v_{11}$.

If $d_{G_1}(v_{12}) = 1$, then we define $G_2 = G_1 - v_{12}$. Let $\{v_1, \ldots, v_t\}$ be the set of vertices with degree one in G_2. We can use the argument in Case 1 to show an upper bound on $s+2$ depending on the value of k. We apply Proposition 2.11 with $(v_{11}, v_{12}, v_1, \ldots, v_t)$. We still have $\Delta(G_i) \le 12 - i$ for $0 \le i \le s-1$. Therefore, Inequalities (4) and (5) are true and the claimed lower bound for $R(G)$ follows.

If $d_{G_1}(v_{12}) \ge 2$, then we can use the argument for Subcase 2.1 to complete the proof of this lemma. □

We will need the following lemma for $n = 12$.

Lemma 3.8. *Let G be a connected graph with 12 vertices. If either of the following holds:*

1. $\Delta(G) = 11$ *and* $e(G) = 12 + k$ *for* $1 \le k \le 8$*;*
2. $\Delta(G) = 10$ *and* $e(G) = 12 + k$ *for* $4 \le k \le 8$*;*
3. $\Delta(G) = 9$*, and* $e(G) = 12 + k$ *for* $7 \le k \le 8$*,*

then we have

$$R(G) > \sqrt{11} + \frac{2(k+1)}{12\sqrt{11}}.$$

We skip the proof here because it uses the same argument as the proof of Lemma 3.7. The next lemma is in the same sprit of Lemma 3.7.

Lemma 3.9. *Let G be a connected graph with $n \geq 13$ vertices. If either of the following holds:*

1. $\Delta(G) = n - 1$ *and* $e(G) = n + k$ *for* $1 \leq k \leq 10$*;*

2. $\Delta(G) = n - 2$ *and* $e(G) = n + k$ *for* $5 \leq k \leq 10$*;*

3. $\Delta(G) = n - 3$*, and* $e(G) = n + k$ *for* $8 \leq k \leq 10$*,*

then we have

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

Proof. We prove the lemma by induction on n. The base case $n = 13$ is given by Lemma 3.7. We assume the lemma holds for $|V(G)| = n$. For the inductive step where $|V(G)| = n + 1$, if $\delta(G) \geq 2$, then the lemma follows from Theorem 2.7. Thus we assume G has at least one vertex with degree one. We assume further v_0 is a vertex with maximum degree. We have three cases.

Case 1: $\Delta(G) = |V(G)| - 1 = n$. Let $v_1 \in N_G(v_0)$ be a vertex with degree one. If we define $G' = G - v_1$, then we have $|V(G')| = n$ and $\Delta(G') = |V(G)'| - 1$. We have $R(G') > \sqrt{n-1} + \frac{2(k+1)}{n\sqrt{n-1}}$ by the inductive hypothesis. Lemma 2.10 completes the proof of this case.

Case 2: $\Delta(G) = |V(G)| - 2 = n - 1$. Assume $\{v_n\} = V(G) \setminus (\{v_0\} \cup N(v_0))$. If $d(v_n) = 1$, then we let $G' = G - v_n$. We get $V(G') = n$ and $\Delta(G') = |V(G')| - 1$. If $d(v_n) \geq 2$, then let $v_1 \in N(v_0)$ such that $d(v_1) = 1$. Set $G' = G - v_1$. We have $V(G') = n$ and $\Delta(G') \geq |V(G')| - 2$. In either case, we have $R(G') > \sqrt{n-1} + \frac{2(k+1)}{n\sqrt{n-1}}$ by the inductive hypothesis. The inductive step then follows from Lemma 2.10.

Case 3: $\Delta(G) = |V(G)| - 3 = n - 2$. Assume $\{v_{n-1}, v_n\} = V(G) \setminus (\{v_0\} \cup N(v_0))$. If one of v_{n-1} and v_n has degree one, say v_n, then we let $G' = G - v_n$. We observe $V(G') = n$ and $\Delta(G') = |V(G')| - 2$. If $d(v_{n-1}), d(v_n) \geq 2$, then let $v_1 \in N(v_0)$ such that $d(v_1) = 1$. Set $G' = G - v_1$. We have $V(G') = n$ and $\Delta(G') \geq |V(G')| - 3$. In either case, the inductive hypothesis gives $R(G') > \sqrt{n-1} + \frac{2(k+1)}{n\sqrt{n-1}}$. We can prove the inductive step by using Lemma 2.10. ☐

The combination of Lemma 3.9 and Lemma 2.4 yields the next lemma.

Lemma 3.10. *Let G be a connected graph with $n \geq 13$ vertices. If either of the following holds:*

1. $\Delta(G) = n - 1$ *and* $e(G) = n + k$ *for* $1 \leq k \leq 10$*;*

2. $\Delta(G) = n - 2$ *and* $e(G) = n + k$ *for* $5 \leq k \leq 10$*;*

3. $\Delta(G) = n - 3$*, and* $e(G) = n + k$ *for* $8 \leq k \leq 10$*,*

then we have

$$\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}.$$

We are now ready to prove the main theorem.

Proof of Theorem 1.2. If $e(G) = n - 1$, then G is a tree. We have $q(G) = n$ and $R(G) \geq \sqrt{n-1}$ by Theorem 2.5. Thus, $\frac{q(G)}{R(G)} \leq \frac{n}{\sqrt{n-1}}$. If $e(G) = n$, then Theorem 2.8

implies $R(G) \geq R(S_n^*) = \frac{n-3}{\sqrt{n-1}} + \sqrt{\frac{2}{n-1}} + \frac{1}{2} > \sqrt{n-1} + \frac{2}{n\sqrt{n-1}}$ when $n \geq 12$. By Lemma 2.4, we have $\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}$. For $n = 12$, we note $\frac{12}{\sqrt{11}} < \frac{11}{3}$. For the rest of the proof, we assume $e(G) = n + k$ with $k \geq 1$. We first prove the second part of the theorem, namely, $n \geq 13$. We shall consider the following three cases depending on the range of $e(G)$.

Case 1: $e(G) \geq 2n^{3/2}$. We get $\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}$ by Lemma 3.3.

Case 2: $n + 11 \leq e(G) \leq \min\{2n^{3/2}, \binom{n}{2}\}$. In this case, $\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}$ is given by Lemma 3.2 and Lemma 3.1.

Case 3: $n + 1 \leq e(G) \leq n + 10$. We consider the following subcases depending on $\Delta(G)$. We claim $\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}$ for each subcase.

Subcase 3.1: $\Delta(G) = n - 1$. Part 1 of Lemma 3.10 proves the claim.

Subcase 3.2: $\Delta(G) = n - 2$. The case of $n + 1 \leq e(G) \leq n + 4$ is proved by Part 3 of Lemma 3.5 and the case of $n + 5 \leq e(G) \leq n + 10$ is proved by Part 2 of Lemma 3.10.

Subcase 3.3: $\Delta(G) = n - 3$. Part 2 of Lemma 3.5 proves the case of $n + 1 \leq e(G) \leq n + 7$ and Part 3 of Lemma 3.10 proves the case of $n + 8 \leq e(G) \leq n + 10$.

Subcase 3.4: $n/2 \leq \Delta(G) \leq n - 4$. Part 1 of Lemma 3.5 implies the claim.

Subcase 3.5: $\Delta(G) < n/2$. Lemma 3.4 gives us the claim.

From the argument for $e(G) \geq n$ and $n \geq 13$, we get $\frac{q(G)}{R(G)} < \frac{n}{\sqrt{n-1}}$ when $e(G) \geq n$. Therefore, $\frac{q(G)}{R(G)} = \frac{n}{\sqrt{n-1}}$ can only occur for $e(G) = n - 1$. By Theorem 2.5, we get the equality holds if and only if G is a star when $n \geq 13$.

We are left with the case where $n = 12$. We shall use the function $g(m)$ from the proof of Theorem 10 in [7]. Specialized to $n = 12$, we get

$$g(m) = \frac{\left(\frac{2m}{11} + 10\right)\sqrt{2m - 11}}{m}.$$

Let $m = e(G)$. With the help of computer, we get $g(m) < \frac{11}{3}$ for $21 \leq m \leq \binom{12}{2} - 1 = 65$ and $g(66) = \frac{11}{3}$. Equivalently, $\frac{q(G)}{R(G)} < \frac{11}{3}$ when $21 \leq m \leq 65$. We need only to prove the case of $m = 12 + k$ for $1 \leq k \leq 8$. Recall Lemmas 2.4, 3.4, 3.6, and 3.8. Repeating the case analysis above, we can show $\frac{q(G)}{R(G)} < \frac{12}{\sqrt{11}} < \frac{11}{3}$ when $13 \leq e(G) \leq 20$. We already have proved $\frac{q(G)}{R(G)} < \frac{11}{3}$ when $e(G) \in \{n - 1, n\}$. Therefore, $\frac{q(G)}{R(G)} = \frac{11}{3}$ may hold only for $e(G) = 66$, which turns out to be true because $G = K_{12}$.

We have completed the proof of the main theorem.

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