Randić index and the diameter of a graph*

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Abstract

The Randić index $R(G)$ of a nontrivial connected graph G is defined as the sum of the weights $(d(u)d(v))^{-\frac{1}{2}}$ over all edges $e = uv$ of G. We prove that $R(G) \geq d(G)/2$, where $d(G)$ is the diameter of G. This immediately implies that $R(G) \geq r(G)/2$, which is the closest result to the well-known Grafiti conjecture $R(G) \geq r(G) - 1$ of Fajtlowicz [4], where $r(G)$ is the radius of G. Asymptotically, our result approaches the bound $\frac{R(G)}{d(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}$ conjectured by Aouchiche, Hansen and Zheng [1].

1 Introduction

All the graphs considered in this paper are simple undirected ones. The *eccentricity* of a vertex v of a graph G is the greatest distance from v to any other vertex of G. The *radius* (resp. *diameter*) of a graph is the minimum (resp. maximum) over eccentricities of all vertices of the graph. The radius and diameter will be denoted by $r(G)$ and $d(G)$, respectively.

There are many different kinds of chemical indices. Some of them are distance based indices like Wiener index, some are degree based indices like Randić index. The *Randić index* $R(G)$ of a graph G is defined as

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

It is also known as connectivity index or branching index. Randić [11] in 1975 proposed this index for measuring the extent of branching of the carbon-atom

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skeleton of saturated hydrocarbons. There is also a good correlation between Randić index and several physicochemical properties of alkanes: boiling points, surface areas, energy levels, etc. In 1998 Bollobás and Erdös [2] generalized this index by replacing the square-root by power of any real number, which is called the *general Randić index.* For a comprehensive survey of its mathematical properties, see the book of Li and Gutman [7], or recent survey of Li and Shi [10]. See also the books of Kier and Hall [5, 6] for chemical properties of this index.

There are several conjectures linking Randić index to other graph parameters. Fajtlowicz [4] posed the following problem:

Conjecture 1. *For every connected graph G, it holds $R(G) \geq r(G) - 1$.*

Caporossi and Hansen [3] showed that $R(T) \geq r(T) + \sqrt{2} - 3/2$ for all trees T. Liu and Gutman [9] verified the conjecture for unicyclic graphs, bicyclic graphs and chemical graphs with cyclomatic number $c(G) \leq 5$. You and Liu [12] proved that the conjecture is true for biregular graphs, tricyclic graphs and connected graphs of order $n \leq 10$.

Regarding the diameter, Aouchiche, Hansen and Zheng [1] conjectured the following:

Conjecture 2. *Any connected graph G of order $n \geq 3$ satisfies*

$$R(G) - d(G) \geq \sqrt{2} - \frac{n+1}{2} \qquad \textit{and} \qquad \frac{R(G)}{d(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2},$$

with equalities if and only if G is a path on n vertices.

Li and Shi [8] proved the first inequality for graphs of minimum degree at least 5. They also proved the second inequality for graphs on $n \geq 15$ vertices with minimum degree at least $n/5$.

The Randić index turns out to be quite difficult parameter to work with. Also, Conjecture 1 is quite weak for graphs with small radius; for instance, $R(K_{1,n}) = \sqrt{n}$, while $r(K_{1,n}) = 1$ for all n. Instead, we work with a different parameter $R'(G)$ defined by

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\max(\deg(u), \deg(v))}.$$

Note that $R(G) \geq R'(G)$ for every graph G, with the equality achieved only if every connected component of G is regular. The main result of this paper is the following:

Theorem 3. *For any connected graph G, $R'(G) \geq d(G)/2$.*

Since $R(G) \geq R'(G)$ and $d(G) \geq r(G)$, by our theorem, we immediately obtain that $R(G) \geq r(G)/2$. This result supports Conjecture 1. Our result solves asymptotically the second claim of Conjecture 2. Let us remark that the bound of Theorem 3 is sharp, with the equality achieved for example by paths of length at least two. Since Conjecture 2 is also tight for paths, in order to prove Conjecture 2 using our technique, it would be necessary to consider the gap $R(G) - R'(G)$.

2 Proof of the main theorem

We prove the theorem by contradiction. In the rest of the paper, assume that G is a connected graph such that $R'(G) < d(G)/2$ and G has the smallest number of edges among the graphs with this property, i.e., $R'(H) \geq d(H)/2$ for every connected graph H with $|E(H)| < |E(G)|$. Let $n = |V(G)|$. For an edge uv, a *weight* of uv is $\frac{1}{\max(\deg(u),\deg(v))}$.

If $d(G) = 0$, then $G = K_1$ and $R'(G) = 0 = d(G)/2$. If $1 \leq d(G) \leq 2$, then G has at least one edge; observe that the sum of the weights of the edges incident with the vertex of G of maximum degree is one, thus $R'(G) \geq 1 \geq d(G)/2$. Therefore, $d(G) \geq 3$.

For two vertices x and y of a graph H, let $d_H(x, y)$ denote the distance between x and y in H.

Lemma 4. *If v is a cut-vertex in G, then all components of $G - v$ except for one consist of a single vertex.*

Proof. Assume for a contradiction that $G - v$ has two components with more than one vertex. Then, there exist induced subgraphs $G_1, G_2 \subseteq G$ such that $G_1 \cup G_2 = G$, $V(G_1) \cap V(G_2) = \{v\}$ and $G_i - v$ has a component with more than one vertex, for $i \in \{1, 2\}$.

For $i \in \{1, 2\}$, let G'_i be the graph obtained from G_i by adding $\deg_{G_{3-i}}(v)$ pendant vertices adjacent to v and let v_i be one of these new vertices. Observe that $R'(G'_1)+R'(G'_2) = R'(G)+1$. Furthermore, consider any two vertices $x, y \in V(G)$. If $x, y \in V(G_1)$, then $d_G(x, y) = d_{G'_1}(x, y) \leq d(G'_1) \leq d(G'_1) + d(G'_2) - 2$. By symmetry, if $x, y \in V(G_2)$, then $d_G(x, y) \leq d(G'_1)+d(G'_2)-2$. Finally, if say $x \in V(G_1)$ and $y \in V(G_2)$, then $d_G(x, y) = d_{G_1}(x, v) + d_{G_2}(y, v) = d_{G'_1}(x, v_1) - 1+d_{G'_2}(y, v_2)-1 \leq d(G'_1)+d(G'_2)-2$. We conclude that $d(G) \leq d(G'_1)+d(G'_2)-2$.

Since both G'_1 and G'_2 have fewer edges than G, the minimality of G implies that

$$R'(G) = R'(G'_1) + R'(G'_2) - 1 \geq \frac{d(G'_1)}{2} + \frac{d(G'_2)}{2} - 1 \geq \frac{d(G)}{2},$$

which contradicts the assumption that G is a counterexample to Theorem 3. $\square$

A vertex v is *locally minimal* if its degree is smaller or equal to the degrees of its neighbors.

Lemma 5. *Let $v \in V(G)$ be a locally minimal vertex. Then* $\deg(v) = 1$, *the neighbor of v has degree at least three and $d(G - v) = d(G) - 1$.*

Proof. Suppose first that $\deg(v) > 1$. Let w be a neighbor of v and k the number of neigbors of w distinct from v whose degree is smaller than $\deg(w)$. Note that $k \leq \deg(w) - 1$. We have

$$\begin{aligned} R'(G - vw) &= R'(G) - \frac{1}{\deg(w)} + k\left(\frac{1}{\deg(w) - 1} - \frac{1}{\deg(w)}\right) \\ &= R'(G) - \frac{1}{\deg(w)} + \frac{k}{\deg(w)(\deg(w) - 1)} \\ &\leq R'(G). \end{aligned}$$

Since v is locally minimal, every neighbor of v has degree at least $\deg(v) \geq 2$, thus by Lemma 4, v is not a cut-vertex. It follows that $G - vw$ is connected, hence $d(G - vw) \geq d(G)$. By the minimality of G, we obtain $R'(G) \geq R'(G - vw) \geq d(G - vw)/2 \geq d(G)/2$, which is a contradiction.

Let us now consider the case that $\deg(v) = 1$. Then $d(G - v)/2 \leq R'(G - v) \leq R'(G) < d(G)/2$, and thus $d(G - v) < d(G)$. Removing the pendant vertex v cannot decrease the diameter by more than one, thus $d(G - v) = d(G) - 1$. Since $d(G) \geq 3$, the neighbor w of v has degree at least two, and if $\deg(w) = 2$, then v is the only neighbor of w of degree smaller than $\deg(w)$. It follows that if $\deg(w) = 2$, then $R'(G - v) = R'(G) - 1/2$. We conclude that $R'(G) = R'(G - v) + 1/2 \geq d(G - v)/2 + 1/2 = d(G)/2$, which is a contradiction. This implies that $\deg(w) \geq 3$. □

Let L be the set of vertices of G of degree one. Note that a vertex of G of the smallest degree is locally minimal, thus by Lemma 5, $L \neq \emptyset$.

Lemma 6. *If the distance between two vertices u and v in G is $d(G)$, then $L \subseteq \{u, v\}$.*

Proof. Suppose that there exists a vertex $w \in L \setminus \{u, v\}$. Then w is locally minimal and $d(G - w) = d(G)$, contradicting Lemma 5. □

Lemma 6 implies that $|L| \leq 2$. Lemma 5 shows that all vertices of degree $d > 1$ are incident with an edge whose weight is $1/d$; thus, if many vertices have small degree, then these edges contribute a lot to $R'(G)$. On the other hand, if many vertices have large degree, then G has many edges and $R'(G)$ is large. Let us now formalize this intuition.

Lemma 7. $d(G) > \sqrt{8(n - 3)} - 1$, *and thus* $n \leq \left\lfloor \frac{d^2(G) + 2d(G)}{8} \right\rfloor + 3$.

Proof. Let $d_1 \geq d_2 \geq \ldots \geq d_n$ be the degree sequence of G. For $1 \leq i \leq n$, let v_i be the vertex of G of degree d_i. For each $i \geq 1$, the sum of the weights of the edges incident with v_i, but not incident with v_j for any $j < i$, is at least $1-(i-1)/d_i$. We conclude that the edges incident with the vertices v_1, v_2, ..., v_t contribute at least $t - \sum_{i=1}^{t} \frac{i-1}{d_i} \geq t - \frac{t(t-1)}{2d_t}$ to $R'(G)$. Let t_0 be the largest integer such that $d_{t_0} \geq t_0 - 1$; thus, for each $i > t_0$, $d_i \leq d_{t_0+1} < (t_0+1)-1 = t_0$. Then the sum of the weights of the edges incident with the vertices v_1, v_2, ..., v_{t_0} is at least $t_0 - \frac{t_0(t_0-1)}{2(t_0-1)} = \frac{t_0}{2}$.

By Lemma 5, any vertex $v \notin L$ has a neighbor $s(v)$ with strictly smaller degree. Let $X = \{v_i s(v_i) | i \geq t_0+1, v_i \notin L\}$. Note that the edges in X are pairwise distinct, thus $|X| \geq n - t_0 - 2$. None of the edges in X is incident with the vertices v_1, ..., v_{t_0}, hence each of them has weight at least $\frac{1}{t_0-1}$, and

$$\begin{aligned} R'(G) &\geq \frac{t_0}{2} + \frac{n-t_0-2}{t_0-1} \\ &= \frac{t_0-1}{2} + \frac{n-3}{t_0-1} - \frac{1}{2} \\ &\geq \sqrt{2(n-3)} - \frac{1}{2}, \end{aligned}$$

where the last inequality holds since $x + y \geq 2\sqrt{xy}$ for all $x, y \geq 0$. As G is a counterexample to Theorem 3, $d(G) > 2R'(G) \geq \sqrt{8(n-3)} - 1$. This is equivalent to $d^2(G) + 2d(G) + 1 > 8(n-3)$. Since both sides of this inequality are integers, $d^2(G) + 2d(G) \geq 8(n-3)$, and thus

$$n \leq \left\lfloor \frac{d^2(G) + 2d(G)}{8} \right\rfloor + 3.$$

□

Let w be a neigbor of a vertex of degree one. By Lemma 5, w has degree at least three, and since $d(G) \geq 3$, at least one vertex of G is not adjacent to w. We conclude that $n \geq 5$, and by Lemma 7, $d(G) > 3$. Lemma 5 also implies that the vertices of G of small degree must be close to L:

Lemma 8. *If the distance of a vertex v from L is at least $k > 0$, then* $\deg(v) \geq k + 2$.

Proof. By Lemma 5, each vertex not in L has a neighbor of strictly smaller degree, thus there exists a path P from v to L such that the degrees on P are decreasing. Also, the vertex in P that has a neighbor in L has degree at least three. Since P has length at least k, we have $\deg(v) \geq 3 + \ell(P) - 1 \geq k + 2$. □

Choose a vertex $v_0 \in L$, and for each integer i, let L_i be the set of vertices of G at the distance i from v_0, as illustrated in Figure 1. Let δ_i be the minimum

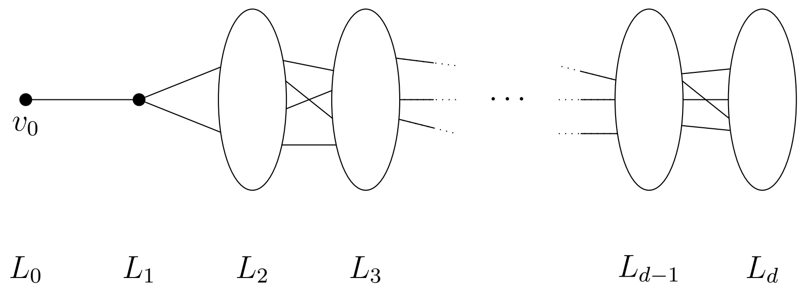

Figure 1: A graph G with vertices partitioned into layers $L_0, L_1, \ldots, L_d$.

and Δ_i the maximum degree of a vertex in L_i, and let $n_i = |L_i|$. Observe that $n_0 = n_1 = 1$, $n_{d(G)} \geq 1$ and $n = \sum_{i=0}^{d(G)} n_i$. Furthermore, by Lemma 6, if $|L| > 1$ then $n_{d(G)} = 1$ and $L = L_0 \cup L_{d(G)}$.

For an integer i, let $\bar{i} = \min(i, d(G) - i)$. Note that the distance between L and L_i is at least $\bar{i}$. By Lemma 8, we have $\Delta_i \geq \delta_i \geq \bar{i} + 2$ for $1 \leq i \leq d(G) - 1$. Also, since all neighbors of a vertex in L_i belong to $L_{i-1} \cup L_i \cup L_{i+1}$, it follows that $\Delta_i \leq n_{i-1} + n_i + n_{i+1} - 1$, and thus $n_{i-1} + n_i + n_{i+1} \geq \bar{i} + 3$.

By Lemma 4, $n_i \geq 2$ for $2 \leq i \leq d(G) - 2$, and thus $n \geq 2d(G) - 2$. Together with Lemma 7, we obtain

$$2d(G) - 2 \leq n \leq \frac{d^2(G) + 2d(G)}{8} + 3,$$

which implies $d(G) \leq 4$ or $d(G) \geq 10$. If $d(G) = 4$, then $n_1 + n_2 + n_3 \geq \bar{2} + 3 = 5$, and thus $n \geq 7 > \frac{d^2(G)+2d(G)}{8} + 3$. This contradicts Lemma 7, hence $d(G) \geq 10$.

Let us now derive some formulas dealing with $\bar{i}$ that we later use to estimate the sizes of the layers L_i.

Lemma 9. *The following holds:*

(a)

$$\sum_{i=0}^{d(G)} \bar{i} \geq \frac{d^2(G) - 1}{4}.$$

(b)

$$\sum_{i=0}^{d(G)} \bar{i}^2 \geq \frac{d^3(G) - d(G)}{12}.$$

Proof. We use the well-known formulas $\sum_{i=0}^{k} i = \frac{k(k+1)}{2}$ and $\sum_{i=0}^{k} i^2 = \frac{k(k+1)(2k+1)}{6}$.

If $d(G)$ is odd, then

$$\sum_{i=0}^{d(G)} \bar{i} = 2 \sum_{i=0}^{(d(G)-1)/2} i = \frac{d^2(G) - 1}{4}$$

and

$$\sum_{i=0}^{d(G)} \bar{i}^2 = 2\sum_{i=0}^{(d(G)-1)/2} i^2 = \frac{d^3(G)-d(G)}{12}.$$

If $d(G)$ is even, then

$$\sum_{i=0}^{d(G)} \bar{i} = \frac{d(G)}{2} + 2\sum_{i=0}^{d(G)/2-1} i = \frac{d^2(G)}{4} > \frac{d^2(G)-1}{4}$$

and

$$\sum_{i=0}^{d(G)} \bar{i}^2 = \frac{d^2(G)}{4} + 2\sum_{i=0}^{d(G)/2-1} i^2 = \frac{d^3(G)+2d(G)}{12} > \frac{d^3(G)-d(G)}{12}.$$

□

Let R_i be the sum of the weights of the edges induced by L_i plus half of the weights of the edges joining vertices of L_i with vertices of L_{i-1} and L_{i+1}. Observe that $R'(G) = \sum_{i\geq 0} R_i$. Also, the weight of each edge incident with a vertex of L_i is at least $\frac{1}{\max(\Delta_{i-1},\Delta_i,\Delta_{i+1})}$, thus $R_i \geq \frac{n_i\delta_i}{2\max(\Delta_{i-1},\Delta_i,\Delta_{i+1})}$. Let $s_i = n_{i-1}+n_i+n_{i+1}$ and $W_i = \frac{n_i(\bar{i}+2)}{\max(s_{i-1},s_i,s_{i+1})-1}$. Since $\Delta_i \leq s_i - 1$ and $\delta_i \geq \bar{i}+2$ for $1 \leq i \leq d(G)-1$, we have $R_i \geq W_i/2$ for $2 \leq i \leq d(G)-2$. Note also that $s_i \geq \delta_i + 1 \geq \bar{i}+3$ for $1 \leq i \leq d(G)-1$.

We can now show that it suffices to consider graphs of small diameter.

Lemma 10. *The diameter of G is at most 35.*

Proof. Suppose that $3 \leq i \leq d(G)-3$. Let

$$X_i = \frac{s_i(\bar{i}+1)}{\max(s_{i-2},s_{i-1},s_i,s_{i+1},s_{i+2})-1}.$$

Observe that $W_{i-1}+W_i+W_{i+1} \geq X_i$. Let

$$M_i = s_{i-2}+s_{i-1}+2s_i+s_{i+1}+s_{i+2}+\alpha X_i,$$

where $\alpha \geq 0$ is a constant to be chosen later. Let $j \in \{i-2,\ldots,i+2\}$ be the index such that $s_j = \max(s_{i-2},s_{i-1},s_i,s_{i+1},s_{i+2})$.

Recall that $s_i \geq \bar{i}+3$, and thus $s_{i-2}, s_{i+2} \geq \bar{i}+1$ and $s_{i-1}, s_{i+1} \geq \bar{i}+2$. If $j = i$, then $\frac{s_i}{\max(s_{i-2},s_{i-1},s_i,s_{i+1},s_{i+2})-1} > 1$, and thus

$$M_i \;>\; 6\bar{i}+12+\alpha(\bar{i}+1) \geq (6+\alpha)\bar{i}+12+\alpha. \qquad (1)$$

On the other hand, if $j \neq i$, then

$$\begin{aligned}
M_i &\geq 5\bar{i} + 11 + (s_j - 1) + \alpha \frac{(\bar{i}+1)(\bar{i}+3)}{s_j - 1} \\
&\geq 5\bar{i} + 11 + 2\sqrt{\alpha(\bar{i}+1)(\bar{i}+3)} \\
&> 5\bar{i} + 11 + 2\sqrt{\alpha}(\bar{i}+1) \\
&= (5 + 2\sqrt{\alpha})\bar{i} + 11 + 2\sqrt{\alpha}. \qquad (2)
\end{aligned}$$

The expression (2) is smaller or equal to (1), giving the lower bound for M_i.

For $m \in \{0, 1, 2\}$, let B_m be the set of integers between 3 and $d(G) - 3$ (inclusive) whose remainder modulo 3 is m, and $b_m = \max B_m$. Let

$$S = 4n_0 + 2n_1 + 2n_{d(G)-1} + 4n_{d(G)} + s_1 + s_2 + s_{d(G)-2} + s_{d(G)-1}.$$

Notice that $S \geq 30$. On one hand, we have $X_i \leq W_{i-1} + W_i + W_{i+1} \leq 2(R_{i-1} + R_i + R_{i+1})$, and thus

$$\begin{aligned}
\sum_{i \in B_m} M_i &\leq s_{1+m} + s_{2+m} + s_{b_m+1} + s_{b_m+2} + 2 \sum_{i=3+m}^{b_m} s_i + 2\alpha \sum_{i=2+m}^{b_m+1} R_i \\
&\leq -S + 4n_0 + 2n_1 + 2n_{d(G)-1} + 4n_{d(G)} + 2 \sum_{i=1}^{d(G)-1} s_i + 2\alpha \sum_{i \geq 0} R_i \\
&= -S + 6n + 2\alpha R'(G) \\
&< -30 + 6n + \alpha d(G).
\end{aligned}$$

On the other hand,

$$\begin{aligned}
\sum_{i \in B_m} M_i &\geq \sum_{i \in B_m} \left((5 + 2\sqrt{\alpha})\bar{i} + 11 + 2\sqrt{\alpha} \right) \\
&= (11 + 2\sqrt{\alpha})|B_m| + (5 + 2\sqrt{\alpha}) \sum_{i \in B_m} \bar{i}.
\end{aligned}$$

Summing the two inequalities above over the three choices of m, we obtain

$$(11 + 2\sqrt{\alpha})(d(G) - 5) + (5 + 2\sqrt{\alpha}) \sum_{i=3}^{d(G)-3} \bar{i} < 18n + 3\alpha d(G) - 90.$$

Applying Lemma 9(a), we obtain $\sum_{i=3}^{d(G)-3} \bar{i} \geq \frac{d^2(G)-25}{4}$, and thus

$$\begin{aligned}
(11 + 2\sqrt{\alpha})(d(G) - 5) + (5 + 2\sqrt{\alpha}) \frac{d^2(G) - 25}{4} &< 18n + 3\alpha d(G) - 90 \\
(5 + 2\sqrt{\alpha}) d^2(G) + 4(11 + 2\sqrt{\alpha} - 3\alpha) d(G) &< 72n + 90\sqrt{\alpha} - 15.
\end{aligned}$$

By Lemma 7, $n \leq \frac{d^2(G)+2d(G)}{8} + 3$, and thus

$$\begin{aligned}(5+2\sqrt{\alpha})d^2(G) + 4(11+2\sqrt{\alpha}-3\alpha)d(G) &< 9(d^2(G)+2d(G)) + 90\sqrt{\alpha} + 201\\ (2\sqrt{\alpha}-4)d^2(G) + (26+8\sqrt{\alpha}-12\alpha)d(G) &< 90\sqrt{\alpha}+201.\end{aligned}$$

Setting $\alpha = 10$, this implies that $d(G) < 35.5$, and since $d(G)$ is an integer, the claim of the lemma follows. □

Lemma 8 gives a lower bound for the minimum degrees δ_i in the layers L_i, which can in turn be used to bound the size of the layers and consequently the number of vertices of G. The lower bound on n obtained in this way is approximately $d^2(G)/12$, and thus it does not directly give a contradiction with Lemma 7. However, the following lemma shows that this lower bound on n can be increased if the maximum degree of G is large (let us note that $\Delta(G) \geq \delta_{\lfloor d(G)/2 \rfloor} \geq \lfloor d(G)/2 \rfloor + 2$). Together with Lemma 7, this can be used to bound $\Delta(G)$.

Lemma 11. *The following holds:* $n \geq (\Delta(G) - \lfloor d(G)/2 \rfloor - 2) + \frac{d^2(G)+12d(G)+3}{12}$.

Proof. Let j be an index such that a vertex of the degree $\Delta(G)$ lies in L_j, and let B be the set of integers i such that $1 \leq i \leq d(G)-1$ and $3|i-j$. Let $a = \min B - 1$ and $b = \max B + 1$. Observe that

$$n = \sum_{i \in B} s_i + \sum_{i=0}^{a-1} n_i + \sum_{i=b+1}^{d(G)} n_i.$$

For $i \in B$, we have that $s_i \geq \delta_i + 1 \geq \bar{i} + 3$. Furthermore, if $j < d(G)$, then $s_j \geq \Delta(G) + 1 \geq (\bar{j} + 3) + (\Delta(G) - \lfloor d(G)/2 \rfloor - 2)$, and if $j = d(G)$, then $b = d(G) - 2$ and $n_{d(G)-1} + n_{d(G)} \geq \Delta(G) + 1 > 2 + (\Delta(G) - \lfloor d(G)/2 \rfloor - 2)$. Also, $\bar{i} \geq (\overline{i-1} + \bar{i} + \overline{i+1})/3$. Using Lemma 9(a), we conclude that

$$\begin{aligned} n &\geq \Delta(G) - \lfloor d(G)/2 \rfloor - 2 + \sum_{i=a}^{b} \left(\frac{\bar{i}}{3} + 1\right) + a + (d(G) - b)\\ &\geq \Delta(G) - \lfloor d(G)/2 \rfloor - 8/3 + \sum_{i=0}^{d(G)} \left(\frac{\bar{i}}{3} + 1\right)\\ &\geq \Delta(G) - \lfloor d(G)/2 \rfloor - 5/3 + d(G) + \frac{d^2(G)-1}{12}\\ &= (\Delta(G) - \lfloor d(G)/2 \rfloor - 2) + \frac{d^2(G)+12d(G)+3}{12}.\end{aligned}$$

□

Next, we show that the maximum degree of G is large. This, combined with the previous lemma, will give us a contradiction.

Lemma 12. *Let $k = \lceil d(G)/2 \rceil$, and let $d_1 \geq d_2 \geq \ldots \geq d_n$ be the degree sequence of G. Then $\sum_{i=1}^{k} d_i \geq \frac{d^3(G)+12d^2(G)+35d(G)+288}{72}$, and thus $\Delta(G) \geq \left\lceil \frac{d^3(G)+12d^2(G)+35d(G)+288}{72k} \right\rceil$.*

Proof. For $1 \leq i \leq n$, let v_i be the vertex of G of degree d_i. Let k_i be the number of neighbors of v_i in $\{v_j | j > i\}$. Note that $\sum_{i=1}^{n} k_i = |E(G)| = \frac{1}{2}\sum_{i=1}^{n} d_i$, $R'(G) = \sum_{i=1}^{n} \frac{k_i}{d_i}$ and $0 \leq k_i \leq d_i$.

Let m be the index such that there exists a sequence $x_1, x_2, \ldots, x_n$ satisfying

- $x_i = d_i$ for $1 \leq i \leq m-1$,
- $0 \leq x_m < d_m$,
- $x_i = 0$ for $m+1 \leq i \leq n$, and
- $\sum_{i=1}^{n} x_i = |E(G)|$.

Since $\frac{a}{b} + \frac{c}{d} \geq \frac{a+1}{b} + \frac{c-1}{d}$ when $b \geq d$, we conclude that

$$\frac{d(G)}{2} > R'(G) = \sum_{i=1}^{n} \frac{k_i}{d_i} \geq \sum_{i=1}^{n} \frac{x_i}{d_i} \geq m-1,$$

i.e., $m \leq \lceil d(G)/2 \rceil$. Furthermore, $\sum_{i=1}^{m} d_i \geq 1 + \sum_{i=1}^{n} x_i = 1 + |E(G)|$.

Let $t_i = n_{i-1}\delta_{i-1} + n_i\delta_i + n_{i+1}\delta_{i+1}$. Note that

$$t_i \geq n_{i-1}(\overline{i-1}+2) + n_i(\bar{i}+2) + n_{i+1}(\overline{i+1}+2) \geq s_i(\bar{i}+1)$$

for $2 \leq i \leq d(G)-2$. Also, $t_2 \geq s_2(\bar{2}+1) + n_2$ and $t_{d(G)-2} \geq s_{d(G)-2}(\overline{d(G)-2}+1) + n_{d(G)-2}$. Using Lemma 9(b), we obtain

$$\begin{aligned}
6|E(G)| &\geq 3\sum_{i=0}^{d(G)} n_i\delta_i \\
&= 3\delta_0 n_0 + 3\delta_{d(G)} n_{d(G)} + 2\delta_1 n_1 + 2\delta_{d(G)-1} n_{d(G)-1} + \delta_2 n_2 + \\
&\quad +\delta_{d(G)-2} n_{d(G)-2} + \sum_{i=2}^{d(G)-2} t_i \\
&\geq 3(n_0 + n_{d(G)}) + 6(n_1 + n_{d(G)-1}) + 5(n_2 + n_{d(G)-2}) + \sum_{i=2}^{d(G)-2} s_i(\bar{i}+1)
\end{aligned}$$

$d(G)$	$LB_{d(G)}$	$UB_{d(G)}$	$d(G)$	$LB_{d(G)}$	$UB_{d(G)}$
10	8	6	23	23	19
11	8	5	24	26	22
12	10	7	25	26	23
13	10	7	26	29	26
14	12	9	27	30	27
15	12	9	28	33	30
16	14	11	29	34	31
17	15	11	30	37	34
18	17	13	31	38	35
19	17	13	32	41	39
20	20	16	33	42	41
21	20	17	34	45	44
22	23	19	35	46	45

Table 1: Values of the lower bound $LB_{d(G)}$ and the upper bound $UB_{d(G)}$ for $\Delta(G)$ from proof of Theorem 3.

$$\begin{aligned}
&\geq 38 + \sum_{i=2}^{d(G)-2} s_i(\bar{i}+1) \\
&\geq 38 + \sum_{i=2}^{d(G)-2} (\bar{i}+3)(\bar{i}+1) \\
&\geq \frac{d^3(G) + 12d^2(G) + 35d(G) + 216}{12}.
\end{aligned}$$

It follows that

$$\sum_{i=1}^{m} d_i \geq \frac{d^3(G) + 12d^2(G) + 35d(G) + 288}{72}.$$

Since $k \geq m$, the lemma holds. □

We are now ready to finish the proof.

Proof of Theorem 3. By Lemma 10, the diameter of the minimal counterexample G is at most 35. Also, as we observed before, $d(G) \geq 10$. Lemmas 7 and 11 imply that

$$\Delta(G) \leq \lfloor d(G)/2 \rfloor + 5 + \left\lfloor \frac{d^2(G) + 2d(G)}{8} \right\rfloor - \left\lceil \frac{d^2(G) + 12d(G) + 3}{12} \right\rceil.$$

We denote this upper bound on $\Delta(G)$ by $UB_{d(G)}$. Lemma 12 gives a lower bound on $\Delta(G)$, which we denote by $LB_{d(G)}$. For $10 \leq d(G) \leq 35$, it holds that

$UB_{d(G)} < LB_{d(G)}$, which is a contradiction. See Table 1 for values of $LB_{d(G)}$ and $UB_{d(G)}$. $\square$

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