Randić index and the diameter of a graph*

Zdeněk Dvořák† Bernard Lidický‡ Riste Škrekovski§

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 Graffiti 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.

---

*Supported by the CZ-SL bilateral project MEB 090805 and BI-CZ/08-09-005.

†Department of Applied Mathematics, Faculty of Mathematics and Physics, Charles University, Malostranské náměstí 25, 118 00 Prague, Czech Republic. E-mail: `rakdver@kam.mff.cuni.cz`. Supported by Institute for Theoretical Computer Science (ITI), project 1M0545 of Ministry of Education of Czech Republic.

‡Department of Applied Mathematics, Faculty of Mathematics and Physics, Charles University, Malostranské náměstí 25, 118 00 Prague, Czech Republic. E-mail: `bernard@kam.mff.cuni.cz`.

§Department of Mathematics, University of Ljubljana, Jadranska 19, 1111 Ljubljana, Slovenia. Partially supported by Ministry of Science and Technology of Slovenia, Research Program P1-0297. E-mail: `skrekovski@gmail.com`.

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 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*

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

with equalities if and only if G is a path 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 $d_G(x,y) = d_{G'_1}(x,y) \le d(G'_1) \le d(G'_1) + d(G'_2) - 2$. By symmetry, if $x, y \in V(G_2)$, then $d_G(x,y) \le d(G'_1) + d(G'_2) - 2$. Finally, if say $x \in V(G_1)$ and $y \in V(G_2)$, then $d_G(x,y) = d_{G_1}(x,v) + d_{G_2}(y,v) = d_{G'_1}(x,v_1) - 1 + d_{G'_2}(y,v_2) - 1 \le d(G'_1) + d(G'_2) - 2$. We conclude that $d(G) \le d(G'_1) + d(G'_2) - 2$.

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

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

which contradicts the assumption that G is a counterexample to Theorem 3. □

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 $k \le \deg(w) - 1$. We have

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

Since v is locally minimal, every neighbor of v has degree at least $\deg(v) \ge 2$, 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, $\ldots$, 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, $\ldots$, 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 $v_1, \ldots, v_{t_0}$, 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 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 $1 \leq i \leq d(G)-1$.

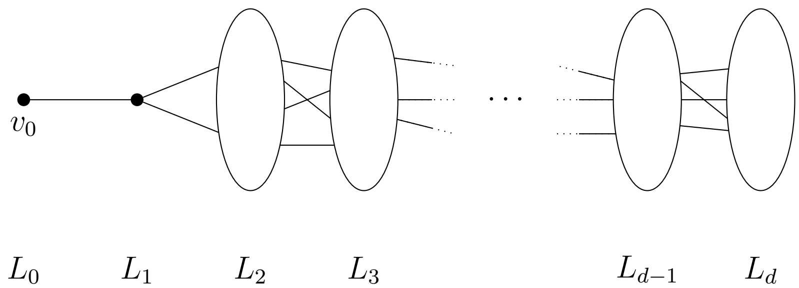

Figure 1: A graph G with vertices partitioned into layers $L_0, L_1, \ldots, L_d$.

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

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

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

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

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

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

On the other hand,

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

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 $\sum_{i=3}^{d(G)-3}\bar{i} \ge \frac{d^2(G)-25}{4}$, 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, $n \le \frac{d^2(G)+2d(G)}{8}+3$, 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 $\Delta(G) \ge \delta_{\lfloor d(G)/2\rfloor} \ge \lfloor d(G)/2\rfloor + 2$). Together with Lemma 7, this can be used to bound $\Delta(G)$.

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

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 $1 \le i \le d(G)-1$ 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

$$\begin{aligned}
6|E(G)| &\geq 3\sum_{i=0}^{d(G)} n_i\delta_i \\
&= 3\delta_0 n_0 + 3\delta_{d(G)}n_{d(G)} + 2\delta_1 n_1 + 2\delta_{d(G)-1}n_{d(G)-1} + \delta_2 n_2 + \delta_{d(G)-2}n_{d(G)-2} + \sum_{i=2}^{d(G)-2} t_i \\
&\geq 3(n_0+n_{d(G)}) + 6(n_1+n_{d(G)-1}) + 5(n_2+n_{d(G)-2}) + \sum_{i=2}^{d(G)-2} s_i(\bar{i}+1) \\
&\geq 38 + \sum_{i=2}^{d(G)-2} s_i(\bar{i}+1) \\
&\geq 38 + \sum_{i=2}^{d(G)-2} (\bar{i}+3)(\bar{i}+1) \\
&\geq \frac{d^3(G)+12d^2(G)+35d(G)+216}{12}.
\end{aligned}$$

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.

$d(G)$	$LB_{d(G)}$	$UB_{d(G)}$	$d(G)$	$LB_{d(G)}$	$UB_{d(G)}$
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.

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 $UB_{d(G)}$. □

References

[1] M. Aouchiche, P. Hansen and M. Zheng, Variable neighborhood search for extremal graphs. 19. Further conjectures and results about the Randić index, *MATCH Commun. Math. Comput. Chem.* **58** (2007), 83–102.

[2] B. Bollobás and P. Erdös, Graphs of extremal weights, *Ars Combin.* **50** (1998), 225–233.

[3] G. Caporossi and P. Hansen, Variable neighborhood search for extremal graphs 1: The AutographiX system, *Discrete Math.* **212** (2000), 29–44.

[4] S. Fajtlowicz, On conjectures of Graffiti, *Discrete Math.* **72** (1988), 113–118.

[5] L. B. Kier and L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research, Academic Press*, New York, 1976.

[6] L. B. Kier and L. H. Hall, *Molecular Connectivity in structure-Activity Analysis, Research Studies Press-Wiley*, Chichester(UK), 1986.

[7] X. Li and I. Gutman, *Mathematical Aspects of Randić - Type Molecular Structure Descriptors, Mathematical Chemistry Monographs No.1*, Kragujevac, 2006.

[8] X. Li and Y. Shi, On the Randić index and the diameter, the average distance, accepted for publication in *MATCH Commun. Math. Comput. Chem.*

[9] B. Liu and I. Gutman, On a conjecture on Randić indices, *MATCH Commun. Math. Comput. Chem.* **62** (2009), 143–154.

[10] X. Li and Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008), 127–156.

[11] M. Randić, On characterization of molecular branching, *J. Amer. Chem. Soc.* **97** (1975), 6609–6615.

[12] Z. You and B. Liu, On a conjecture of the Randić index, *Discrete Appl. Math.* **157** (2009), 1766–1772.