Randić index, Diameter and Average Distance[1]

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Abstract

The Randić index of a graph G, denoted by $R(G)$, is defined as the sum of $1/\sqrt{d(u)d(v)}$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. In this paper, we partially solve two conjectures on the Randić index $R(G)$ with relations to the diameter $D(G)$ and the average distance $\mu(G)$ of a graph G. We prove that for any connected graph G of order n with minimum degree $\delta(G)$, if $\delta(G) \geq 5$, then $R(G) - D(G) \geq \sqrt{2} - \frac{n+1}{2}$; if $\delta(G) \geq n/5$ and $n \geq 15$, $\frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}$ and $R(G) \geq \mu(G)$. Furthermore, for any arbitrary real number ε $(0 < \varepsilon < 1)$, if $\delta(G) \geq \varepsilon n$, then $\frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}$ and $R(G) \geq \mu(G)$ hold for sufficiently large n.

1 Introduction

The *Randić index* $R(G)$ of a (molecular) graph G was introduced by the chemist Milan Randić [8] in 1975 as the sum of $1/\sqrt{d(u)d(v)}$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G, i.e., $R(G) = \sum\limits_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$. Recently, many results on the extremal theory of the Randić index have been reported (see [6]).

Given a connected, simple and undirected graph $G = (V, E)$ of order n. The distance between two vertices u and v in G, denoted by $d_G(u, v)$ (or $d(u, v)$ for short), is the length of a shortest path connecting u and v in G. The *diameter* $D(G)$ of G is the maximum distance $d(u, v)$ over all pairs of vertices u and v of G. The *average distance* $\mu(G)$, an interesting graph-theoretical invariant, is defined as the average value of the distances between all pairs of vertices of G, i.e.,

$$\mu(G) = \frac{\sum_{u,v \in V} d(u, v)}{\binom{n}{2}}.$$

For terminology and notations not given here, we refer to the book of Bondy and Murty [2].

There are many results on the relations between the Randć index and some other graph invariants, such as the minimum degree, the chromatic number, the radius,

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and so on. In this paper, we will consider the relations of the Randić index with the diameter and the average distance.

In [1], Aouchiche, Hansen and Zheng proposed the following conjecture on the relation between the Randić index and the diameter.

Conjecture 1.1 ([1]). *For any connected graph of order $n \geq 3$ with Randić index $R(G)$ and diameter $D(G)$,*

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

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

In [4], Fajtlowicz proposed the following conjecture on the relation between the Randić index and the average distance.

Conjecture 1.2 ([4]). *For all connected graphs G, $R(G) \geq \mu(G)$, where $\mu(G)$ denotes the average distance of G.*

In the following, we will prove that for any connected graph G of order n with minimum degree $\delta(G)$, if $\delta(G) \geq 5$, then $R(G) - D(G) \geq \sqrt{2} - \frac{n+1}{2}$; if $\delta(G) \geq n/5$ and $n \geq 15$, $\frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}$ and $R(G) \geq \mu(G)$. Furthermore, for any arbitrary real number ε $(0 < \varepsilon < 1)$, if $\delta(G) \geq \varepsilon n$, then $\frac{R(G)}{D(G)} \geq \frac{n-3+2\sqrt{2}}{2n-2}$ and $R(G) \geq \mu(G)$ hold for sufficiently large n.

2 Main results

At first, we recall some lemmas which will be used in the sequel.

Lemma 2.1 (Erdös et al. [3]). *Let G be a connected graph with n vertices and minimum degree $\delta(G) \geq 2$. Then $D(G) \leq \frac{3n}{\delta(G)+1} - 1$.*

Lemma 2.2 (Kouider and Winkler [5]). *If G is a graph with n vertices and minimum degree $\delta(G)$, then the average distance satisfying $\mu(G) \leq \frac{n}{\delta(G)+1} + 2$.*

Lemma 2.3 (Li, Liu and Liu [7]). *Let G be a graph of order n with minimum degree $\delta(G) = k$. Then*

$$R(G) \geq \begin{cases} \frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} & \text{if } k \leq \frac{n}{2} \\ \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+k-n)}{2k} + \frac{p(n-p)}{\sqrt{k(n-1)}} & \text{if } k > \frac{n}{2} \end{cases}$$

where p is an integer given as follows:

$$p = \begin{cases} \frac{n}{2} & \text{if } n \equiv 0 \pmod 4 \\ \lfloor \frac{n}{2} \rfloor \text{ or } \lceil \frac{n}{2} \rceil & \text{if } n \equiv 1 \pmod 4 \text{ and } k \text{ is even} \\ \lfloor \frac{n}{2} \rfloor & \text{if } n \equiv 1 \pmod 4 \text{ and } k \text{ is odd} \\ \frac{n-2}{2} \text{ or } \frac{n+2}{2} & \text{if } n \equiv 2 \pmod 4 \text{ and } k \text{ is even} \\ \frac{n}{2} & \text{if } n \equiv 2 \pmod 4 \text{ and } k \text{ is odd} \\ \lfloor \frac{n}{2} \rfloor \text{ or } \lceil \frac{n}{2} \rceil & \text{if } n \equiv 3 \pmod 4 \text{ and } k \text{ is even} \\ \lceil \frac{n}{2} \rceil & \text{if } n \equiv 3 \pmod 4 \text{ and } k \text{ is odd.} \end{cases}$$

It is easy to see from Lemma 2.3 that p is among the numbers $\frac{n-2}{2}$, $\frac{n-1}{2}$, $\frac{n}{2}$, $\frac{n+1}{2}$ and $\frac{n+2}{2}$.

Lemma 2.4. *Denote by $g(n,k) = \frac{2k-1}{2(n-1)} + \frac{n-3k}{2\sqrt{k(n-1)}}$. Then for $1 \le k \le n/2$, $g(n,k) \ge 0$.*

Proof. If $n \ge 3k$, we can directly obtain that $g(n,k) > 0$. Now we assume that $2k \le n < 3k$. Then

$$g(n,k) = \frac{1}{2\sqrt{n-1}}\left(\frac{2k-1}{\sqrt{n-1}} - \frac{3k-n}{\sqrt{k}}\right) = \frac{1}{2\sqrt{n-1}}\left(\frac{2k-1}{\sqrt{n-1}} - 3\sqrt{k} + \frac{n}{\sqrt{k}}\right).$$

Since

$$\begin{aligned} \frac{\partial g(n,k)}{\partial k} &= \frac{1}{2\sqrt{n-1}}\left(\frac{2}{\sqrt{n-1}} - \frac{3}{2\sqrt{k}} - \frac{n}{2k\sqrt{k}}\right) \\ &< \frac{1}{2\sqrt{n-1}}\left(\frac{2}{\sqrt{n-1}} - \frac{3}{2\sqrt{k}} - \frac{2k}{2k\sqrt{k}}\right) < 0, \end{aligned}$$

for $n \ge 2$, we have

$$g(n,k) > g(n, \frac{n}{2}) = \sqrt{n-1} - \sqrt{\frac{n}{2}} \ge 0.$$

Therefore, the lemma follows. ∎

Theorem 2.5. *For any connected graph G of order n with minimum degree $\delta(G)$.*

(1) If $\delta(G) \ge 5$, then $R(G) - D(G) \ge \sqrt{2} - \frac{n+1}{2}$;

(2) If $\delta(G) \ge n/5$ and $n \ge 15$, then $\frac{R(G)}{D(G)} \ge \frac{n-3+2\sqrt{2}}{2n-2}$. Furthermore, for any arbitrary real number ε $(0 < \varepsilon < 1)$, if $\delta(G) \ge \varepsilon n$, then $\frac{R(G)}{D(G)} \ge \frac{n-3+2\sqrt{2}}{2n-2}$ holds for sufficiently large n.

(3) If $\delta(G) \ge n/5$ and $n \ge 15$, then $R(G) \ge \mu(G)$. Furthermore, for any arbitrary real number ε $(0 < \varepsilon < 1)$, if $\delta(G) \ge \varepsilon n$, then $R(G) \ge \mu(G)$ holds for sufficiently large n.

Proof. Let G be a connected graph of order n with minimum degree $\delta(G) = k$. By Lemma 2.1, we have $D(G) \leq \frac{3n}{k+1} - 1$.

(1) Suppose $k \geq 5$, we will show $R(G) - D(G) \geq \sqrt{2} - \frac{n+1}{2}$. We consider the following two cases:

Case 1. $k \leq \frac{n}{2}$.

By Lemma 2.3, we only need to consider the following inequality,

$$\frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} \geq \frac{3n}{k+1} - 1 + \sqrt{2} - \frac{n+1}{2}.$$

Let

$$f(n,k) = \frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} - \frac{3n}{k+1} - \sqrt{2} + \frac{n+3}{2}.$$

Then by Lemma 2.4, $\frac{\partial f(n,k)}{\partial k} > \frac{2k-1}{2(n-1)} + \frac{n-3k}{2\sqrt{k(n-1)}} > 0$. If $k \geq 5$, we have $f(n,k) \geq f(n,5) = \frac{10}{n-1} + \frac{5(n-5)}{\sqrt{5(n-1)}} - \sqrt{2} + \frac{3}{2} > 0$.

Case 2. $\frac{n}{2} < k \leq n-1$.

Let $q(n,p) = \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+k-n)}{2k} + \frac{p(n-p)}{\sqrt{k(n-1)}}$. In the following, we will show that for every $p \in \{\frac{n-2}{2}, \frac{n-1}{2}, \frac{n}{2}, \frac{n+1}{2}, \frac{n+2}{2}\}$,

$$q(n,p) \geq \frac{3n}{k+1} - 1 + \sqrt{2} - \frac{n+1}{2}.$$

In fact, if $p = \frac{n-2}{2}$, denote by

$$\begin{aligned} h(n,k) &= q(n, \frac{n-2}{2}) - \frac{3n}{k+1} - \sqrt{2} + \frac{n+3}{2} \\ &= \frac{n(n+2)}{8(n-1)} + \frac{(n-2)(2k-(n+2))}{8k} + \frac{n^2-4}{4\sqrt{k(n-1)}} \\ &\quad - \frac{3n}{k+1} - \sqrt{2} + \frac{n+3}{2}. \end{aligned}$$

Notice that

$$\frac{\partial h(n,k)}{\partial k} = \frac{n^2-4}{8k^2} - \frac{n^2-4}{8k\sqrt{k(n-1)}} + \frac{3n)}{(k+1)^2} > 0,$$

since $8k^2 \leq 8k\sqrt{k(n-1)}$, i.e., $\sqrt{k} \leq \sqrt{n-1}$. Thus, we have

$$\begin{aligned} h(n,k) > h(n, \frac{n}{2}) &= \frac{n(n+2)}{8(n-1)} - \frac{n-2}{2n} + \frac{n^2-4}{2\sqrt{2n(n-1)}} - \frac{6n}{n+2} - \sqrt{2} + \frac{n+3}{2} \\ &> \frac{n}{8} + \frac{n-2}{8} - \frac{n}{4} + \frac{n^2-4}{n} - 6 - \sqrt{2} + \frac{n+3}{2} \\ &= \frac{2n+5}{4} + \frac{n^2-4}{2\sqrt{2}} - 6 - \sqrt{2}. \end{aligned}$$

By some calculations, we have that $\frac{2n+5}{4} + \frac{n^2-4}{2\sqrt{2}} - 6 - \sqrt{2} > 0$ for $n \geq 8$. For $4 \leq n \leq 7$, it is easy to verify $h(n, \frac{n}{2}) > 0$.

In a similar way, we can verify the inequality for each of the cases for $p = \frac{n-1}{2}$, $\frac{n}{2}$, $\frac{n+1}{2}$ or $\frac{n+2}{2}$. The details are omitted.

(2) Similarly, we consider the following two cases:

Case 1. $k \leq \frac{n}{2}$.

By Lemma 2.3, we only need to consider the following inequality,

$$\frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} \geq \left(\frac{3n}{k+1} - 1\right) \frac{n-3+2\sqrt{2}}{2n-2}.$$

Let

$$f(n,k) = \frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} - \left(\frac{3n}{k+1} - 1\right) \frac{n-3+2\sqrt{2}}{2n-2}.$$

Then by Lemma 2.4, $\frac{\partial f(n,k)}{\partial k} > \frac{2k-1}{2(n-1)} + \frac{n-3k}{2\sqrt{k(n-1)}} > 0$.

If $k \geq \frac{n}{5}$ and $n \geq 15$, we have $f(n,k) \geq f(n, \frac{n}{5}) = \frac{n(n-5)}{50(n-1)} + \frac{4n^2}{5\sqrt{5n(n-1)}} - \frac{(14n-5)(n-3+2\sqrt{2})}{2(n-1)(n+5)} > 0$. Actually, for any arbitrary positive number ε $(0 < \varepsilon < 1)$, if $k \geq \varepsilon n$, then $f(n,k) > f(n, \varepsilon n) > \frac{\varepsilon(1-\varepsilon)n^2}{\sqrt{\varepsilon n(n-1)}} - \left(\frac{3n}{\varepsilon n+1} - 1\right) \frac{n-3+2\sqrt{2}}{2n-2} > 0$ for sufficiently large n.

Case 2. $\frac{n}{2} < k \leq n-1$.

Let $q(n,p) = \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+k-n)}{2k} + \frac{p(n-p)}{\sqrt{k(n-1)}}$. In the following, we will show that for every $p \in \{\frac{n-2}{2}, \frac{n-1}{2}, \frac{n}{2}, \frac{n+1}{2}, \frac{n+2}{2}\}$,

$$q(n,p) \geq \left(\frac{3n}{k+1} - 1\right) \frac{n-3+2\sqrt{2}}{2n-2}.$$

In fact, if $p = \frac{n-2}{2}$, denote by

$$\begin{aligned} h(n,k) &= q(n, \frac{n-2}{2}) - \left(\frac{3n}{k+1} - 1\right) \frac{n-3+2\sqrt{2}}{2n-2} \\ &= \frac{n(n+2)}{8(n-1)} + \frac{(n-2)(2k-(n+2))}{8k} + \frac{n^2-4}{4\sqrt{k(n-1)}} \\ &\quad - \left(\frac{3n}{k+1} - 1\right) \frac{n-3+2\sqrt{2}}{2n-2}. \end{aligned}$$

Notice that

$$\frac{\partial h(n,k)}{\partial k} > \frac{n^2-4}{8k^2} - \frac{n^2-4}{8k\sqrt{k(n-1)}} > 0,$$

since $8k^2 \leq 8k\sqrt{k(n-1)}$, i.e., $\sqrt{k} \leq \sqrt{n-1}$. Thus, we have

$$\begin{aligned} h(n,k) > h(n,\frac{n}{2}) &= \frac{n(n+2)}{8(n-1)} - \frac{n-2}{2n} + \frac{n^2-4}{2\sqrt{2n(n-1)}} \\ &\quad - \left(\frac{6n}{n+2} - 1\right)\frac{n-3+2\sqrt{2}}{2n-2} \\ &> \frac{n}{8} + \frac{n-2}{8} - \frac{n}{4} + \frac{n^2-4}{n} - \frac{(6-1)n}{2n-2} \\ &= \frac{n^2-4}{n} - \frac{11n-1}{4(n-1)}. \end{aligned}$$

By some calculations, we have that $\frac{n^2-4}{n} - \frac{11n-1}{4(n-1)} > 0$ for $n \geq 5$.

In a similar way, we can verify the inequality for each of the cases for $p = \frac{n-1}{2}$, $\frac{n}{2}$, $\frac{n+1}{2}$ or $\frac{n+2}{2}$. The details are omitted.

By the method similar to (2), we can obtain the result of (3).

The proof is now complete. ∎

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