MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **64** (2010) 425-431

ISSN 0340 - 6253

Randić Index, Diameter and Average Distance[1]

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(Received October 9, 2009)

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

[1]Supported by NSFC No.10831001, PCSIRT and the "973" program.

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, 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:

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

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 $1 \leq k \leq n/2$, $g(n,k) \geq 0$.*

Proof. If $n \geq 3k$, we can directly obtain that $g(n,k) > 0$. Now we assume that $2k \leq n < 3k$. 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 $n \geq 2$, we have

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

Therefore, the lemma follows. ∎

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

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

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

(3) If $\delta(G) \geq n/5$ and $n \geq 15$, then $R(G) \geq \mu(G)$. Furthermore, for any arbitrary real number ε $(0 < \varepsilon < 1)$, if $\delta(G) \geq \varepsilon n$, then $R(G) \geq \mu(G)$ 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 $8k^2 \le 8k\sqrt{k(n-1)}$, i.e., $\sqrt{k} \le \sqrt{n-1}$. 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 $n \ge 5$.

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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