On a relation between the Randić index and the chromatic number*

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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. Caporossi and Hansen proposed a conjecture on the relation between the Randić index $R(G)$ and the chromatic number $\chi(G)$ of a graph G: for any connected graph G of order $n \geq 2$, $R(G) \geq \frac{\chi(G)-2}{2} + \frac{1}{\sqrt{n-1}}\left(\sqrt{\chi(G)-1} + n - \chi(G)\right)$, and furthermore the bound is sharp for all n and $2 \leq \chi(G) \leq n$. We prove this conjecture.

Keywords: Randić index; chromatic number; minimum degree

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1 Introduction

The *Randić index* $R(G)$ of a graph G was introduced by 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. Recently many researches on the extremal theory of Randić index have been reported (see [6]).

A vertex coloring of a graph G is *proper* if any two adjacent vertices are assigned different colors. The *chromatic number* $\chi(G)$ of G is the minimum

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number of colors in a proper coloring of G. For terminology and notation not given here, we refer to the book of Bondy and Murty [2].

Many papers [1, 3, 4, 7] have been written on the relation between the Randić index and other graph invariants, such as the minimum degree, the radius, the diameter, the average distance, etc. Caporossi and Hansen [3] proposed the following conjecture on the relation between the chromatic number and Randić index, which is also referred in [6].

Conjecture 1 *[3] For any connected graph G of order $n \geq 2$ with chromatic number $\chi(G)$ and Randić index $R(G)$,*

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

Moreover, the bound is sharp for all n and $2 \leq \chi(G) \leq n$.

This paper proves the conjecture.

2 Main results

First, we recall some lemmas that will be used in the sequel.

Lemma 1 *[5] Let G be a simple graph with Randić index $R(G)$, minimum degree δ, and maximum degree Δ. If v is a vertex of G with minimum degree, then*

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

Lemma 2 *[7] If G is 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

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

From Lemma 2, we know that $p \in \{\frac{n-2}{2}, \frac{n-1}{2}, \frac{n}{2}, \frac{n+1}{2}, \frac{n+2}{2}\}$.

Lemma 3 *Let* $g(n,k) = -\frac{n^2}{8k} + \frac{n^2}{4\sqrt{k(n-1)}} - \frac{k-1}{2} - \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}}$. *For* $n \geq 5$, $g(n,k)$ *is a decreasing function in* k *with* $\frac{n}{2} < k \leq n-1$.

Proof. Note that

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

Let $h(n,k) = 8k^2 + (n^2-4k^2)\sqrt{n-1} - (n^2+4k)\sqrt{k}$. We have $\frac{\partial h(n,k)}{\partial k} = 16k - 8k\sqrt{n-1} - 6\sqrt{k} - \frac{n^2}{2\sqrt{k}}$ and $\frac{\partial^2 h(n,k)}{\partial k^2} = 16 - 8\sqrt{n-1} - \frac{3}{\sqrt{k}} + \frac{n^2}{4k\sqrt{k}}$. For $n \geq 6$, $\frac{\partial^2 h(n,k)}{\partial k^2} < 16 - 8\sqrt{n-1} - \frac{3}{\sqrt{n-1}} + \frac{n}{\sqrt{2n}} < 0$. It is easy to verify that $\frac{\partial^2 h(n,k)}{\partial k^2} \leq 0$ for $n = 5$ and $3 \leq k \leq 4$. Thus, for $n \geq 5$, we have

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

We then have

$$h(n,k) < h(n,\frac{n}{2}) = 2n^2 - \frac{(n^2+2n)\sqrt{2n}}{2} < 0.$$

Therefore, $\frac{\partial g(n,k)}{\partial k} < 0$ for $n \geq 5$. ∎

Theorem 1 *For any connected graph G of order $n \geq 2$ with chromatic number $\chi(G)$ and Randić index $R(G)$, we have $R(G) \geq f(\chi(G))$, where f is defined by $f(x) = \frac{x-2}{2} + \frac{1}{\sqrt{n-1}}\left(\sqrt{x-1} + n - x\right)$. Moreover, the bound is sharp for all n and $2 \leq \chi(G) \leq n$.*

Proof. Since we only consider connected graphs of order at least 2, we may assume $\chi(G) \geq 2$ in the following.

If the claimed inequality fails, then let G be a graph with fewest vertices such that $R(G) < f(\chi(G))$. Let $k = \delta(G)$. We begin by proving the following claim:

Claim. $k \geq \chi(G) - 1$.

Suppose to the contrary that $k < \chi(G) - 1$. Let v be a vertex with minimum degree k. If $\chi(G - v) = \chi(G)$, then by Lemma 1, $R(G - v) < R(G) < f(\chi(G)) = f(\chi(G - v))$, which contradicts the choice of G. Now we suppose $\chi(G - v) < \chi(G)$. Hence $G - v$ has a proper coloring with $\chi(G) - 1$ colors. Since $d(v) = k < \chi(G) - 1$, there exists a vertex u such that the color of u does not appeared on the neighbors of v. Thus v can be colored with that color, which implies that G has a proper coloring with $\chi(G) - 1$ colors, a contradiction. The claim is thus proved.

Note that $f(x)$ is increasing in x for $x \geq 2$. Since $f'(x) = \frac{1}{2} + \frac{1}{2\sqrt{(n-1)(x-1)}} - \frac{1}{\sqrt{n-1}}$, $f'(x) > 0$ for all $x \geq 2$ when $n \geq 3$. Thus for $n \geq 3$, $f(\chi(G)) \leq f(k+1)$. If $n = 2$, then $G \cong K_2$, and it is easy to verify that $f(\chi(G)) = f(k+1)$ since $\chi(K_2) = 2$ and $\delta(K_2) = 1$. Thus for $n \geq 2$, we have

$$R(G) < f(\chi(G)) \leq f(k+1) = \frac{k-1}{2} + \frac{\sqrt{k} + n - k - 1}{\sqrt{n-1}}. \tag{1}$$

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

By Lemma 2 and the Inequality (1), we have

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

However, since $k \le \frac{n}{2}$, we have $\frac{\sqrt{k}+1}{2\sqrt{n-1}} \le \frac{\sqrt{n/2}+1}{2\sqrt{n-1}} \le 1$. Now,

$$\begin{aligned}
& \frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} - \frac{k-1}{2} - \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}} \\
= & \frac{(n-k-1)(k-\sqrt{k})}{\sqrt{k(n-1)}} - \frac{(k-1)(n-k-1)}{2(n-1)} \\
= & \frac{(n-k-1)(\sqrt{k}-1)}{\sqrt{n-1}} \left(1 - \frac{\sqrt{k}+1}{2\sqrt{n-1}}\right) \ge 0,
\end{aligned}$$

a contradiction.

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

Let $q(n,p) = \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+k-n)}{2k} + \frac{p(n-p)}{\sqrt{k(n-1)}}$. By Lemma 2 and (1), we have

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

By some elementary calculations, we have

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

Now, we have $q(n, \frac{n-2}{2}) - q(n, \frac{n+2}{2}) = 0$, $q(n, \frac{n-1}{2}) - q(n, \frac{n+1}{2}) = 0$, $q(n, \frac{n}{2}) - q(n, \frac{n-2}{2}) = \frac{1}{\sqrt{k(n-1)}} - \frac{1}{2k} - \frac{1}{2(n-1)} < 0$ and $q(n, \frac{n}{2}) - q(n, \frac{n-1}{2}) = \frac{1}{4\sqrt{k(n-1)}} - \frac{1}{8k} - \frac{1}{8(n-1)} < 0$ since $\frac{1}{\sqrt{x(n-1)}} - \frac{1}{2x}$ is an increasing function in x for $x \in (\frac{n}{2}, n-1)$. Therefore, $q(n, \frac{n}{2})$ is minimum among all the above five values. Thus, we only need to prove $q(n, \frac{n}{2}) \ge \frac{k-1}{2} + \frac{\sqrt{k}+n-k-1}{\sqrt{n-1}}$, which contradicts (2). By some elementary calculations, we obtain that $q(n,\frac{n}{2})-\frac{k-1}{2}-\frac{\sqrt{k}+n-k-1}{\sqrt{n-1}}\geq 0$ for $2\leq n\leq 4$ and $\frac{n}{2}<k\leq n-1$. In the following, we assume that $n\geq 5$ and then

$$\begin{aligned}
& q(n,\frac{n}{2})-\frac{k-1}{2}-\frac{\sqrt{k}+n-k-1}{\sqrt{n-1}} \\
= & \frac{n(n-2)}{8(n-1)}+\frac{n(2k-n)}{8k}+\frac{n^2}{4\sqrt{k(n-1)}}-\frac{k-1}{2}-\frac{\sqrt{k}+n-k-1}{\sqrt{n-1}} \\
= & \frac{n(n-2)}{8(n-1)}+\frac{n}{4}+g(n,k) \\
\geq & \frac{n(n-2)}{8(n-1)}+\frac{n}{4}+g(n,n-1) \\
= & \frac{n(n-2)}{8(n-1)}+\frac{n}{4}-\frac{n^2}{8(n-1)}+\frac{n^2}{4(n-1)}-\frac{n-2}{2}-1=0,
\end{aligned}$$

where the inequality holds by Lemma 3 and $g(n,k)$ is defined in Lemma 3. Thus we have the require inequality $R(G)\geq f(\chi(G))$.

Note that the bound is sharp for all n and $2\leq\chi(G)\leq n$. For example, if G is the complete graph K_n on n vertices, then $\chi(G)=n$ and $R(G)=f(\chi(G))=\frac{n}{2}$. ∎

Remark. Although the complete graph K_n is a graph such that equality holds in Theorem 1, more effort is needed to determine all the graphs for which the equality holds.

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References

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

[2] J.A. Bondy and U.S.R. Murty, Graph Theory, Springer, 2008.

[3] G. Caporossi, 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] P. Hansen, D. Vukicević, Variable neighborhood search for extremal graphs. 23. On the Randić index and the chromatic number, *Discrete Math.* **309**(2009), 4228–4234.

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

[7] X. Li, B. Liu, J. Liu, Complete solution to a conjecture on Randić index, *European J. Operational Research* **200**(2010), 9–13.

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