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ON GENERAL RANDIĆ INDICES

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Abstract

The Randić index is a graph invariant defined as $\sum\limits_{i\sim j} \frac{1}{\sqrt{d_i\, d_j}}$, where d_i denotes the degree of the vertex i in the graph G, and the summation goes over all pairs of adjacent vertices i, j. The general Randić index is $R_\alpha = R_\alpha(G) = \sum\limits_{i\sim j} (d_i\, d_j)^\alpha$, where α is a real number. Up to now most works concerned with bounds for $R_\alpha(G)$ focus on the case $|\alpha| \leq 1$. In this paper we investigate bounds for $R_\alpha(G)$ for $|\alpha| > 1$ and arrive at some new results.

1. INTRODUCTION

Let $G = (V, E)$ be a simple graph with vertex set $V = \{1, 2, \ldots, n\}$, and edge set E, such that $|E| = m$. Sometimes we refer to G as an (n, m)-graph. For $i, j \in V$, if

i is adjacent to j then we write $i \sim j$. The degree of the vertex i is denoted by d_i. A chemical graph is a graph in which no vertex has degree greater than four.

The general Randić index (or connectivity index [1]) of a (molecular) graph G is defined as

$$R_\alpha(G) = \sum_{i \sim j} (d_i\, d_j)^\alpha$$

where α is a real number. In particular, $R_{-1/2}(G)$ is the ordinary Randić index of G.

The Randić index is an important molecular descriptor and has been closely correlated with many chemical properties (see [2, 3]). Many mathematical properties of $R_{-1/2}$ and of its generalized version R_α have been established, including lower and upper bounds [1]; for some most recent results along these lines see [4–10]. Let $Q_\alpha = Q_\alpha(G) = \sum_{i \sim j} (d_i)^\alpha$. Then Q_2 and R_1 are called the first and the second Zagreb index, respectively [11]. Up to now, many results on the bounds of Q_α and R_α have been reported (see [1]). Recently, some bounds for $R_\alpha(G)$ for $-1 \le \alpha < 0$ and $0 < \alpha \le 1$ were obtained in [4]. The purpose of this work is to present bounds for $R_\alpha(G)$ for $\alpha < -1$ and $\alpha > 1$.

2. MAIN RESULTS

Using the Cauchy–Schwartz inequality, the authors of [4] (also see [1] p. 112) have deduced the inequality $R_\alpha(G)\, R_{-\alpha}(G) \ge m^2$. We now get a somewhat stronger result, namely:

Lemma 2.1. *For an (n,m)-graph G,*

$$R_\alpha(G)\, R_{-\alpha}(G) \ge m^2 \qquad \text{and} \qquad Q_\alpha(G)\, Q_{-\alpha}(G) \ge n^2 .$$

As we know (see [1]), the estimates for R_α and $R_{-\alpha}$ are usually restricted to $-1 \le \alpha < 0$ and $0 < \alpha \le 1$. A natural question is: What about the bounds for $R_\alpha(G)$ for $\alpha < -1$ and $\alpha > 1$? We now give such bounds as follows.

By the Hölder inequality (see [12], p. 135), he have:

Lemma 2.2. *Let α, β be real numbers such that $\alpha + \beta = 1$, $\alpha, \beta \ne 0, 1$. Then*

$$\sum_{v=1}^{n} a_v\, b_v \ge \left[\sum_{v=1}^{n} (a_v)^{1/\alpha}\right]^\alpha \left[\sum_{v=1}^{n} (b_v)^{1/\beta}\right]^\beta \qquad \text{for } \alpha > 1 .$$

Equality holds if and only if $(a_v)^{1/\alpha}/(b_v)^{1/\beta}$ = constant or $a_v = b_v = 0$.

Lemma 2.3. (The Pólya–Szegő inequality) *Let* $0 < m_1 \le a_k \le M_1$, $0 < m_2 \le b_k \le M_2$ $(k = 1, 2, \dots, n)$. *Then*

$$\left[\sum_{k=1}^{n} (a_k)^2\right] \left[\sum_{k=1}^{n} (b_k)^2\right] \le \frac{1}{4} \left(\sqrt{\frac{M_1\,M_2}{m_1\,m_2}} + \sqrt{\frac{m_1\,m_2}{M_1\,M_2}}\right)^2 \left(\sum_{k=1}^{n} a_k\,b_k\right)^2$$

where the equality holds if and only if $a_1 = a_2 = \cdots = a_n$, $b_1 = b_2 = \cdots = b_n$, $m_1 = M_1 = a_1$, $m_2 = M_2 = b_1$.

Denote $b(x) := (x + 1/x)/2$. It is easy to see that $b(x)$ is an increasing function for $x \ge 1$, and that $b(1/x) = b(x)$.

Lemma 2.4. *For an* (n, m)*-graph* G *with maximum vertex degree* Δ *and minimum vertex degree* δ ,

$$R_\alpha(G)\,R_{-\alpha}(G) \le b^2\left(\left(\frac{\Delta}{\delta}\right)^\alpha\right) m^2$$

where the equality holds if and only if G *is regular.*

Proof. Assume first that $\alpha > 0$. Since $0 < \delta^2 \le d_i\,d_j \le \Delta^2$, in view of Lemma 2.3, let $m_1 = \delta^\alpha$, $M_1 = \Delta^\alpha$, $m_2 = \Delta^{-\alpha}$, and $M_2 = \delta^{-\alpha}$. Then

$$\begin{aligned} R_\alpha(G)\,R_{-\alpha}(G) &= \sum_{i\sim j} (d_i\,d_j)^\alpha \cdot \sum_{i\sim j} (d_i\,d_j)^{-\alpha} \\ &\le \frac{1}{4}\left(\frac{\Delta^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{\Delta^\alpha}\right)^2 \left[\sum_{i\sim j} (d_i\,d_j)^{\alpha/2} \cdot (d_i\,d_j)^{-\alpha/2}\right]^2 \\ &= b^2\left(\left(\frac{\Delta}{\delta}\right)^\alpha\right) m^2 \end{aligned}$$

where the equality holds if and only if $\Delta = \delta$, i. e., if G is regular.

The proof of Lemma 2.4 for $\alpha < 0$ is fully analogous. □

Note that if $i \sim j$, then it is impossible that both i and j are pendent vertices (provided $n > 2$). Thus $2 \le (d_i\,d_j) \le (n-1)^2$, from which follows $\sqrt{2}^\alpha \le (d_i\,d_j)^{\alpha/2} \le (n-1)^\alpha$. By means of a method similar to what was used in the proof of Lemma 2.4, and noticing that $b(x)$ is an increasing function for $x \ge 1$, we get:

Corollary 2.1. *For an* (n, m)*-graph* G ,

$$R_\alpha(G)\,R_{-\alpha}(G) \le b^2\left(\left(\frac{n-1}{\sqrt{2}}\right)^\alpha\right) m^2 \qquad \text{for } \alpha > 0\ .$$

If G is a connected chemical graph (and $n > 2$), then $2 \le d_i\,d_j \le 16$, and we have

Corollary 2.2. *For a connected (n,m) chemical graph G, $n>2$,*

$$R_\alpha(G)\,R_{-\alpha}(G) \le b^2((2\sqrt{2})^\alpha)\,m^2 \qquad \text{for } \alpha > 0 \,.$$

Using the Hölder inequality we have (see [12] p. 137):

Lemma 2.5. *Let a_i, b_i, and c_i be positive real numbers, $i=1,2,\ldots,n$. Then*

$$\left(\sum_{i=1}^{n} a_i\,b_i\,c_i\right)^3 \le \left[\sum_{i=1}^{n}(a_i)^3\right]\left[\sum_{i=1}^{n}(b_i)^3\right]\left[\sum_{i=1}^{n}(c_i)^3\right]$$

where equality holds if and only if $a_i=b_i=c_i$, $i=1,2,\ldots,n$.

Lemma 2.6. *For an (n,m)-graph G with maximum vertex degree Δ and minimum vertex degree δ,*

$$R_1(G) \ge \frac{4\,m^3}{n^2\,b(\Delta/\delta)} \,.$$

Proof. By Lemma 2.3, note that $0<\delta\le d_i\le\Delta$. Let $m_1=m_2=\delta$ and $M_1=M_2=\Delta$. Then

$$\frac{1}{4}\left(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\right)^2\left(\sum_{i\sim j} d_i\,d_j\right)^2 \ge \left(\sum_{i\sim j}(d_i)^2\right)\left(\sum_{i\sim j}(d_j)^2\right) = \left(\frac{1}{2}\sum_{i=1}^{n}(d_i)^3\right)^2 \,.$$

Then

$$\frac{1}{2}\left(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\right) R_1(G) \;\ge\; \frac{1}{2}\sum_{i=1}^{n}(d_i)^3 \,,$$

$$b(\Delta/\delta)\,R_1(G) \;\ge\; \frac{1}{2}\sum_{i=1}^{n}(d_i)^3 \,,$$

and by Lemma 2.5 (by setting $b_i=c_i=1$),

$$n^2\sum_{i=1}^{n}(d_i)^3 \;\ge\; \left(\sum_{i=1}^{n} d_i\right)^3 = 8\,m^3$$

$$\sum_{i=1}^{n}(d_i)^3 \;\ge\; \frac{8\,m^3}{n^2}$$

and therefore

$$b(\Delta/\delta)\,R_1(G) \;\ge\; \frac{1}{2}\cdot\frac{8\,m^3}{n^2} \,,$$

$$R_1(G) \;\ge\; \frac{4\,m^3}{n^2\,b(\Delta/\delta)} \,. \qquad \square$$

Corollary 2.3. *For an* (n,m)*-graph* G *,*

$$R_1(G) \geq \frac{4\,m^3}{n^2\,b(n-1)} \ .$$

Corollary 2.4. *For a connected* (n,m) *chemical graph* G *,* $n > 2$ *,*

$$R_1(G) \geq \frac{4\,m^3}{n^2\,b(4)} = \frac{32\,m^3}{17\,n^2} \ .$$

Theorem 2.1. *Let* G *be an* (n,m)*-graph with maximum vertex degree* Δ *and minimum vertex degree* δ *. Then*

$$R_\alpha(G) \geq 4^\alpha\, n^{-2\alpha}\, m^{2\alpha+1}\, b^{-\alpha}(\Delta/\delta) \quad \text{for } \alpha > 1$$

and

$$R_\alpha(G) \leq 4^\alpha\, n^{-2\alpha}\, m^{2\alpha+1}\, b^{-\alpha}(\Delta/\delta)\, b^2((\Delta/\delta)^2) \quad \text{for } \alpha < -1 \ .$$

Proof. Let $\alpha + \beta = 1$, $\alpha, \beta \notin \{0,1\}$. By Lemmas 2.2 and 2.6,

$$\begin{aligned}
R_\alpha(G) &= \sum_{i\sim j} (d_i\, d_j)^\alpha \cdot 1^\beta \\
&\geq \left(\sum_{i\sim j} (d_i\, d_j)^{\alpha \cdot 1/\alpha} \right)^\alpha \cdot \left(\sum_{i\sim j} 1^{\beta \cdot 1/\beta} \right)^\beta \qquad \text{for } \alpha > 1 \\
&= \left(\sum_{i\sim j} d_i\, d_j \right)^\alpha \cdot m^\beta \\
&= R_1(G)^\alpha \cdot m^{1-\alpha} \qquad\qquad (1) \\
&\geq \frac{4^\alpha\, m^{3\alpha}}{n^{2\alpha}\, b^\alpha(\Delta/\delta)} \cdot m^{1-\alpha} = 4^\alpha\, n^{-2\alpha}\, m^{2\alpha+1}\, b^{-\alpha}(\Delta/\delta) \ .
\end{aligned}$$

For $\alpha < -1$, i. e., $-\alpha > 1$, by Lemma 2.4, Lemma 2.6, and the above result

$$\begin{aligned}
R_\alpha(G) &\leq \frac{b^2((\Delta/\delta)^2)\, m^2}{R_{-\alpha}(G)} \\
&\leq \frac{b^2((\Delta/\delta)^2)\, m^2}{R_1(G)^{-\alpha}\, m^{1+\alpha}} \qquad\qquad (2) \\
&\leq 4^\alpha\, n^{-2\alpha}\, m^{2\alpha+1}\, b^{-\alpha}\left(\frac{\Delta}{\delta}\right) b^2\left(\left(\frac{\Delta}{\delta}\right)^2\right) \ . \qquad \Box
\end{aligned}$$

Corollary 2.5. *For an* (n,m)*-graph* G *,*

$$R_\alpha(G) \geq 4^\alpha \cdot n^{-2\alpha} \cdot m^{2\alpha+1} \cdot b^{-\alpha}(n-1) \qquad \textit{for } \alpha > 1$$

and

$$R_\alpha(G) \leq 4^\alpha \cdot n^{-2\alpha} \cdot m^{2\alpha+1} \cdot b^{-\alpha}(n-1) \cdot b^2((n-1)^2) \qquad \textit{for } \alpha < -1 \ .$$

Corollary 2.6. *For a connected* (n,m) *chemical graph* G *,*

$$R_\alpha(G) \geq 4^\alpha \cdot n^{-2\alpha} \cdot m^{2\alpha+1} \cdot b^{-\alpha}(4) \qquad \textit{for } \alpha > 1$$

and

$$R_\alpha(G) \leq 4^\alpha \cdot n^{-2\alpha} \cdot m^{2\alpha+1} \cdot b^{-\alpha}(4) \cdot b^2(16) \qquad \text{for } \alpha < -1 \ .$$

In order to obtain another form of Theorem 2.1, we first prove:

Lemma 2.7. *Let* G *be an* (n,m)*-graph,* $(n \geq 2)$ *, with maximum vertex degree* Δ *and minimum vertex degree* δ *. Then*

$$\begin{aligned} R_1(G) &\geq 2\,m^2 + [(\Delta-1)(\Delta+\delta) - (n-1)\Delta]\,m \\ &- \frac{1}{8}\,(\Delta-1)[4n\,\delta\,\Delta + (\Delta-\delta)^2\,(n-2)] \end{aligned}$$

where the equality holds if and only if G *is regular.*

Proof.

$$\begin{aligned} R_1(G) &= \sum_{i\sim j} d_i\,d_j = \frac{1}{2}\sum_{i=1}^{n} d_i \sum_{i\sim j} d_j \\ &\geq \frac{1}{2}\sum_{i=1}^{n} d_i\,[2m - d_i - (n-1-d_i)\,\Delta] \\ &= 2\,m^2 + \frac{1}{2}\,(\Delta-1)\sum_{i=1}^{n}(d_i)^2 - (n-1)m\,\Delta \\ &= 2\,m^2 - (n-1)m\,\Delta + \frac{1}{2}\,(\Delta-1)\,Q_2(G) \end{aligned} \qquad (3)$$

where the equality holds if and only if G is regular. $\square$

Let n_i be the number of vertices of degree i in G , $\delta \leq i \leq \Delta$. From a result in [13] (formula (9), p. 235, note a printing error),

$$Q_2(G) = 2m\,(\Delta+\delta) - n\,\Delta\,\delta + \sum_{i=\delta+1}^{\Delta-1}(\delta-i)(\Delta-i)\,n_i \ . \qquad (4)$$

By the arithmetic–geometric inequality

$$\begin{aligned}
\sum_{i=\delta+1}^{\Delta-1} (\delta - i)(\Delta - i)\, n_i &= - \sum_{i=\delta+1}^{\Delta-1} (i-\delta)(\Delta - i)\, n_i \\
&\geq -\frac{(\Delta-\delta)^2}{4} \sum_{i=\delta+1}^{\Delta-1} n_i = -\frac{(\Delta-\delta)^2}{4}\,(n - n_\Delta - n_\delta) \\
&\geq -\frac{(\Delta-\delta)^2}{4}\,(n-2)
\end{aligned}$$

where the equality holds if and only if either $\delta = \Delta$ or $n_\Delta = n_\delta = 1$, $n_{(\delta+\Delta)/2} = n-2$, $\delta + \Delta \equiv 0 \ mod\ 2$. From formula (4),

$$Q_2(G) \geq 2m\,(\Delta+\delta) - n\,\Delta\,\delta - \frac{(\Delta-\delta)^2}{4}\,(n-2)\ .$$

Hence by inequality (3)

$$\begin{aligned}
R_1(G) \ \geq\ & 2\,m^2 + [(\Delta-1)(\Delta+\delta) - (n-1)\,\Delta]\,m \\
& - \frac{1}{8}(\Delta-1)[4n\,\delta\,\Delta + (\Delta-\delta)^2\,(n-2)]\ .
\end{aligned}$$

Clearly, equalities in the above formulas hold if and only if $\delta = \Delta$, i. e., if G is regular. □

By combining inequalities (1), (2) and Lemma 2.7, we get

Theorem 2.2. *Let G be an (n,m)-graph with maximum vertex degree Δ and minimum vertex degree δ . Then*

$$R_\alpha(G) \geq a^\alpha(n,m,\delta,\Delta)\, m^{1-\alpha} \qquad \text{for } \alpha > 1$$

and

$$R_\alpha(G) \leq a^\alpha(n,m,\delta,\Delta)\, m^{1-\alpha} \cdot b^2((\Delta/\delta)^2) \qquad \text{for } \alpha < -1$$

where

$$\begin{aligned}
a(n,m,\delta,\Delta) \ :=\ & 2\,m^2 + [(\Delta-1)(\Delta+\delta) - (n-1)\Delta]\,m \\
& - \frac{1}{8}\,(\Delta-1)[4n\,\delta\,\Delta + (\Delta-\delta)^2\,(n-2)]\ .
\end{aligned}$$

Corollaries 2.5 and 2.6 follow also from Theorem 2.2.

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