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A NOTE ON GENERAL RANDIĆ INDEX

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Abstract

The general Randić index of a graph G is a graph invariant defined as $R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$, where d_u denotes the degree of vertex u in G, $E(G)$ denotes the edge set of G, and α is a real number. In this note, we report some bounds for R_α, especially when $|\alpha| \geq 1$.

INTRODUCTION

We consider graphs without loops and multiple edges. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, the degree of u is denoted by d_u. Denote by uv or vu the edge connecting the vertices u and v.

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

$$R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$$

where α is a real number. In particular, $R_{-1/2}$ is the ordinary Randić index [2], while R_1 is the second Zagreb index [3]. Both of them have been continuously used in QSPR and QSAR studies, see, e.g., [4].

There is a lot of research on the mathematical properties of the general Randić index of a graph. On the basis of Bollobás and Erdős [5], Bollobás *et al.* [6] gave an upper bound for R_α when $\alpha > 0$ and a lower bound for R_α when $\alpha < 0$ using the number of edges. Lu *et al.* [7] gave an upper bound for R_α when $0 < \alpha \leq 1$ and a lower bound for R_α when $-1 \leq \alpha < 0$ using the number of vertices, the number of edges and the maximum eigenvalue of the adjacency matrix of the graph. Li and Yang [8] obtained some bounds for R_α of a graph using the number of vertices. Hu *et al.* [9] studied R_α of a tree. Clark and Moon [10] found the expected value and variance of R_α for certain families of trees. Rodríguez and Sigarreta [11] derived relations between R_{α_1} and R_{α_2} for different nonzero α_1 and α_2. Recently, Liu and Gutman [12] reported some lower bounds for R_α when $\alpha > 1$ and upper bounds for R_α when $\alpha < -1$. Results on the relations between R_α and $Q_\alpha = \sum_{\substack{u \in V(G) \\ d_u \geq 1}} d_u^\alpha$ (which is called the general zeroth-order Randić index) can be found in [13, 14]. In this note, we report bounds for R_α, especially when $|\alpha| \geq 1$.

RESULTS

First we give various lower bounds for R_α when $\alpha \geq 1$ and upper bounds for R_α when $\alpha \leq -1$.

Theorem 1. *Let G be a graph with n vertices and $m \geq 1$ edges. Then for $\alpha \geq 1$,*

$$R_\alpha \geq 4^\alpha n^{-2\alpha} m^{1+2\alpha} \tag{1}$$

with equality if and only if G is a regular graph.

Proof. First suppose that $\alpha = 1$. By the Cauchy–Schwarz inequality,

$$R_{1/2} R_{-1/2} \geq m^2$$

$$m R_1 \geq R_{1/2}^2$$

with either equality if and only if $d_u d_v$ is a constant for every edge $uv \in E(G)$. Note that $R_{-1/2} \leq \frac{n}{2}$ with equality if and only if G has no isolated vertices and every component of G is regular [1]. It is easy to see that

$$R_1 \geq \frac{1}{m} R_{1/2}^2 \geq \frac{1}{m} \left(\frac{m^2}{R_{-1/2}} \right)^2 \geq \frac{1}{m} \left(\frac{m^2}{\frac{n}{2}} \right)^2 = \frac{4m^3}{n^2} \,.$$

This proves (1) for $\alpha = 1$. Equality holds in (1) for $\alpha = 1$ if and only if all the inequality above are equalities, i.e., G is a regular graph.

Now suppose that $\alpha > 1$. By Hölder's inequality (see [15, p. 24]) or by Theorem 4 of [11],

$$R_\alpha = \sum_{uv \in E(G)} \left[(d_u d_v)^\alpha \cdot 1^{1-\alpha} \right] \geq R_1^\alpha \cdot m^{1-\alpha}$$

with equality if and only if $d_u d_v$ is a constant for every edge $uv \in E(G)$. Now the result follows from the conclusion in the case $\alpha = 1$. $\square$

Let G be a connected graph with $n \geq 2$ vertices, m edges, maximum vertex degree Δ and minimum vertex degree $\delta \geq 1$. Then

$$\begin{aligned} R_{-1/2} &= \frac{n}{2} - \frac{1}{2} \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}} \right)^2 \\ &\leq \frac{n}{2} - \frac{1}{2m} \left(\sum_{uv \in E(G)} \left| \frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}} \right| \right)^2 \\ &\leq \frac{n}{2} - \frac{1}{2m} \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right)^2 . \end{aligned}$$

Thus, for $\alpha \geq 1$, from the proof of Theorem 1, we may improve the lower bound in (1) as

$$R_\alpha \geq 4^\alpha \left(nm\Delta\delta - \Delta - \delta + 2\sqrt{\Delta\delta} \right)^{-2\alpha} \Delta^{2\alpha} \delta^{2\alpha} m^{1+4\alpha}$$

with equality if and only if G is regular.

Let $b(x) = \frac{1}{2}\left(x + \frac{1}{x}\right)$. Obviously, $b(x)$ is increasing for $x \geq 1$.

Theorem 2. *Let G be a graph with n vertices, m edges, maximum vertex degree Δ and minimum vertex degree $\delta \geq 1$. Then for $\alpha \leq -1$,*

$$R_\alpha \leq 4^\alpha n^{-2\alpha} m^{1+2\alpha} b^2 \left((\Delta/\delta)^\alpha \right) \tag{2}$$

with equality if and only if G is a regular graph.

Proof. It was shown in Lemma 2.4 of [12] by using the Pólya–Szegő inequality [16] that

$$R_\alpha R_{-\alpha} \leq b^2 \left((\Delta/\delta)^\alpha \right) m^2$$

with equality if and only if G is a regular graph. Since $\alpha \leq -1$, we have $-\alpha \geq 1$. By Theorem 1,

$$R_{-\alpha} \geq 4^{-\alpha} n^{2\alpha} m^{1-2\alpha}$$

with equality if and only if G is a regular graph. Thus

$$R_\alpha \leq \frac{b^2 \left((\Delta/\delta)^\alpha \right) m^2}{R_{-\alpha}} \leq \frac{b^2 \left((\Delta/\delta)^\alpha \right) m^2}{4^{-\alpha} n^{2\alpha} m^{1-2\alpha}} = 4^\alpha n^{-2\alpha} m^{1+2\alpha} b^2 \left((\Delta/\delta)^\alpha \right) .$$

This proves (2). Equality holds in (2) if and only if all the inequality above are equalities, i.e., G is a regular graph. $\square$

As noted above, for $\alpha \leq -1$ and connected graph G, (2) can be improved as

$$R_\alpha \leq 4^\alpha \left(nm\Delta\delta - \Delta - \delta + 2\sqrt{\Delta\delta}\right)^{-2\alpha} \Delta^{2\alpha}\delta^{2\alpha}m^{1+4\alpha}b^2\left((\Delta/\delta)^\alpha\right)$$

with equality if and only if G is regular.

Theorem 3. *Let G be a graph with $n \geq 3$ vertices, m edges, maximum vertex degree Δ and minimum vertex degree $\delta \geq 1$. Then for $\alpha \geq 1$,*

$$R_\alpha \geq c^\alpha m^{1-\alpha} \tag{3}$$

and for $\alpha \leq -1$,

$$R_\alpha \leq c^\alpha m^{1-\alpha} b^2\left((\Delta/\delta)^\alpha\right) \tag{4}$$

with equality in (3) *or in* (4) *if and only if G is a regular graph, where* $c = c(n, m, \Delta, \delta) = 2m^2 - (n-1)m\Delta + \frac{\Delta-1}{2}\left[\Delta^2 + \delta^2 + \frac{(2m-\Delta-\delta)^2}{n-2}\right]$.

Proof. Note that [12]

$$R_1 = \frac{1}{2}\sum_{u\in V(G)} d_u \sum_{uv\in E(G)} d_v \geq 2m^2 - (n-1)m\Delta + \frac{\Delta-1}{2}Q_2$$

with equality if and only G is a regular graph. It was shown in Theorem 2.3 of [17] that

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

with equality if and only if except a vertex of degree Δ and a vertex of degree δ, all other vertices have equal degrees. It follows that $R_1 \geq c$ with equality if and only if G is a regular graph.

By similar arguments as in Theorems 1 and 2, the result follows. $\square$

Let G be a graph with n vertices and m edges. Note that [17, 18]

$$Q_2 \geq 2m\left(2\left\lfloor\frac{2m}{n}\right\rfloor + 1\right) - \left\lfloor\frac{2m}{n}\right\rfloor\left(1 + \left\lfloor\frac{2m}{n}\right\rfloor\right)n$$

with equality if and only if the difference of the degrees of any two vertices of G is at most one. Similarly, we have

Theorem 4. *Let G be a graph with n vertices, m edges, maximum vertex degree Δ and minimum vertex degree $\delta \geq 1$. Then for $\alpha \geq 1$,*

$$R_\alpha \geq d^\alpha m^{1-\alpha} \tag{5}$$

and for $\alpha \leq -1$,

$$R_\alpha \leq d^\alpha m^{1-\alpha} b^2 \left((\Delta/\delta)^\alpha \right) \tag{6}$$

with equality in (5) *or in* (6) *if and only if* G *is a regular graph, where* $d = d(n, m, \Delta, \delta) = 2m^2 - (n-1)m\Delta + \frac{\Delta - 1}{2} \left[2m \left(2 \left\lfloor \frac{2m}{n} \right\rfloor + 1 \right) - \left\lfloor \frac{2m}{n} \right\rfloor \left(1 + \left\lfloor \frac{2m}{n} \right\rfloor \right) n \right]$.

Remark 1. Let G be a graph with n vertices, m edges, maximum vertex degree Δ and minimum vertex degree $\delta \geq 1$. Then by Theorem 2.1 of [12] (note a printing error: $b^2\left((\Delta/\delta)^2\right)$ should be $b^2\left((\Delta/\delta)^\alpha\right)$),

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

$$R_\alpha \leq 4^\alpha n^{-2\alpha} m^{1+2\alpha} b^2 \left((\Delta/\delta)^\alpha \right) b^{-\alpha} (\Delta/\delta) \qquad \text{if } \alpha < -1\,.$$

Since $b^{-\alpha}(\Delta/\delta) \leq 1$ if $\alpha \geq 1$ and $b^{-\alpha}(\Delta/\delta) \geq 1$ if $\alpha \leq -1$, the lower bound in (1) and upper bound in (2) improve the ones above, respectively.

Remark 2. Let G be a graph with $n \geq 3$ vertices, m edges, maximum vertex degree Δ and minimum vertex degree $\delta \geq 1$. Then by Theorem 2.2 of [12] (note a printing error again),

$$R_\alpha \geq h^\alpha m^{1-\alpha} \qquad \text{if } \alpha > 1\,,$$

$$R_\alpha \leq h^\alpha m^{1-\alpha} b^2 \left((\Delta/\delta)^\alpha \right) \qquad \text{if } \alpha < -1\,,$$

where $h = h(n, m, \Delta, \delta) = 2m^2 - (n-1)m\Delta + \frac{\Delta-1}{2} \left[2m(\Delta + \delta) - n\Delta\delta - \frac{(\Delta-\delta)^2}{4}(n-2) \right]$. Obviously, the lower bound in (3) and upper bound in (4) are improvement of the ones above respectively if and only if $c \geq h$, or equivalently,

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

i.e.,

$$(n-1)(\Delta + \delta)^2 + 4m^2 + \Delta\delta(n-2)^2 + \frac{(\Delta - \delta)^2}{4}(n-2)^2 \geq 2nm(\Delta + \delta)$$

which is transformed into the obvious inequality

$$\left[\frac{(\Delta + \delta)n}{2} - 2m \right]^2 \geq 0\,.$$

Now we discuss upper bounds for R_α when $0 < \alpha \leq 1$ and lower bounds for R_α when $\alpha < 0$. Let G be a graph with $m \geq 1$ edges. If $0 < \alpha < 1$, then as in [5], $R_\alpha \leq R_1^\alpha m^{1-\alpha}$ with equality if and only if $d_u d_v$ is a constant for any $uv \in E(G)$. Thus from an upper bound B for R_1, we have

$$R_\alpha \leq B^\alpha m^{1-\alpha} \quad \text{if } 0 < \alpha < 1\,,$$

and by similar arguments as in the proof of Theorem 9 in [6],

$$R_\alpha \geq B^\alpha m^{1-\alpha} \quad \text{if} \ \ \alpha < 0\,,$$

and either bound for R_α is attained if and only if $R_1 = B$ and $d_u d_v$ is a constant for any $uv \in E(G)$. We note that upper bounds for R_1 of various classes of graphs can be found in, e.g., [19–21]. Recall that a semiregular bipartite graph of degrees r and s is a bipartite graph, for which each vertex in one part of a bipartition has degree r and each vertex in the other part has degree s.

Example 1. Let G be a graph with n vertices, $m \geq 1$ edges and clique number (the number of vertices in a largest complete subgraph) ω. Suppose that G has no isolated vertices. Then [14] $R_1 \leq \frac{2(\omega-1)}{\omega} m^2$ with equality if and only if G is either a complete bipartite graph for $\omega = 2$ or a regular complete ω-partite graphs for $\omega \geq 3$. Thus

$$R_\alpha \leq 2^\alpha(\omega-1)^\alpha \omega^{-\alpha} m^{1+\alpha} \quad \text{if} \ \ 0 < \alpha \leq 1\,,$$

$$R_\alpha \geq 2^\alpha(\omega-1)^\alpha \omega^{-\alpha} m^{1+\alpha} \quad \text{if} \ \ \alpha < 0\,,$$

and either bound for R_α is attained if and only if G is either a complete bipartite graph for $\omega = 2$ or a regular complete ω-partite graphs for $\omega \geq 3$.

Example 2. Let G be a graph with n vertices and $m \geq 1$ edges, and let ρ be the maximum eigenvalue of the adjacency matrix of G. Note that $\rho^2 \geq \frac{Q_2}{n}$ with equality if and only if every component of G is either a regular graph of degree ρ or a semiregular bipartite graph the product of whose degrees (of any two adjacent vertices) is equal to ρ^2 [22, 23], and by the Rayleigh–Ritz theorem, see, e.g., [24, p. 176], $\rho \geq \frac{2R_1}{Q_2}$. It follows that $R_1 \leq \frac{n\rho^3}{2}$ [7] with equality if and only if $\rho = \frac{2R_1}{Q_2} = \frac{2m\rho^2}{n\rho^2} = \frac{2m}{n}$, i.e., G is a regular graph. So a result in [7] concerning lower (resp. upper) bound for $0 < \alpha \leq 1$ (resp. $-1 \leq \alpha < 0$) may be extended a little as:

$$R_\alpha \leq 2^{-\alpha} n^\alpha m^{1-\alpha} \rho^{3\alpha} \quad \text{if} \ \ 0 < \alpha \leq 1\,,$$

$$R_\alpha \geq 2^{-\alpha} n^\alpha m^{1-\alpha} \rho^{3\alpha} \quad \text{if} \ \ \alpha < 0\,,$$

and either bound for R_α is attained if and only if G is regular graph.

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