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Remark on upper bounds of Randić index of a graph

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ABSTRACT. Let $G = (V, E)$ be an undirected simple graph of order n with m edges without isolated vertices. Further, let $d_1 \geq d_2 \geq \cdots \geq d_n$ be vertex degree sequence of G. General Randić index of graph $G = (V, E)$ is defined by $R_\alpha = \sum_{(i,j)\in E} (d_i d_j)^\alpha$, where $\alpha \in \mathbb{R} - \{0\}$. We consider the case when $\alpha = -1$ and obtain upper bound for R_{-1}.

1. INTRODUCTION

Let $G = (V, E)$ be an undirected simple graph of order n with no isolated vertices. The general Randic index R_α defined by Bollobas and Erdos [2]

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

where α is a given parameter and d_i the degree of vertex i, is generalization of the classic index, where $\alpha = -\frac{1}{2}$, introduced by Randic in 1975 [16] for studies organic compounds and boiling points in chemistry. Since then, studies for general Randić index pay attention on the case where graph is a tree or a chemical graph (see for example [7, 8, 19]). Besides, general Randić index, particulary its upper/lower bounds on general graphs has attracted recently the attention of many mathematicians and computer scientists. For a survey of its mathematical properties and application in spectral graph theory, see [6, 9, 10, 18, 20]. Since the invariant R_α can be exactly determined for only a small number of graph classes, other methods for approximate calculation, asymptotic assessments, as well as inequalities that establish upper/lower bounds for this graph invariant depending of other graph parameters are of interest. This paper concerns with upper bounds for R_{-1}.

2. PRELIMINARIES

In what follows, we outline a few results of spectral graph theory and state a few analytical inequalities that will be needed in the subsequent considerations.

In [13] Lu *et all* proved the following result:

Theorem 2.1. [13] *Let G be undirected, simple graph of order n, $n \geq 2$, with no isolated vertices. Then*

$$R_{-1} \leq \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d_i}. \tag{2.1}$$

Equality holds if and only if G is isomorph with k-regular graph, $1 \leq k \leq n-1$.

Zhou and Luo [21] proved the following result.

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Theorem 2.2. [21]. *Let G be a graph with n vertices, m edges, maximum vertex degree d_1 and minimum vertex degree $d_n \geq 1$. Then for $\alpha \leq -1$*

$$R_\alpha \leq 4^{\alpha-1} n^{-2\alpha} m^{1+2\alpha} \left(\sqrt{\frac{d_1^\alpha}{d_n^\alpha}} + \sqrt{\frac{d_n^\alpha}{d_1^\alpha}} \right)^2 ,$$

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

For our consideration the case $\alpha = -1$ is of interest. In that case the above inequality becomes

$$R_{-1} \leq \frac{n^2}{16m} \left(\sqrt{\frac{d_1}{d_n}} + \sqrt{\frac{d_n}{d_1}} \right)^2 \tag{2.2}$$

In [18] Shi proved the following.

Theorem 2.3. [18]. *Let $G = (V, E)$ be a graph of order n and minimum degree d_n. Let $\alpha \in (-\infty, -\frac{1}{2}]$. Then*

$$R_\alpha \leq \frac{n}{2} d_n^{1+2\alpha},$$

with equality if and only if G is regular.

For $\alpha = -1$ the above inequality becomes

$$R_{-1} \leq \frac{n}{2d_1} \tag{2.3}$$

Andrica and Badea [1] (see also Cerone, Dragomir [4]) proved the following result:

Theorem 2.4. *Let $a_1, a_2, \ldots, a_n$ be a sequence of positive real numbers, for which there are real constants r and R so that $0 < r \leq a_i \leq R < +\infty$, for each $i = 1, 2, \ldots, n$. Then*

$$\left(\sum_{i=1}^n a_i \right) \left(\sum_{i=1}^n \frac{1}{a_i} \right) \leq n^2 \left(1 + \left(\sqrt{\frac{R}{r}} - \sqrt{\frac{r}{R}} \right)^2 \alpha(n) \right) \tag{2.4}$$

where

$$\alpha(n) = \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor \right).$$

3. Main results

In the following theorem we establish an upper bound for R_{-1} in terms of the parameters n, m, d_1 and d_n.

Theorem 3.5. *Let G be undirected, simple graph of order n, $n \geq 2$, with m edges and with no isolated vertices. Then*

$$R_{-1} \leq \frac{n^2}{4m} \left(1 + \left(\sqrt{\frac{d_1}{d_n}} - \sqrt{\frac{d_n}{d_1}} \right)^2 \alpha(n) \right). \tag{3.5}$$

Equality holds if and only if G is k-regular graph, $1 \leq k \leq n-1$.

Proof. For $a_i = d_i$, $i = 1, 2, \ldots, n$, $r = d_n$ and $R = d_1$, the inequality (2.4) transforms into

$$\sum_{i=1}^n d_i \sum_{i=1}^n \frac{1}{d_i} \leq n^2 \left(1 + \left(\sqrt{\frac{d_1}{d_n}} - \sqrt{\frac{d_n}{d_1}} \right)^2 \alpha(n) \right) \tag{3.6}$$

Since $\sum_{i=1}^{n} d_i = 2m$, the inequality (3.6) becomes

$$\sum_{i=1}^{n} \frac{1}{d_i} \leq \frac{n^2}{2m} \left(1 + \left(\sqrt{\frac{d_1}{d_n}} - \sqrt{\frac{d_n}{d_1}} \right)^2 \alpha(n) \right).$$

From this and the inequality (2.1) we obtain inequality (3.5).

Since equalities in (3.6) and (2.1) hold if and only if $d_1 = d_2 = \cdots = d_n$, we conclude that equality in (3.5) holds if and only if G is k-regular graph, $1 \leq k \leq n-1$. □

Remark 3.1. Since the following is valid (see [14])

$$\alpha(n) = \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor \right) = \frac{1}{4} \left(1 - \frac{1 + (-1)^{n+1}}{2n^2} \right),$$

inequality (3.5) can be represented in a form

$$R_{-1} \leq \begin{cases} \frac{n^2}{16m} \left(\sqrt{\frac{d_1}{d_n}} + \sqrt{\frac{d_n}{d_1}} \right)^2, & n \text{ is even} \\ \frac{n^2-1}{16m} \left(\sqrt{\frac{d_1}{d_n}} + \sqrt{\frac{d_n}{d_1}} \right)^2 + \frac{1}{4m}, & n \text{ is odd} \end{cases}$$

This means that inequality (3.5) is stronger than (2.2) for odd n.

Corollary 3.1. *Let G be an undirected simple graph of order n, $n \geq 2$, with m edges and with no isolated vertices.*

If $d_n = 1$ then

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

Equality holds if and only if $G \cong K_2$.

If $d_n \geq 2$ then

$$R_{-1} \leq \frac{n^2}{4m} \left(1 + \frac{(n-3)^2}{2(n-1)} \alpha(n) \right).$$

Equality holds if and only if $G \cong K_3$.

Remark 3.2. The inequalities (3.5) and (2.3) are incomparable. Thus, for example, for $G = P_n$, $n \geq 3$, the inequality (3.5) is stronger than (2.3), whereas for $G = K_{1,n-1}$ the opposite is valid.

Our next result is an upper bound for R_{-1} in terms of n, m, d_2, and d_n.

Theorem 3.6. *Let G be an undirected simple graph of order n, $n \geq 3$, with m edges and with no isolated vertices. Then*

$$R_{-1} \leq \frac{1}{2d_2} + \frac{(n-1)^2}{2(2m-n+1)} \left(1 + \left(\sqrt{\frac{d_2}{d_n}} - \sqrt{\frac{d_n}{d_2}} \right)^2 \alpha(n-1) \right) \tag{3.7}$$

where

$$\alpha(n-1) = \frac{1}{4} \left(1 - \frac{1 + (-1)^n}{2(n-1)^2} \right).$$

Equality holds if and only if $G \cong K_n$.

Proof. For $a_i = d_i$, $i = 1, 2, \dots, n$, $r = d_n$ and $R = d_2$, inequality

$$\left(\sum_{i=2}^{n} a_i\right)\left(\sum_{i=2}^{n} \frac{1}{a_i}\right) \le (n-1)^2 \left(1 + \left(\sqrt{\frac{R}{r}} - \sqrt{\frac{r}{R}}\right)^2 \alpha(n-1)\right)$$

where

$$\alpha(n-1) = \frac{1}{4}\left(1 - \frac{1+(-1)^n}{2(n-1)^2}\right),$$

transforms into

$$\left(\sum_{i=2}^{n} d_i\right)\left(\sum_{i=2}^{n} \frac{1}{d_i}\right) \le (n-1)^2 \left(1 + \left(\sqrt{\frac{d_2}{d_n}} - \sqrt{\frac{d_n}{d_2}}\right)^2 \alpha(n-1)\right). \tag{3.8}$$

Since $\sum_{i=2}^{n} d_i = 2m - d_1$, the inequality (3.8) becomes

$$\sum_{i=1}^{n} \frac{1}{d_i} \le \frac{1}{d_1} + \frac{(n-1)^2}{2m-d_1}\left(1 + \left(\sqrt{\frac{d_2}{d_n}} - \sqrt{\frac{d_n}{d_2}}\right)^2 \alpha(n-1)\right).$$

Bearing in mind the above and the inequality (2.1) we obtain

$$R_{-1} \le \frac{1}{2d_1} + \frac{(n-1)^2}{2(2m-d_1)}\left(1 + \left(\sqrt{\frac{d_2}{d_n}} - \sqrt{\frac{d_n}{d_2}}\right)^2 \alpha(n-1)\right).$$

Since

$$d_2 \le d_1 \qquad \text{and} \qquad d_1 \le n-1\,, \qquad \text{i.e.} \quad 2m - d_1 \ge 2m - n + 1 \tag{3.9}$$

from the last inequality we arrive at (3.7).

Equality in (3.8) holds if and only if $d_2 = d_3 = \cdots = d_n$, and in (3.9) if and only if $d_1 = d_2$ and $d_1 = n - 1$. This means that equality in (3.7) holds if and only if $d_1 = d_2 = \cdots = d_n = n - 1$, i.e. if $G \cong K_n$. □

Remark 3.3. Since $\alpha(n-1) = \frac{1}{4}\left(1 - \frac{1+(-1)^n}{2(n-1)^2}\right)$, $n \ge 3$, inequality (3.7) can be represented in the following way

$$R_{-1} \le \begin{cases} \frac{1}{2d_2} + \frac{(n-1)^2}{8(2m-n+1)}\left(\sqrt{\frac{d_2}{d_n}} + \sqrt{\frac{d_n}{d_2}}\right)^2, & \text{if } n \text{ is odd} \\ \frac{1}{2d_2} + \frac{1}{8(2m-n+1)}\left(n(n-2)\left(\sqrt{\frac{d_2}{d_n}} + \sqrt{\frac{d_n}{d_2}}\right)^2 + 4\right), & \text{if } n \text{ is even} \end{cases}$$

Remark 3.4. The inequalities (3.7) and (2.3) are incomparable. Suppose $K_n - e$ is a graph obtained after removing an edge e from a complete graph K_n. For $G = K_n - e$ the inequality (3.7) is stronger than (2.3). For $G = K_{1,n-1}$ the inequality (2.3) is stronger than (3.7).

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