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SHARP BOUNDS FOR THE GENERAL RANDIĆ INDEX R_{-1} OF A GRAPH

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ABSTRACT. Let G be an undirected simple, connected graph with $n \geq 3$ vertices and m edges, with vertex degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. The general Randić index is defined by

$$R_{-1} = \sum_{(i,j)\in E} \frac{1}{d_i d_j}.$$

Lower and upper bounds for R_{-1} are obtained in this paper.

1. Introduction. Let $G = (V, E)$ be an undirected simple, connected graph with $n \geq 3$ vertices and m edges, with vertex degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. Denote by $\mathbf{A}$ the adjacency matrix of the graph G and by $\mathbf{D}$ the diagonal matrix of its vertex degrees. Then $\mathbf{L}^* = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$ is the normalized Laplacian matrix of G. Its eigenvalues

$$\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n = 0$$

are normalized Laplacian eigenvalues of graph G. If $\rho_{n-1} \neq 0$, the graph G is connected, i.e., it has only one component. If $\rho_{n-k} \neq 0$ and

$$\rho_{n-k+1} = \cdots = \rho_{n-1} = 0 \quad \text{for some } k,\ 1 \leq k \leq n-1,$$

then the graph G has k connected components, see [**2**].

The general Randić index R_{-1} is defined [**8, 9**] by

$$R_{-1} = \sum_{(i,j)\in E} \frac{1}{d_i d_j}.$$

Here, d_i and d_j are the degrees of vertices i and j, respectively.

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The Randić index is an important molecular descriptor and has been closely related with many physico-chemical properties of alkanes, such as boiling points, surface areas, energy levels, etc. For details on chemical applications of the general Randić index, see for example, [**1, 4, 5, 6, 13**]. For a survey of its mathematical properties and new results, see [**3, 11, 12**].

Since the invariant R_{-1} 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 and lower bounds for R_{-1} depending on other graph parameters are of interest. In this paper, we are concerned with determining upper and lower bounds for R_{-1} in terms of the number of vertices, number of edges, vertex degrees and extremal (the greatest and the smallest non-zero) normalized Laplacian eigenvalues.

2. Preliminaries. In what follows, we outline a few results of spectral graph theory and state a few analytical inequalities necessary for subsequent considerations.

In [**13**], Zumstein proved the following result:

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

$$\sum_{i=1}^{n-1} \rho_i = n \quad \textit{and} \quad \sum_{i=1}^{n-1} \rho_i^2 = n + 2R_{-1}. \tag{2.1}$$

Lemma 2.2 ([**6**]). *Let G be an undirected, simple graph of order $n \geq 2$ with no isolated vertices. Then*

$$R_{-1} \leq \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d_i}. \tag{2.2}$$

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

Lemma 2.3 ([**5**]). *Let G be an undirected, simple graph of order $n \geq 2$ with no isolated vertices. Then*

$$\frac{n}{2(n-1)} \leq R_{-1} \leq \left\lfloor \frac{n}{2} \right\rfloor \tag{2.3}$$

with equality in the lower bound if G is a complete graph, and equality in the upper bound if and only if either (i) *n is even and G is the disjoint union of $n/2$ paths of length* 1*, or* (ii) *n is odd and G is the disjoint union of $(n-3)/2$ paths of length* 1 *and one path of length* 2*.*

In **[10]**, also see **[7]**, Rennie proved the following result:

Lemma 2.4 ([**10**])**.** *Let $p_1, p_2, \ldots, p_n$ be non-negative real numbers with the property*

$$p_1 + p_2 + \cdots + p_n = 1.$$

Further, let

$$a_1 \geq a_2 \geq \ldots \geq a_n,$$

be real numbers, and assume that there are $r, R \in \mathbb{R}$ such that

$$0 < r \leq a_i \leq R < +\infty, \quad \textit{for each } i,\ i = 1, 2, \ldots, n.$$

Then

$$\sum_{i=1}^{n} p_i a_i + rR \sum_{i=1}^{n} \frac{p_i}{a_i} \leq r + R. \tag{2.4}$$

Equality in equation (2.4) *is obtained if and only if*

$$R = a_1 = \cdots = a_k \geq a_{k+1} = \cdots = a_n = r$$

for some k, $1 \leq k \leq n$.

Remark 2.5. Let us note that inequality (2.4) can be easily proved by induction or by maximizing the function

$$F(x_1, x_2, \ldots, x_n) = \sum_{i=1}^{n} p_i x_i + rR \sum_{i=1}^{n} \frac{p_i}{x_i}$$

on

$$\{[x_1, x_2, \ldots, x_n] \mid r \leq x_i \leq R\}.$$

3. Main results. We now obtain the lower bound for R_{-1} in terms of the parameters n, ρ_1 and ρ_{n-1}.

Theorem 3.1. *Let G be an undirected, connected graph with $n \geq 2$ vertices and m edges. Then*

$$R_{-1} \geq \frac{n}{2(n-1)} + \frac{1}{4}(\rho_1 - \rho_{n-1})^2. \tag{3.1}$$

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

Proof. Let

$$\rho_1 \geq \rho_2 \geq \cdots \geq \rho_{n-1} > \rho_n = 0$$

be the normalized Laplacian eigenvalues of the graph G. Then

$$\begin{aligned}
&(n-1)\sum_{i=1}^{n-1}\rho_i^2 - \left(\sum_{i=1}^{n-1}\rho_i\right)^2 \\
&= \sum_{1\leq i<j\leq n-1}(\rho_i - \rho_j)^2 \\
&\geq \sum_{i=2}^{n-2}((\rho_1-\rho_i)^2 + (\rho_i - \rho_{n-1})^2) + (\rho_1 - \rho_{n-1})^2 \qquad (3.2)\\
&\geq \frac{1}{2}\sum_{i=2}^{n-2}(\rho_1 - \rho_{n-1})^2 + (\rho_1 - \rho_{n-1})^2 \\
&= \frac{n-1}{2}(\rho_1 - \rho_{n-1})^2
\end{aligned}$$

Bearing in mind Lemma 2.1 and the above inequality, we get

$$n(n-1) + 2(n-1)R_{-1} - n^2 \geq \frac{n-1}{2}(\rho_1 - \rho_{n-1})^2.$$

By rearranging the above inequality we arrive at (3.1).

Equality in (3.2) holds if and only if

$$\rho_1 = \rho_2 = \cdots = \rho_{n-1};$$

hence, the equality in (3.1) holds if and only if $G \cong K_n$. □

Remark 3.2. Since $(\rho_1 - \rho_{n-1})^2 \geq 0$, inequality (3.1) is stronger than the left hand side inequality in (2.3).

Our next result is the upper bound for R_{-1} in terms of n, m, d_1, and d_n.

Theorem 3.3. *Let G be an undirected, simple graph of order $n \geq 2$, with m edges and with no isolated vertices. Then*

$$R_{-1} \leq \frac{n(d_1 + d_n) - 2m}{2d_1 d_n}. \tag{3.3}$$

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

Proof. For

$$p_i = \frac{1}{n}, \qquad a_i = d_i, \quad i = 1, 2, \dots, n,$$

$r = d_n$ and $R = d_1$, inequality (2.4) becomes

$$\frac{1}{n}\sum_{i=1}^{n} d_i + \frac{d_1 d_n}{n}\sum_{i=1}^{n}\frac{1}{d_i} \leq d_1 + d_n. \tag{3.4}$$

Since

$$\sum_{i=1}^{n} d_i = 2m,$$

inequality (3.4) becomes

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

According to the above inequality and inequality (2.2) we obtain the desired result.

Equality in (3.4) holds if and only if

$$d_1 = \cdots = d_k \quad \text{and} \quad d_{k+1} = \cdots = d_n,$$

for some k, $1 \leq k \leq n-1$, and in equation (2.2) if and only if

$$d_1 = d_2 = \cdots = d_n.$$

Consequently, equality in (3.3) holds if and only if G is a k-regular graph, $1 \leq k \leq n-1$. □

Remark 3.4. Inequality (3.3) and the right term in inequality (2.3) are incomparable. It is easy to see that inequality (3.3) is stronger than the right term in inequality (2.3) if G is a k-regular graph, $1 \leq k \leq n-1$, or if $G \cong K_{1,n-1}$. Moreover, inequality (3.3) is stronger than the right term in inequality (2.3) if n is even. However, if n is odd and G is the union of paths of length 1 and a path of length 2, then the right term in inequality (2.3) is stronger than that of inequality (3.3).

In the following theorem, we establish the upper bound for R_{-1} depending on the parameters n, m, d_2 and d_n.

Theorem 3.5. *Let G be an undirected, simple graph of order $n \geq 3$, with m edges and with no isolated vertices. Then*:

$$R_{-1} \leq \frac{1}{2d_2} + \frac{(n-1)(d_2+d_n) - (2m-n+1)}{2d_2 d_n}. \tag{3.5}$$

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

Proof. For

$$p_i = \frac{1}{n-1}, \qquad a_i = d_i, \quad i = 2, \dots, n,$$

$r = d_n$ and $R = d_2$, the inequality

$$\sum_{i=2}^{n} p_i a_i + rR \sum_{i=2}^{n} \frac{p_i}{a_i} \leq r + R$$

transforms into

$$\frac{1}{n-1} \sum_{i=2}^{n} d_i + \frac{d_2 d_n}{n-1} \sum_{i=2}^{n} \frac{1}{d_i} \leq d_2 + d_n, \tag{3.6}$$

i.e.,

$$\sum_{i=1}^{n} \frac{1}{d_i} \leq \frac{1}{d_1} + \frac{(n-1)(d_2+d_n) - (2m-d_1)}{d_2 d_n}. \tag{3.7}$$

Since

$$d_1 \geq d_2 \quad \text{and} \quad 2m - d_1 \geq 2m - n + 1,$$

from inequality (3.7), it follows that

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

From inequality (3.8) and inequality (2.2) we obtain inequality (3.5).

Equality in (3.6) holds if and only if

$$d_2 = \cdots = d_k \quad \text{and} \quad d_{k+1} = \cdots = d_n,$$

for some k, $1 \le k \le n-1$, and in inequality (2.2) if and only if

$$d_1 = d_2 = \cdots = d_n.$$

Equality $2m - d_1 = 2m - n + 1$ holds if and only if $d_1 = n - 1$. This means that equality in (3.5) holds if and only if $G \cong K_n$. □

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