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SOME NEW BOUNDS ON RANDIĆ ENERGY

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Abstract. Let $G = (V, E)$ be a simple graph of order n with vertex set $V = V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E = E(G)$. Let d_i be the degree of the vertex v_i in G for $i = 1, 2, \dots, n$. The Randić matrix $\mathbf{R} = \mathbf{R}(G) = ||R_{ij}||_{nxn}$ is defined by

$$R_{ij} = \begin{cases} \dfrac{1}{\sqrt{d_i d_j}}, & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases}$$

The eigenvalues of matrix $\mathbf{R}$, denoted by $\rho_1, \rho_2, \dots, \rho_n$, are called the Randić eigenvalues of graph G. The Randić energy of graph G, denoted by RE, is defined as

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i|.$$

In this paper we establish some new upper and lower bounds on Randić energy.

1. Introduction

Let $G = (V, E)$ be a simple graph with vertex set $V = V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E = E(G)$. Denote by d_i the degree of vertex $v_i \in V$, i.e., the number of the vertices adjacent to v_i, $i = 1, 2, \dots, n$. A vertex of degree zero is said to be isolated. In this paper we consider graphs without such vertices. Let $\mathbf{A} = \mathbf{A}(G)$ be the adjacency matrix of G and denote by $\mathbf{D} = \mathbf{D}(G)$ the diagonal matrix whose diagonal elements are vertex degrees of G.

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The Randić matrix of G is the $n \times n$ matrix $\mathbf{R} = \mathbf{R}(G) = ||R_{ij}||$, defined by

$$R_{ij} = \begin{cases} \dfrac{1}{\sqrt{d_i d_j}}, & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases}$$

The eigenvalues $\rho_1, \rho_2, \dots, \rho_n$ of matrix $\mathbf{R}$ are called the Randić eigenvalues of a graph G, and suppose they are labeled in a non-increasing order, i.e., $\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_n$. The Randić energy $RE = RE(G)$ of a graph G is defined as [2, 3, 12]

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i|.$$

For recent results on Randić energy we refer the reader to the papers [1, 9–11, 13, 16]. Also, several lower and upper bounds on Randić energy were obtained in [2, 3, 7, 12, 14] and [15].

Randić matrix occurs in a natural way within Laplacian spectral theory and provides the non-trivial part of the so-called normalized Laplacian matrix [3]. Let $\mathbf{D} = \mathbf{D}(G)$ be the diagonal matrix of order n whose i-th diagonal entry is d_i. Then the Laplacian matrix of G is defined as $\mathbf{L} = \mathbf{L}(G) = \mathbf{D} - \mathbf{A}$. If graph G has no isolated vertices, then the matrix $\mathbf{D}^{-1/2}$ exists. For a graph without isolated vertices, the normalized Laplacian matrix can be defined [6] as

$$\tilde{\mathbf{L}} = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2},$$

where $\mathbf{I}$ is the unit matrix of order n.

Recall that $\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2} = \mathbf{R}$ for a graph without isolated vertices, implying the following relation [3] between the Randić matrix and the normalized Laplacian matrix of a graph without isolated vertices

$$\tilde{\mathbf{L}} = \mathbf{I} - \mathbf{R}. \tag{1.1}$$

The rest of the paper is organized as follows. In Section 2 we state some previously known results needed for the subsequent considerations. In Section 3 we obtain some new upper and lower bounds for the Randić energy. In addition, we determine a new lower bound on RE which is better than the lower bound obtained in [7, 15].

2. Preliminaries

In this section we review some properties of normalized Laplacian eigenvalues, Randić eigenvalues and Randić energy. Besides, we recall some analytic inequalities for real number sequences that are of interest for the subsequent considerations.

If we denote by $\tilde{\mu}_1 \geqslant \tilde{\mu}_2 \geqslant \cdots \geqslant \tilde{\mu}_{n-1} \geqslant \tilde{\mu}_n$ the normalized Laplacian eigenvalues of a graph G, then from (1.1) it follows

$$\rho_i = 1 - \tilde{\mu}_{n-i+1}, \quad i = 1, 2, \dots, n. \tag{2.1}$$

There are numerous results for the $\tilde{\mathbf{L}}$-eigenvalues, see [4] for example. From [4] it follows that $0 \leqslant \tilde{\mu}_i \leqslant 2$, $i = 1, 2, \ldots, n$, which implies, by (2.1),

$$-1 \leqslant \rho_i \leqslant 1, \quad i = 1, 2, \ldots, n. \tag{2.2}$$

Besides, the following results for the Randić eigenvalues are known.

Lemma 2.1. [12, 17] *Let G be a graph on n vertices, $n \geq 1$, and let ρ_1 be the largest eigenvalue of its Randić matrix. Then $\rho_1 = 0$ if and only if $G \cong \overline{K}_n$. If G possesses at least one edge, then $\rho_1 = 1$.*

Lemma 2.2. [12] *Let G be a graph on n vertices, and let $\mathbf{A}$ and $\mathbf{R}$ be its adjacency and Randić matrices. If $\mathbf{A}$ has n_+, n_0, and n_- positive, zero, and negative eigenvalues, respectively ($n_+ + n_0 + n_- = n$), then $\mathbf{R}$ has n_+, n_0, and n_- positive, zero, and negative eigenvalues, respectively.*

Lemma 2.3. [12] *Let G be a graph on n vertices, and let $\mathbf{A}$ and $\mathbf{R}$ be its adjacency and Randić matrices. If G possesses isolated vertices, then* $\det \mathbf{R} = \det \mathbf{A} = 0$, *otherwise*

$$\det \mathbf{R} = \frac{1}{d_1 d_2 \cdots d_n} \det \mathbf{A}.$$

Denote by η the nullity of a graph G, i.e., the multiplicity of 0 as an eigenvalue of $\mathbf{A} = \mathbf{A}(G)$. Lemma 2.2 implies that η is also the multiplicity of 0 as an eigenvalue of the matrix $\mathbf{R}$. In addition, as we are concerned with graphs without isolated vertices, it holds $\eta(G) < n$.

Denote by $\rho_1^* \geqslant \rho_2^* \geqslant \cdots \geqslant \rho_n^*$ the absolute values of the Randić eigenvalues of G labeled in a non-increasing order. Then, by (2.2), $\rho_i^* \in [0, 1]$, for $i = 1, 2, \ldots, n$.

In the sequel we review some known inequalities needed for subsequent considerations.

Lemma 2.4. [5] *Let $a_1, a_2, \ldots, a_n$ be positive real numbers such that $0 < a_1 \leq \cdots \leq a_i \leq \cdots \leq a_k \leq \cdots \leq a_n$. Then*

$$a_1 + a_2 + \cdots + a_n - n\sqrt[n]{a_1 a_2 \cdots a_n} \geq P(\sqrt{a_k} - \sqrt{a_i})^2, \tag{2.3}$$

where

$$P = \begin{cases} \dfrac{2i(n-k+1)}{n+i-k+1}, & i+k \leq n+1, \\ n-k+1, & i+k \geq n+1. \end{cases}$$

Lemma 2.5. [19] *Let $a_i \in \mathbb{R}^+, i = 1, \ldots, n$. Then*

$$(n-1)\sum_{i=1}^{n} a_i + n\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}} \geq \left(\sum_{i=1}^{n} \sqrt{a_i}\right)^2 \geq \sum_{i=1}^{n} a_i + n(n-1)\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}. \tag{2.4}$$

Lemma 2.6. [18] *Let $a_1, \ldots, a_n$ and $b_1, \ldots, b_n$ be real numbers such that $a \leq a_i \leq A$ and $b \leq b_i \leq B$, $i = 1, \ldots, n$. Then*

$$-(A-a)(B-b)n\alpha(n) \le \sum_{i=1}^{n} a_i b_i - \frac{1}{n}\sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \le (A-a)(B-b)n\alpha(n), \tag{2.5}$$

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

3. Main Results

In recent papers [7, 15] the following lower bound on RE was obtained.

Theorem 3.1. [7, 15] *Let G be a graph on n vertices. Then*

$$RE(G) \ge 1 + (n-1)|\det \mathbf{R}|^{\frac{1}{n-1}}, \tag{3.1}$$

with equality if and only if G is a complete graph or a non-bipartite graph with three distinct Randić eigenvalues

$$\left(1, \sqrt{\frac{2\sum\limits_{v_iv_j\in E(G)} \frac{1}{d_id_j}}{n-1}}, -\sqrt{\frac{2\sum\limits_{v_iv_j\in E(G)} \frac{1}{d_id_j}}{n-1}}\right).$$

In the sequel we obtain the lower bound on RE which improves the result (3.1).

Theorem 3.2. *Let G be a graph on n vertices, $n \geqslant 2$, and let $\rho_1^* \ge \rho_2^* \ge \cdots \ge \rho_n^*$ be the absolute values of its Randić eigenvalues labeled in a non-increasing order.*

(a) *If G is a non-singular graph, i.e., $\eta(G) = 0$, then*

$$RE(G) \ge 1 + (n-1)|\det \mathbf{R}|^{\frac{1}{n-1}} + (\sqrt{\rho_n^*} - \sqrt{\rho_2^*})^2. \tag{3.2}$$

(b) *If $\eta(G) = n - j$, $0 < j < n$, then*

$$RE(G) \ge 1 + (j-1)\left(\prod_{i=2}^{j-1} \rho_i^*\right)^{\frac{1}{j-1}} + (\sqrt{\rho_j^*} - \sqrt{\rho_2^*})^2. \tag{3.3}$$

Proof. (a) Since $\eta(G) = 0$, it follows that $\rho_i^* \in (0, 1]$, implying $RE(G) = \rho_1^* + \sum\limits_{i=2}^{n} \rho_i^*$. If we apply the inequality (2.3) to $\sum\limits_{i=2}^{n} \rho_i^*$ letting $a_{i-1} = \rho_i^*$, $i = 2, \dots, n$, whereas $k = n - 1$ and $i = 1$, we obtain that $P = 1$, and so

$$\begin{aligned}\sum_{i=2}^{n} \rho_i^* \ge& (n-1)\sqrt[n-1]{\rho_2^* \cdots \rho_n^*} + (\sqrt{\rho_n^*} - \sqrt{\rho_2^*})^2 \\ =& (n-1)|\det \mathbf{R}|^{\frac{1}{n-1}} + (\sqrt{\rho_n^*} - \sqrt{\rho_2^*})^2.\end{aligned}$$

By Lemma 2.1, $\rho_1^* = 1$, which completes the proof.

(b) We now turn to the case $\eta(G) = n - j$, $0 < j < n$. If we apply the inequality (2.3) in the same manner as in case (a) to non-zero absolute values of Randić eigenvalues $1 = \rho_1^* \geqslant \rho_2^* \geqslant \cdots \geqslant \rho_j^* > 0$, we obtain (3.3). □

Remark 3.1. If G is a non-singular graph, then the lower bound (3.2) is better than the lower bound (3.1) from [7, 15]. If $\eta(G) > 0$, then $\det \mathbf{R} = 0$ and the lower bound (3.3) is also better than the lower bound (3.1) from [7, 15].

Theorem 3.3. *Let G be a non-singular graph on n vertices, $n \geqslant 2$, and let $\rho_1^* \geq \rho_2^* \geq \cdots \geq \rho_n^*$ be the absolute values of its Randić eigenvalues labeled in a non-increasing order. Then*

(3.4)
$$-\frac{n^2}{n-1}\alpha(n)(\sqrt{\rho_1^*}-\sqrt{\rho_n^*})^2+n|\det \mathbf{R}|^{\frac{1}{n}} \leq RE(G) \leq n^2\alpha(n)(\sqrt{\rho_1^*}-\sqrt{\rho_n^*})^2+n|\det \mathbf{R}|^{\frac{1}{n}},$$

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

Proof. In deducing the left-hand side of the inequality (3.4) we make use of the inequality (2.5) for $A = B = \sqrt{\rho_1^*}, a = b = \sqrt{\rho_n^*}$, $a_i = b_i = \sqrt{\rho_i^*}$, $i = 1, \ldots, n$. In addition, having in mind the right-hand side of the inequality (2.4), we obtain

$$\begin{aligned} RE(G) &\geqslant -(\sqrt{\rho_1^*} - \sqrt{\rho_n})^2 n\alpha(n) + \frac{1}{n}\left(\sum_{i=1}^{n} \sqrt{\rho_i^*}\right)^2 \\ &\geqslant -(\sqrt{\rho_1^*} - \sqrt{\rho_n})^2 n\alpha(n) + \frac{1}{n}\sum_{i=1}^{n} \rho_i^* + (n-1)\left|\prod_{i=1}^{n} \rho_i^*\right|^{\frac{1}{n}} \\ &= -(\sqrt{\rho_1^*} - \sqrt{\rho_n})^2 n\alpha(n) + \frac{1}{n} RE(G) + (n-1)|\det \mathbf{R}|^{\frac{1}{n}}, \end{aligned}$$

and hence the proof follows from the last inequality.

In order to prove the right-hand side of the inequality (3.4) we will again use the inequalities (2.5) and (2.4). Letting $A = B = \sqrt{\rho_1^*}$, $a = b = \sqrt{\rho_n^*}$, $a_i = b_i = \sqrt{\rho_i^*}$, $i = 1, \ldots, n$, in the inequality (2.5), and then using the left-hand side of the inequality (2.4), we obtain

$$\begin{aligned} RE(G) &\leqslant (\sqrt{\rho_1^*} - \sqrt{\rho_n^*})^2 n\alpha(n) + \frac{1}{n}\left(\sum_{i=1}^{n} \sqrt{\rho_i^*}\right)^2 \\ &\leqslant (\sqrt{\rho_1^*} - \sqrt{\rho_n^*})^2 n\alpha(n) + \frac{1}{n}(n-1)\sum_{i=1}^{n} \rho_i^* + \left|\prod_{i=1}^{n} \rho_i^*\right|^{\frac{1}{n}} \\ &= (\sqrt{\rho_1^*} - \sqrt{\rho_n^*})^2 n\alpha(n) + \frac{1}{n}(n-1) RE(G) + |\det \mathbf{R}|^{\frac{1}{n}}, \end{aligned}$$

which completes the proof. □

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