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SOME REMARKS ON THE RANDIĆ ENERGY OF GRAPHS

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Abstract. Let G be a graph of order n. The Randić energy of G is defined as $RE(G) = \sum_{i=1}^{n} |\rho_i|$, where $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$ are the Randić eigenvalues of G. In this study, we present improved bounds for $RE(G)$ as well as a relationship between (ordinary) graph energy and $RE(G)$.

1. Introduction

Let $G = (V, E)$, $V = \{v_1, v_2, \ldots, v_n\}$, be a simple connected graph of order n and size m, with vertex degree sequence $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$, $d_i = d(v_i)$. Denote by $D = \operatorname{diag}(d_1, d_2, \ldots, d_n)$ the diagonal matrix of its vertex degrees. If vertices v_i and v_j are adjacent in G, it will be denoted as $i \sim j$.

Let $A = (a_{ij})$, be the $(0, 1)$ adjacency matrix of G. The eigenvalues of matrix A, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, are the (ordinary) eigenvalues of G [4]. Some well known properties of these eigenvalues are [4]:

$$\sum_{i=1}^{n} \lambda_i = \operatorname{tr}(A) = 0, \quad \sum_{i=1}^{n} \lambda_i^2 = \operatorname{tr}(A^2) = \sum_{i=1}^{n} d_i = 2m, \quad \prod_{i=1}^{n} \lambda_i = \det A.$$

Denote with $|\lambda_1^*| \geq |\lambda_2^*| \geq \cdots \geq |\lambda_n^*|$ the non-increasing arrangement of the absolute values of eigenvalues of G. The notion of (ordinary) graph energy was introduced in [12]. It is defined to be

$$E(G) = \sum_{i=1}^{n} |\lambda_i| = \sum_{i=1}^{n} |\lambda_i^*|.$$

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The Randić matrix of G [2] is defined as

$$R = R(G) = D^{-1/2} A D^{-1/2}.$$

The eigenvalues of matrix R , $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$, form the Randić spectrum of G. Some properties of Randić eigenvalues are (see, e.g., [2]):

$$\sum_{i=1}^{n} \rho_i = \operatorname{tr}(R) = 0, \quad \sum_{i=1}^{n} \rho_i^2 = \operatorname{tr}(R^2) = 2R_{-1}(G),$$

where $R_{-1}(G)$ is a vertex–degree based graph invariant introduced in [3] defined as

$$R_{-1}(G) = \sum_{i \sim j} \frac{1}{d_i d_j}.$$

It is known as general Randić index R_{-1}, as well as modified second Zagreb index [24].

In [14] it was proven that the following identity is valid

$$\det R = \frac{\det A}{\prod_{i=1}^{n} d_i}. \tag{1.1}$$

The other two vertex–degree based topological indices that are of interest for the present paper are the first Zagreb index [17]

$$M_1(G) = \sum_{i=1}^{n} d_i^2 = \sum_{i \sim j} (d_i + d_j),$$

and the inverse degree index [9] defined as

$$ID(G) = \sum_{i=1}^{n} \frac{1}{d_i} = \sum_{i \sim j} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right).$$

Denote with $|\rho_1^*| \geq |\rho_2^*| \geq \cdots \geq |\rho_n^*|$ the non-increasing arrangement of the absolute values of Randić eigenvalues of G. The Randić energy of G is defined as [2]

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

More on its mathematical properties can be found in [1–3, 5, 7, 14, 20, 22].

In this paper, we obtain improved bounds for $RE(G)$ as well as a relationship between $E(G)$ and $RE(G)$.

2. Preliminaries

In this section we recall some results from spectral graph theory and analytical inequalities that are of interest for the present paper.

Lemma 2.1 ([20]). *The Randić spectral radius is $\rho_1 = 1$.*

Remark 2.1. In [14] it was observed that when $G \cong \overline{K}_n$ then $\rho_1 = 0$. Therefore, if G has at least one edge, then $\rho_1 = 1$.

Let $G_1 \bigvee G_2$ denote the complete product of two graphs G_1 and G_2. This graph is obtained from $G_1 \cup G_2$ by joining every vertex of G_1 with every vertex of G_2.

Lemma 2.2 ([8])**.** *Let G be a connected graph of order n with maximum vertex degree $\Delta = n-1$. Then $|\rho_2| = |\rho_3| = \cdots = |\rho_n|$ if and only if $G \cong K_n$, or $G \cong K_1 \bigvee r\, K_2$, with $n = 2r+1$ ($r \geq 2$).*

Lemma 2.3 ([20])**.** *Let G be a connected graph of order n. Then*

$$RE(G) \leq 1 + \sqrt{(n-1)(2R_{-1}(G)-1)}. \tag{2.1}$$

Remark 2.2. The inequality (2.1) was also proved in [19, 21], as well as in [5] as a special case of one more general result. In [8] it was proved that when $\Delta = n-1$, equality in (2.1) holds if and only if $G \cong K_n$, or $G \cong K_1 \bigvee r\, K_2$, with $n = 2r+1$ ($r \geq 2$).

Lemma 2.4 ([1])**.** *Let G be a connected bipartite graph of order $n \geq 2$. Then*

$$RE(G) \leq 2 + \sqrt{(n-2)(2R_{-1}(G)-2)}. \tag{2.2}$$

Remark 2.3. The inequality (2.2) was also proved in [21]. In [8] it was proven that equality in (2.2) holds if and only if $G \cong K_{p,q}$, $p+q=n$, for odd n.

Lemma 2.5 ([11])**.** *Let G be a connected bipartite graph of order $n \geq 3$ with Randić eigenvalues $\rho_1 = 1 \geq \rho_2 \geq \cdots \geq \rho_{n-1} \geq \rho_n = -1$ and let $\rho = \max_{2 \leq i \leq n-1} \{|\rho_i|\}$. Then, for any real k, $\rho \geq k \geq \sqrt{\frac{2R_{-1}(G)-2}{n-2}}$, holds*

$$RE(G) \leq 2 + k + \sqrt{(n-3)(2R_{-1}(G)-2-k^2)}. \tag{2.3}$$

Equality holds if G is a complete bipartite graph, in which case $k=0$.

Remark 2.4. In [18, Theorem 3.4] it was claimed that when

$$\frac{1}{\Delta} \geq \sqrt{\frac{2R_{-1}(G)-1}{n-1}}, \tag{2.4}$$

then

$$RE(G) \leq 1 + \frac{1}{\Delta} + \sqrt{(n-2)\left(2R_{-1}(G) - 1 - \frac{1}{\Delta^2}\right)}, \tag{2.5}$$

which would mean that (2.5) is stronger than (2.1). However, if (2.4) is true, then $\Delta \geq n-1$, which is not possible. Therefore, the inequality (2.5) is not correct.

Lemma 2.6 ([6, 18])**.** *Let G be a connected graph of order n. Then*

$$RE(G) \geq 1 + (n-1)\left(\frac{|\det A|}{\prod_{i=1}^{n} d_i}\right)^{\frac{1}{n-1}}. \tag{2.6}$$

The following analytical inequality would be used in proofs of theorems in the present paper.

Lemma 2.7 ([23]). *Let $p = (p_i)$, $i = 1, 2, \dots, n$, be a sequence of positive real numbers and $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \dots, n$, two similarly ordered sequences of non–negative real numbers. Then*

$$\sum_{i=1}^{n} p_i \sum_{i=1}^{n} p_i a_i b_i \geq \sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} p_i b_i. \tag{2.7}$$

When $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \dots, n$, are of different monotonicity, then opposite inequality is valid. Equality holds if and only if $a_1 = \cdots = a_n$ or $b_1 = \cdots = b_n$.

3. Main Results

In the next theorem we establish a lower bound on $RE(G)$.

Theorem 3.1. *Let G be a connected graph of order n. Then, for any real k, $|\rho_2^*| \geq k \geq \sqrt{\frac{2R_{-1}(G)-1}{n-1}}$, holds*

$$RE(G) \geq 1 + k + (n-2)\left(\frac{|\det A|}{k \prod_{i=1}^{n} d_i}\right)^{\frac{1}{n-2}}. \tag{3.1}$$

Equality holds if and only if G is a graph with the property $\rho_1 = |\rho_1^*| = 1$, $|\rho_2^*| = k$, and $|\rho_i^*| = \sqrt{\frac{2R_{-1}(G)-1-k^2}{n-2}}$, for $i = 3, 4, \dots, n$.

Proof. Using arithmetic-geometric mean inequality (see, e.g., [23]), Lemma 2.1 and (1.1) we obtain

$$\begin{aligned} RE(G) =& \sum_{i=1}^{n} |\rho_i^*| = 1 + |\rho_2^*| + \sum_{i=3}^{n} |\rho_i^*| \\ \geq& 1 + |\rho_2^*| + (n-2)\left(\frac{|\det R|}{|\rho_2^*|}\right)^{\frac{1}{n-2}} \\ =& 1 + |\rho_2^*| + (n-2)\left(\frac{|\det A|}{|\rho_2^*| \prod_{i=1}^{n} d_i}\right)^{\frac{1}{n-2}}. \end{aligned} \tag{3.2}$$

Let us consider the following function defined by

$$f(k) = x + (n-2)\left(\frac{|\det A|}{x \prod_{i=1}^{n} d_i}\right)^{\frac{1}{n-2}}.$$

Observe that f is increasing for $x \geq \left(\frac{|\det A|}{\prod_{i=1}^{n} d_i}\right)^{\frac{1}{n-1}}$. Considering Lemmas 2.1 and 2.3 together with (1.1), for any real k, $|\rho_2^*| \geq k \geq \sqrt{\frac{2R_{-1}(G)-1}{n-1}}$, we have that

$$|\rho_2^*| \geq k \geq \sqrt{\frac{2R_{-1}(G)-1}{n-1}} \geq \frac{RE(G)-1}{n-1} = \frac{\sum_{i=2}^{n} |\rho_i^*|}{n-1} \geq \left(\prod_{i=2}^{n} |\rho_i^*|\right)^{\frac{1}{n-1}} = \left(\frac{|\det A|}{\prod_{i=1}^{n} d_i}\right)^{\frac{1}{n-1}}.$$

Then, we deduce that $f(|\rho_2^*|) \geq f(k)$. Combining this with (3.2), the inequality (3.1) is obtained. The equality in (3.1) holds if and only if

$$|\rho_2^*| = k \quad \text{and} \quad |\rho_3^*| = \cdots = |\rho_n^*|.$$

Since $\sum_{i=2}^n |\rho_i^*|^2 = 2R_{-1}(G) - 1$, the above conditions imply that $|\rho_3^*| = \cdots = |\rho_n^*| = \sqrt{\frac{2R_{-1}(G)-1-k^2}{n-2}}$. This completes the proof. □

Corollary 3.1. *Let G be a connected graph of order n. Then*

$$RE(G) \geq 1 + \sqrt{\frac{2R_{-1}(G)-1}{n-1}} + (n-2)\left(\frac{|\det A|}{\sqrt{\frac{2R_{-1}(G)-1}{n-1}}\prod_{i=1}^n d_i}\right)^{\frac{1}{n-2}}. \tag{3.3}$$

If the maximum vertex degree Δ is equal to $n-1$, the equality in (3.3) *holds if and only if $G \cong K_n$, or $G \cong K_1 \bigvee r\,K_2$, with $n = 2r+1$ $(r \geq 2)$.*

Proof. The inequality (3.3) is obtained from (3.1) for $k = \sqrt{\frac{2R_{-1}(G)-1}{n-1}}$. Now, assume that equality in (3.3) holds. Then

$$|\rho_2^*| = \sqrt{\frac{2R_{-1}(G)-1}{n-1}} \quad \text{and} \quad |\rho_3^*| = \cdots = |\rho_n^*|.$$

Since $\sum_{i=2}^n |\rho_i^*| = 2R_{-1}(G) - 1$, we get

$$|\rho_3^*| = \cdots = |\rho_n^*| = \sqrt{\frac{2R_{-1}(G)-1}{n-1}}.$$

The above results state that $|\rho_2^*| = |\rho_3^*| = \cdots = |\rho_n^*|$, that is $|\rho_2| = |\rho_3| = \cdots = |\rho_n|$. Then, by Lemma 2.2 if $\Delta = n-1$, the equality in (3.3) holds if and only if $G \cong K_n$, or $G \cong K_1 \bigvee r\,K_2$, with $n = 2r+1$ $(r \geq 2)$. □

Remark 3.1. The lower bounds (3.1) and (3.3) are stronger than the lower bound (2.6). Moreover, by Theorem 3.1, it is possible to derive stronger lower bound than (3.3) using any real k such that $|\rho_2^*| \geq k \geq \sqrt{\frac{2R_{-1}(G)-1}{n-1}}$.

In the next theorem we establish a relationship between Randić energy and general Randić index R_{-1}.

Theorem 3.2. *Let G be a connected graph of order $n \geq 3$. Then, for any real k, such that $|\rho_2^*| \geq k \geq \sqrt{\frac{2R_{-1}(G)-1}{n-1}}$, we have*

$$RE(G) \leq 1 + k + \sqrt{(n-2)(2R_{-1}(G) - 1 - k^2)}. \tag{3.4}$$

Equality holds if and only if G is a graph with the property $\rho_1 = |\rho_1^*| = 1$, $|\rho_2^*| = k$ and $|\rho_i^*| = \sqrt{\frac{2R_{-1}(G)-1-k^2}{n-2}}$, for $i = 3, 4, \ldots, n$.

Proof. By the Cauchy–Schwarz inequality (see, e.g., [23]), we have that

$$\sum_{i=3}^n |\rho_i^*| \leq \left(\sum_{i=3}^n 1\right)^{1/2} \left(\sum_{i=3}^n |\rho_i^*|^2\right)^{1/2},$$

that is

$$RE(G) \le |\rho_1^*| + |\rho_2^*| + \sqrt{(n-2)(2R_{-1}(G) - |\rho_1^*|^2 - |\rho_2^*|^2)}.$$

By Lemma 2.1, we have that $\rho_1 = |\rho_1^*| = 1$. Considering this fact with the above inequality, we get

$$RE(G) \le 1 + |\rho_2^*| + \sqrt{(n-2)(2R_{-1}(G) - 1 - |\rho_2^*|^2)}. \tag{3.5}$$

Now, observe the function

$$f(x) = x + \sqrt{(n-2)(2R_{-1}(G) - 1 - x^2)}, \quad x \ge 0.$$

This function is monotone decreasing for $x \ge \sqrt{\frac{2R_{-1}(G)-1}{n-1}}$. Therefore for any $k \ge 0$ with the property $|\rho_2^*| \ge k \ge \sqrt{\frac{2R_{-1}(G)-1}{n-1}}$, holds that $f(|\rho_2^*|) \le f(k)$. From this inequality and (3.5) we obtain (3.4).

The equality case for (3.4) can be proved similarly as in case of Theorem 3.1. □

Remark 3.2. When $k = \sqrt{\frac{2R_{-1}(G)-1}{n-1}}$, from (3.4) the inequality (2.1) is obtained, which means that inequality (3.4) is stronger than (2.1).

Remark 3.3. Recall that the Randić spectrum of a bipartite graph is symmetric with respect to the origin, that is, $\rho_i = -\rho_{n-i+1}$, for $i = 1, 2, \ldots, n$ [10]. In this case, $|\rho_1^*| = \rho_1 = 1 = |\rho_n| = |\rho_2^*|$. On the other hand, $\rho = |\rho_3^*| = |\rho_4^*|$.

Having in mind the above remark, by a similar procedure as in Theorem 3.2, the following result can be proven.

Theorem 3.3. *Let G be a connected bipartite graph of order $n \ge 5$. Then, for any real k such that $|\rho_3^*| \ge k \ge \sqrt{\frac{2R_{-1}(G)-2}{n-2}}$, we have*

$$RE(G) \le 2 + 2k + \sqrt{(n-4)(2R_{-1}(G) - 2 - 2k^2)}. \tag{3.6}$$

Equality holds if and only if G is a graph with the property $\rho_1 = |\rho_1^*| = |\rho_2^*| = 1$, $|\rho_3^*| = |\rho_4^*| = k$ and $|\rho_i^*| = \sqrt{\frac{2R_{-1}(G)-2-2k^2}{n-4}}$, for $i = 5, \ldots, n$.

Remark 3.4. When $k = \sqrt{\frac{2R_{-1}(G)-2}{n-2}}$, from (3.6) the inequality (2.2) is obtained. Furthermore, the inequality (3.6) is stronger than (2.2) and (2.3).

Theorem 3.4. *Let G be a connected graph of order $n \ge 2$. Then*

$$RE(G) \le 1 + \sqrt{(n-1)\left(2R_{-1}(G) - 1 - \frac{1}{2}(|\rho_2^*| - |\rho_n^*|)^2\right)}. \tag{3.7}$$

Equality holds if and only if G is a graph with the property $\rho_1 = |\rho_1^*| = 1$ and $|\rho_3^*| = \cdots = |\rho_{n-1}^*| = \frac{|\rho_2^*|+|\rho_n^*|}{2}$.

Proof. Based on the Lagrange's identity (see e.g. [23]), we have that

$$\begin{aligned}(n-1)\sum_{i=2}^{n}|\rho_i^*|^2-\left(\sum_{i=2}^{n}|\rho_i^*|\right)^2 &=\sum_{2\le i<j\le n}(|\rho_i^*|-|\rho_j^*|)^2\\ &\ge(|\rho_2^*|-|\rho_n^*|)^2+\sum_{i=3}^{n-1}\left((|\rho_i^*|-|\rho_n^*|)^2+(|\rho_2^*|-|\rho_i^*|)^2\right)\\ &\ge(|\rho_2^*|-|\rho_n^*|)^2+\frac{1}{2}\sum_{i=3}^{n-1}(|\rho_2^*|-|\rho_n^*|)^2 \qquad (3.8)\\ &=\frac{n-1}{2}(|\rho_2^*|-|\rho_n^*|)^2.\end{aligned}$$

Since

$$(n-1)\sum_{i=2}^{n}|\rho_i^*|^2-\left(\sum_{i=2}^{n}|\rho_i^*|\right)^2=(n-1)(2R_{-1}(G)-1)-(RE(G)-1)^2,$$

from (3.8) the inequality (3.7) is obtained.

Equality in (3.8) holds if and only if $|\rho_3^*|=\cdots=|\rho_{n-1}^*|$ and $|\rho_i^*|-|\rho_n^*|=|\rho_2^*|-|\rho_i^*|$, for $i=3,\ldots,n-1$, which implies that equality in (3.7) holds if and only if $\rho_1=|\rho_1^*|=1$ and $|\rho_3^*|=\cdots=|\rho_{n-1}^*|=\frac{|\rho_2^*|+|\rho_n^*|}{2}$. □

Remark 3.5. Let us note that the inequality (3.7) is stronger than (2.1).

The proof of the next theorem is analogous to that of Theorem 3.4, hence omitted.

Theorem 3.5. *Let G be a connected bipartite graph of order $n\ge 4$. Then*

$$RE(G)\le 2+\sqrt{(n-2)\left(2R_{-1}(G)-2-\frac{1}{2}(|\rho_3^*|-|\rho_n^*|)^2\right)}. \qquad (3.9)$$

Equality holds if and only if G is a graph with the property $\rho_1=|\rho_1^*|=|\rho_2^*|=1$ and $|\rho_4^*|=\cdots=|\rho_{n-1}^*|=\frac{|\rho_3^*|+|\rho_n^*|}{2}$.

Remark 3.6. Notice that the inequality (3.9) is stronger than (2.2).

We now give a relationship between $E(G)$ and $RE(G)$.

Theorem 3.6. *Let G be a graph of order $n\ge 2$ and size m, without isolated vertices. Then we have*

$$E(G)RE(G)\le 2n\sqrt{mR_{-1}(G)}. \qquad (3.10)$$

Equality holds if and only if $G\cong\frac{n}{2}K_2$, for even n.

Proof. For $p_i=1$, $a_i=|\lambda_i^*|$, $b_i=|\rho_i^*|$, $i=1,2,\ldots,n$, the inequality (2.7) becomes

$$\sum_{i=1}^{n}1\sum_{i=1}^{n}|\lambda_i^*|\,|\rho_i^*|\ge\sum_{i=1}^{n}|\lambda_i^*|\,\sum_{i=1}^{n}|\rho_i^*|,$$

that is

$$E(G)RE(G) \leq n\sum_{i=1}^{n}|\lambda_i^*|\,|\rho_i^*|. \tag{3.11}$$

On the other hand, having in mind Cauchy–Schwarz inequality, we have that

$$n\sum_{i=1}^{n}|\lambda_i^*|\,|\rho_i^*| \leq n\left(\sum_{i=1}^{n}|\lambda_i^*|^2\right)^{1/2}\left(\sum_{i=1}^{n}|\rho_i^*|^2\right)^{1/2},$$

that is

$$n\sum_{i=1}^{n}|\lambda_i^*|\,|\rho_i^*| \leq 2n\sqrt{mR_{-1}(G)}. \tag{3.12}$$

Now, from (3.11) and (3.12) we arrive at (3.10).

Equality in (3.11) holds if and only if $|\lambda_1^*| = \cdots = |\lambda_n^*|$, or $|\rho_1^*| = \cdots = |\rho_n^*|$. Equality in (3.12) holds if and only if $|\lambda_i^*| = C\,|\rho_i^*|$, $C = Const$, for $i = 1, 2, \ldots, n$. Thus, equalities in both (3.11) and (3.12) hold if and only if $|\lambda_1^*| = \cdots = |\lambda_n^*|$ and $|\rho_1^*| = \cdots = |\rho_n^*|$. Since G has no isolated vertices, equality in (3.10) holds if and only if $G \cong \frac{n}{2}K_2$, for even n. □

Recall that the Sombor energy of a graph G, denoted by $E_{SO}(G)$, is introduced as the sum of the absolute values of the eigenvalues of its Sombor matrix [13]. The following relationship between graph energy and Sombor energy can be found in [15].

Theorem 3.7 ([15]). *If G is a bipartite graph whose all cycles (if any) have size not divisible by 4, then*

$$E_{SO}(G) \leq \sqrt{2}\Delta E(G).$$

From Theorem 3.6 and Theorem 3.7, we directly have the following.

Corollary 3.2. *If G is a bipartite graph whose all cycles (if any) have size not divisible by 4, then*

$$E_{SO}(G)\, RE(G) \leq 2\Delta n\sqrt{2mR_{-1}(G)}.$$

Corollary 3.3. *Let G be a graph of order $n \geq 2$ and size m, without isolated vertices. Then we have*

$$E(G) \leq n\sqrt{mR_{-1}(G)}.$$

Proof. In [3] it was proven that $RE(G) \geq 2$. Considering this with inequality (3.10) we obtain the required result. □

Corollary 3.4. *Let G be a graph of order $n \geq 2$ and size m, without isolated vertices. Then we have*

$$E(G) \leq n\sqrt{\frac{M_2(G)}{m}}, \tag{3.13}$$

where $M_2(G) = \sum_{i\sim j} d_i d_j$ is the second Zagreb index [16].

Proof. In [3] it was also proven that

$$RE(G) \geq 2R_{-1}(G).$$

From the above and inequality (3.10) we obtain

$$E(G) \leq n\sqrt{\frac{m}{R_{-1}(G)}}. \tag{3.14}$$

On the other hand, by the inequality between arithmetic and harmonic means (see, e.g., [23]), we have that

$$M_2(G)R_{-1}(G) \geq m^2.$$

Combining the above and inequality (3.14) we arrive at (3.13). □

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