

A Note on Randić Energy¹

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Abstract

The Randić energy of a graph is the sum of the absolute values of its Randić eigenvalues. In this note, new bounds on the Randić energy of a graph are established.

1 Introduction

All graphs considered here are simple, undirected and finite. Let G be a graph with vertex set $\mathcal{V}(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $\mathcal{E}(G)$. Its *order* is $|\mathcal{V}(G)|$, denoted by n , and its *size* is $|\mathcal{E}(G)|$, denoted by m . For $i = 1, 2, \dots, n$, let d_i be the degree of the vertex $v_i \in \mathcal{V}(G)$.

Randić [15] invented a molecular structure descriptor which is defined as

$$R = R(G) = \sum_{v_i v_j \in \mathcal{E}(G)} \frac{1}{\sqrt{d_i d_j}}$$

where the summation is over all (unordered) edges $v_i v_j$ of the underlying (molecular) graph G . Nowadays, R is referred to as the Randić index. It has been found countless chemical applications and became a popular topic of research in mathematics and mathematical chemistry, for more details see [10, 13, 14, 20, 21].

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Gutman et al. [8] pointed out that the Randić-index-concept is purposeful to associate the graph G a symmetric square matrix of order n , named Randić matrix $\mathcal{R}(G)$, whose (i, j) -entry is defined as

$$r_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}} & \text{if } v_i v_j \in \mathcal{E}(G); \\ 0 & \text{otherwise} \end{cases} .$$

Let $A(G)$ and $D(G)$ be the adjacency matrix and the diagonal matrix of vertex degrees of G , respectively. Clearly, $\mathcal{R}(G) = D(G)^{-1/2} A(G) D(G)^{-1/2}$. Hence $rank(A(G)) = rank(\mathcal{R}(G))$. As usual, we shall index the eigenvalues of $A(G)$ and $\mathcal{R}(G)$ (or the eigenvalues and the Randić eigenvalues of G , respectively) in non-increasing order and denote them as $\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$ and $\rho_1(G) \geq \rho_2(G) \geq \dots \geq \rho_n(G)$, respectively. When only one graph G is under consideration, we sometimes use A , D , \mathcal{R} , λ_i and ρ_i instead of $A(G)$, $D(G)$ and $\mathcal{R}(G)$, $\lambda_i(G)$ and $\rho_i(G)$ for $i = 1, 2, \dots, n$, respectively.

The (ordinary) energy $E(G)$ of a graph G is defined as the sum of the absolute values of its eigenvalues:

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

Details and more information on graph energy can be found in the reviews [9, 11, 12] and the recent papers [16, 19].

The concept of the Randić energy of a graph G , denoted by $RE(G)$, was introduced in [2] as:

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

and was conceived in full analogy with the ordinary graph energy, Eq. (1). Some basic properties of the Randić energy were determined in the papers [1-3, 5, 7, 8, 18], including upper and lower bounds. In particular, the authors [8] conjectured that the connected graphs of order n with maximal Randić energy is a tree. And explored the structure of the maximum-RE trees.

Remark 1. Recall that the normalized Laplacian matrix of G is $\mathcal{L}(G) = I_n - \mathcal{R}(G)$ [4] and its normalized Laplacian energy is $E_{\mathcal{L}}(G) = \sum_{i=1}^n |\mu_i - 1|$ [3], where $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$ are the eigenvalues of $\mathcal{L}(G)$. Then $\rho_i = 1 - \mu_{n-i+1}$ for $i = 1, 2, \dots, n$ and $E_{\mathcal{L}}(G) = RE(G)$ [8]. Therefore, results obtained for μ_i ($i = 1, 2, \dots, n$) and $E_{\mathcal{L}}(G)$ can be immediately re-stated for ρ_i ($i = 1, 2, \dots, n$) and $RE(G)$, respectively.

In this note, some further properties on $RE(G)$ are established, mainly upper and lower bounds on $RE(G)$.

2 Main result

Recall that the general Randić index R_{-1} of a connected graph G is

$$R_{-1} = R_{-1}(G) = \sum_{v_i v_j \in \mathcal{E}(G)} \frac{1}{d_i d_j},$$

where the summation is over all (unordered) edges $v_i v_j$ in G [3]. Some basic properties of the general Randić index were determined in the paper [3], including upper and lower bounds.

In this section, further properties on $RE(G)$ are explored, mainly upper and lower bounds. We begin with the following well-known facts on the Randić eigenvalues of G .

Fact 2 ([4, 17]). Let G be a connected graph of order n with Randić eigenvalues $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$. Then

(i) $\rho_1 = 1, \sum_{i=1}^n \rho_i = 0, \sum_{i=1}^n \rho_i^2 = 2R_{-1}$ and $\sum_{i < j} \rho_i \rho_j = -R_{-1}$.

(ii) When $G \cong K_n$, then $\rho_1 = 1$ and $\rho_2 = \dots = \rho_n = \frac{-1}{n-1}$.

(iii) When $G \neq K_n$, then $\rho_2 \geq 0$. Moreover, the equality holds if and only if G is a complete multipartite graph.

(iv) When G is bipartite, then $\rho_i = -\rho_{n-i+1}$ for $i = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor$.

Proposition 3 ([8]). Let G be a connected graph of order n . Then $RE(G) \geq 2$. Moreover, the equality holds if and only if G is a complete multipartite graph.

Proof. From Fact 2(i), we have $RE(G) \geq 2\rho_1 = 2$. The equality holds if and only if $\rho_2 \leq 0$. That is G is complete multipartite graph from Fact 2(ii) and (iii). ■

In [3], bounds on $E_{\mathcal{L}}(G)$ in terms of R_{-1} were established. Those can be re-stated for $RE(G)$ as follows.

Lemma 4 ([3]). Let G be a graph of order n with no isolated vertices. Then

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

We now give another bounds on $RE(G)$ in terms of R_{-1} as follows.

Theorem 5. *Let G be a connected graph of order n with Randić eigenvalues $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$. Then*

$$\sqrt{2R_{-1} - 1 + 2|1 - R_{-1}|} + 1 \leq RE(G) \leq \sqrt{(n-1)(2R_{-1} - 1)} + 1. \quad (3)$$

Moreover, the lower bound is attained if and only if G is a complete multipartite graph; and the upper bound is attained if and only if $|\rho_2| = \dots = |\rho_n|$.

Proof. Form Fact 2(i), we have $\sum_{2 \leq i < j} \rho_i \rho_j = 1 - R_{-1}$ and $\rho_n < 0$ for the connected graph G . Note that $\sum_{2 \leq i < j} |\rho_i| |\rho_j| \geq |\sum_{2 \leq i < j} \rho_i \rho_j| = |1 - R_{-1}|$. The equality holds if and only if $\rho_i \leq 0$ for $i = 2, \dots, n$ since $\rho_n < 0$. That is G is a complete multipartite graph from Fact 2(ii) and (iii). Note that

$$\begin{aligned} RE^2 &= \left(\sum_{i=1}^n |\rho_i| \right)^2 = \sum_{i=1}^n |\rho_i|^2 + \sum_{i \neq j} |\rho_i| |\rho_j| \\ &= \sum_{i=1}^n |\rho_i|^2 + 2 \sum_{i=2}^n |\rho_i| + \sum_{2 \leq i \neq j} |\rho_i| |\rho_j| \\ &\geq 2R_{-1} + 2(RE - 1) + 2|1 - R_{-1}|. \end{aligned}$$

That is $(RE - 1)^2 \geq 2R_{-1} - 1 + 2|1 - R_{-1}|$ with equality if and only if G is a complete multipartite graph. This implies that $RE(G) \geq \sqrt{2R_{-1} - 1 + 2|1 - R_{-1}|} + 1$ with equality if and only if G is a complete multipartite graph.

Moreover, note that

$$\begin{aligned} 4nR_{-1} - 2RE^2 &= \sum_{i=1}^n \sum_{j=1}^n (|\rho_i| - |\rho_j|)^2 \\ &= 2 \sum_{i=2}^n (|\rho_1| - |\rho_i|)^2 + \sum_{i=2}^n \sum_{j=2}^n (|\rho_i| - |\rho_j|)^2 \\ &= 2(n + 2R_{-1} - 2RE) + \sum_{i=2}^n \sum_{j=2}^n (|\rho_i| - |\rho_j|)^2 \\ &\geq 2(n + 2R_{-1} - 2RE). \end{aligned}$$

That is $(RE - 1)^2 \leq (n-1)(2R_{-1} - 1)$ with equality if and only if $\sum_{i=2}^n \sum_{j=2}^n (|\rho_i| - |\rho_j|)^2 = 0$. This implies that $RE(G) \leq \sqrt{(n-1)(2R_{-1} - 1)} + 1$ with equality if and only if $|\rho_2| = \dots = |\rho_n|$. This completes the proof. ■

Remark 6. The lower bound in (3) is an improvement of Proposition 3 since

$$\begin{cases} \sqrt{2R_{-1} - 1 + 2|1 - R_{-1}|} + 1 = 2 & \text{if } R_{-1} \leq 1; \\ \sqrt{2R_{-1} - 1 + 2|1 - R_{-1}|} + 1 > 2 & \text{if } R_{-1} > 1 . \end{cases}$$

And the upper bound in (3) is also an improvement of that in (2) since

$$\sqrt{(n-1)(2R_{-1}-1)} + 1 \leq \sqrt{2nR_{-1}} .$$

But the lower bounds (2) and (3) are incomparable since

$$\begin{cases} 2R_{-1} \leq \sqrt{2R_{-1} - 1 + 2|1 - R_{-1}|} + 1 = 2 & \text{if } R_{-1} \leq 1; \\ 2R_{-1} > \sqrt{2R_{-1} - 1 + 2|1 - R_{-1}|} + 1 > 2 & \text{if } R_{-1} > 1 . \end{cases}$$

Remark 7. It should be pointed out that when $G = K_n$, then $|\rho_2| = \dots = |\rho_n| = \frac{1}{n-1}$ from Fact 2(ii). Hence the upper bound in (3) is attained for K_n . However, the problem of determining all connected graphs for which the upper bound in (3) is attained appears to be somewhat more difficult.

To deduce more bounds on RE , the following lemma is needed.

Lemma 8 ([6]). *Let $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and let $A(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n x_i$, $A(\mathbf{y}) = \frac{1}{n} \sum_{i=1}^n y_i$. If $\phi \leq x_i \leq \Phi$ and $\gamma \leq y_i \leq \Gamma$, then*

$$\left| \frac{1}{n} \sum_{i=1}^n x_i y_i - \frac{1}{n^2} \sum_{i=1}^n x_i \sum_{i=1}^n y_i \right| \leq \sqrt{(\Phi - A(\mathbf{x}))(A(\mathbf{x}) - \phi)(\Gamma - A(\mathbf{y}))(A(\mathbf{y}) - \gamma)} .$$

Now we turn to new bounds on $RE(G)$.

Theorem 9. *Let G be a connected graph of order n with Randić eigenvalues $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$. Then*

$$RE \geq \frac{2R_{-1} + (n-1)\alpha\beta - 1}{\alpha + \beta} + 1, \tag{4}$$

where $\alpha = \min_{1 \leq i \leq n} \{|\rho_i|\}$ and $\beta = \max\{\rho_2, |\rho_n|\}$.

Proof. Note that

$$RE^2 = \left(1 + \sum_{i=2}^n |\rho_i| \right)^2 = 1 + \sum_{i=2}^n |\rho_i|^2 + \sum_{2 \leq i \neq j} |\rho_i||\rho_j| + 2 \sum_{i=2}^n |\rho_i| .$$

That is

$$RE^2 - 2RE + 2 = 2R_{-1} + \sum_{2 \leq i \neq j} |\rho_i||\rho_j|, \text{ as } \sum_{i=1}^n |\rho_i|^2 = 2R_{-1} . \tag{5}$$

Let $P = \sum_{2 \leq i \neq j}^n |\rho_i| |\rho_j|$, $x_i = |\rho_i|$ and $y_i = RE - 1 - |\rho_i|$ for $i = 2, \dots, n$. Then $P = \sum_{i=2}^n x_i y_i$.

Recall that $\alpha = \min_{1 \leq i \leq n} \{|\rho_i|\}$ and $\beta = \max\{\rho_2, |\rho_n|\}$. Then $\alpha \leq x_i \leq \beta$ and $RE - 1 - \beta \leq y_i \leq RE - 1 - \alpha$. Also $A(x) = \frac{RE-1}{n-1}$ and $A(y) = \frac{(n-2)(RE-1)}{n-1}$. Hence by Lemma 8, we have

$$\left| \frac{P}{n-1} - \frac{(n-2)(RE-1)^2}{(n-1)^2} \right| \leq \sqrt{\left(\beta - \frac{RE-1}{n-1}\right)^2 \left(\frac{RE-1}{n-1} - \alpha\right)^2}.$$

It follows that

$$P \geq (RE - 1)^2 + (n - 1)\alpha\beta - (\alpha + \beta)(RE - 1).$$

This together with (5) imply that

$$RE^2 - 2RE + 2 = 2R_{-1} + P \geq 2R_{-1} + (RE - 1)^2 + (n - 1)\alpha\beta - (\alpha + \beta)(RE - 1).$$

It follows that

$$RE \geq \frac{2R_{-1} + (n - 1)\alpha\beta - 1}{\alpha + \beta} + 1.$$

This completes the proof. ■

Note that the right-hand side of (4) is a non-decreasing function on $\alpha \geq 0$. Then we have

Corollary 10. *Let G be a connected graph of order n with Randić eigenvalues $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$. Then*

$$RE \geq \frac{2R_{-1} - 1}{\beta} + 1, \tag{6}$$

where $\beta = \max\{\rho_2, |\rho_n|\}$.

Remark 11. The equalities of (4) and (6) are attained for $G \cong K_n$ and G is complete bipartite graph, respectively. Moreover, note that the right-hand sides of (4) and (6) are non-decreasing functions on R_{-1} , respectively. Hence lower bounds on R_{-1} in [3] can be used to deduce more bounds on RE .

Recall that $rank(A) = rank(R)$ for any graph G . And note that 0 is a Randić eigenvalue of G when $rank(R) < n$. Then we have the following general result.

Theorem 12. *Let G be a connected graph of order n with Randić eigenvalues $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$. If $rank(A) = r$, then*

$$RE \geq \frac{2R_{-1} + (r - 1)\alpha^*\beta - 1}{\alpha^* + \beta} + 1, \tag{7}$$

where $\alpha^* = \min\{|\rho_i| \mid \rho_i \neq 0, i = 1, 2, \dots, n\}$ and $\beta = \max\{\rho_2, |\rho_n|\}$.

Proof. Note that there are r non-zero Randić eigenvalues in G since $\text{rank}(A) = r$. Let $\rho_1^* \geq \rho_2^* \geq \dots \geq \rho_r^*$ be r non-zero Randić eigenvalues of G . Clearly, $\rho_1^* = 1$. Hence

$$\begin{aligned} RE^2 &= \left(1 + \sum_{i=2}^r |\rho_i^*|\right)^2 = 1 + \sum_{i=2}^r |\rho_i^*|^2 + \sum_{2 \leq i \neq j}^r |\rho_i^*||\rho_j^*| + 2 \sum_{i=2}^r |\rho_i^*| \\ &= 2R_{-1} + 2RE - 2 + \sum_{2 \leq i \neq j}^r |\rho_i^*||\rho_j^*|. \end{aligned}$$

Then similar argument as the proof of Theorem 9 leads to $RE \geq \frac{2R_{-1} + (r-1)\alpha^*\beta - 1}{\alpha^* + \beta} + 1$. This completes the proof. ■

In particular, if G is bipartite, then we have the following.

Theorem 13. *Let G be a connected bipartite graph of order n with Randić eigenvalues $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$. If G is not a complete bipartite graph, then*

$$RE \geq 2 \left(\frac{R_{-1} + (\lfloor \frac{n}{2} \rfloor - 1) \alpha \rho_2 - 1}{\alpha + \rho_2} + 1 \right), \tag{8}$$

where $\alpha = \min_{2 \leq i \leq \lfloor \frac{n}{2} \rfloor} \{|\rho_i|\}$.

Proof. Note that G is a bipartite graph. Then from Fact 2(iv), we have $\rho_i = -\rho_{n+1-i}$ and $\rho_i \geq 0$ for $i = 1, \dots, \lfloor \frac{n}{2} \rfloor$. In particular, $\rho_1 = -\rho_n = 1$. Therefore,

$$RE^2 = \left(2 + 2 \sum_{i=2}^{\lfloor \frac{n}{2} \rfloor} \rho_i\right)^2 = 4 + 4 \sum_{i=2}^{\lfloor \frac{n}{2} \rfloor} \rho_i^2 + 4 \sum_{2 \leq i \neq j}^{\lfloor \frac{n}{2} \rfloor} \rho_i \rho_j + 8 \sum_{i=2}^{\lfloor \frac{n}{2} \rfloor} \rho_i.$$

That is

$$(RE - 2)^2 = 4R_{-1} - 4 + 4 \sum_{2 \leq i \neq j}^{\lfloor \frac{n}{2} \rfloor} \rho_i \rho_j. \tag{9}$$

Let $P = \sum_{2 \leq i \neq j}^{\lfloor \frac{n}{2} \rfloor} \rho_i \rho_j$. Note that $\sum_{i=2}^{\lfloor \frac{n}{2} \rfloor} \rho_i = \frac{RE}{2} - 1$, $\alpha \leq \rho_i \leq \rho_2$ for $i = 2, \dots, \lfloor \frac{n}{2} \rfloor$ and $\rho_2 > 0$ since G is not a complete bipartite graph. Then similar argument as the proof of Theorem 9 leads to

$$P \geq \left(\frac{RE}{2} - 1\right)^2 + \left(\lfloor \frac{n}{2} \rfloor - 1\right) \alpha \rho_2 - (\alpha + \rho_2) \left(\frac{RE}{2} - 1\right).$$

This together with (9) imply that

$$RE \geq 2 \left(\frac{R_{-1} + (\lfloor \frac{n}{2} \rfloor - 1) \alpha \rho_2 - 1}{\alpha + \rho_2} + 1 \right),$$

which completes the proof. ■

Note that the right-hand side of (8) is also a non-decreasing function on $\alpha \geq 0$. Then we have

Corollary 14. *Let G be a connected bipartite graph of order n with Randić eigenvalues $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$. If G is not a complete bipartite graph, then*

$$RE \geq 2 \left(\frac{R_{-1} - 1}{\rho_2} + 1 \right).$$

Note that for a bipartite graph G , if $\text{rank}(A) = r$, then r is even. Similarly, we have the following general result for bipartite graphs.

Theorem 15. *Let G be a connected bipartite graph of order n with Randić eigenvalues $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$. If $\text{rank}(A) = r$ and G is not a complete bipartite graph, then*

$$RE \geq 2 \left(\frac{R_{-1} + \left(\frac{r}{2} - 1\right) \alpha^* \rho_2 - 1}{\alpha^* + \rho_2} + 1 \right),$$

where $\alpha^* = \min \{ |\rho_i| \mid \rho_i \neq 0, i = 1, 2, \dots, n \}$.

Proof. Note that G is a bipartite graph with $\text{rank}(A) = r$. Then there are r non-zero Randić eigenvalues in G . Let $\rho_1^* \geq \rho_2^* \geq \dots \geq \rho_r^*$ be r non-zero Randić eigenvalues of G . Clearly, $\rho_i^* = -\rho_{r-i+1}^*$ for $i = 1, 2, \dots, \frac{r}{2}$. Hence

$$\begin{aligned} RE^2 &= \left(2 + 2 \sum_{i=2}^{\frac{r}{2}} \rho_i^* \right)^2 = 4 + 4 \sum_{i=2}^{\frac{r}{2}} (\rho_i^*)^2 + 4 \sum_{2 \leq i \neq j}^{\frac{r}{2}} \rho_i^* \rho_j^* + 8 \sum_{i=2}^{\frac{r}{2}} \rho_i^* \\ &= 4R_{-1} + 4(RE - 2) + 4 \sum_{2 \leq i \neq j}^{\frac{r}{2}} \rho_i^* \rho_j^*. \end{aligned}$$

Then similar argument as the proof of Theorem 13 leads to

$$RE \geq 2 \left(\frac{R_{-1} + \left(\frac{r}{2} - 1\right) \alpha^* \rho_2 - 1}{\alpha^* + \rho_2} + 1 \right).$$

This completes the proof. ■

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