A Note on Randić Energy

Jianxi Li\textsuperscript{a}, Ji–Ming Guo\textsuperscript{b}, Wai Chee Shiu\textsuperscript{c}

\textsuperscript{a} School of Mathematics and Statistics, Minnan Normal University, Zhangzhou, Fujian, P. R. China
\textsuperscript{b} Department of Mathematics, East China University of Science and Technology, Shanghai, P. R. China
\textsuperscript{c} Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong, P. R. China

(Received August 27, 2014)

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 $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. Its order is $|V(G)|$, denoted by $n$, and its size is $|E(G)|$, denoted by $m$. For $i = 1, 2, \ldots, n$, let $d_i$ be the degree of the vertex $v_i \in V(G)$.

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

$$R = R(G) = \sum_{v_iv_j \in E(G)} \frac{1}{\sqrt{d_id_j}}$$

where the summation is over all (unordered) edges $v_iv_j$ 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].

\textsuperscript{1}The first author is supported by NSF of China (Nos. 11101358, 61379021, 11471077) and China Postdoctoral Science Foundation (No. 2014M551831) and NSF of Fujian (No. 2014J01020), the second author is supported by NSF of China (No. 11371372), the third author is supported by General Research Fund of Hong Kong and Faculty Research Grant of Hong Kong Baptist University. E-mail addresses: ptjxli@hotmail.com(J. Li), jimingguo@hotmail.com(J.-M. Guo), weshiu@hkbu.edu.hk(W.C. Shiu).
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 $\text{rank}(A(G)) = \text{rank}(\mathcal{R}(G))$. 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 $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ and $\rho_1(G) \geq \rho_2(G) \geq \cdots \geq \rho_n(G)$, respectively. When only one graph $G$ is under consideration, we sometimes use $A$, $D$, $\mathcal{R}$, $\lambda_i$ and $\rho_i$ instead of $A(G)$, $D(G)$ and $\mathcal{R}(G)$, $\lambda_i(G)$ and $\rho_i(G)$ for $i = 1, 2, \ldots, n$, respectively.

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

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|.$$  \hfill (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 $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ are the eigenvalues of $\mathcal{L}(G)$. Then $\rho_i = 1 - \mu_{n-i+1}$ for $i = 1, 2, \ldots, n$ and $E_{\mathcal{L}}(G) = RE(G)$ [8]. Therefore, results obtained for $\mu_i$ ($i = 1, 2, \ldots, n$) and $E_{\mathcal{L}}(G)$ can be immediately re-stated for $\rho_i$ ($i = 1, 2, \ldots, n$) 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

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

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 $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. Then

1. $\rho_1 = 1$, $\sum_{i=1}^{n} \rho_i = 0$, $\sum_{i=1}^{n} \rho_i^2 = 2R_{-1}$ and $\sum_{i<j} \rho_i \rho_j = -R_{-1}$ .
2. When $G \cong K_n$, then $\rho_1 = 1$ and $\rho_2 = \cdots = \rho_n = \frac{-1}{n-1}$ .
3. When $G \neq K_n$, then $\rho_2 \geq 0$. Moreover, the equality holds if and only if $G$ is a complete multipartite graph.
4. When $G$ is bipartite, then $\rho_i = -\rho_{n-i+1}$ for $i = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$ .

**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.** Form 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 form Fact 2(ii) and (iii). \hfill \blacksquare

In [3], bounds on $E_L(G)$ 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 $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. 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 $|\rho_2| = \cdots = |\rho_n|$. 

**Proof.** Form Fact 2(i), we have

$$\sum_{2 \leq i < j} \rho_i \rho_j = 1 - R_{-1} \quad \text{and} \quad \rho_n < 0 \quad \text{for the connected graph } G.$$ 

Note that

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

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

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

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

$$4nR_{-1} - 2RE^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} (|\rho_i| - |\rho_j|)^2$$

$$= 2 \sum_{i=2}^{n} (|\rho_i| - |\rho_1|)^2 + \sum_{i=2}^{n} \sum_{j=2}^{n} (|\rho_i| - |\rho_j|)^2$$

$$= 2(n + 2R_{-1} - 2RE) + \sum_{i=2}^{n} \sum_{j=2}^{n} (|\rho_i| - |\rho_j|)^2$$

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

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 $|\rho_2| = \cdots = |\rho_n|$. This completes the proof. \hfill \blacksquare
Remark 6. The lower bound in (3) is an improvement of Proposition 3 since
\[
\begin{align*}
\sqrt{2R - 1} - 1 + 2|1 - R| + 1 & = 2 \quad \text{if } R \leq 1; \\
\sqrt{2R - 1} - 1 + 2|1 - R| + 1 & > 2 \quad \text{if } R > 1.
\end{align*}
\]
And the upper bound in (3) is also an improvement of that in (2) since
\[
\sqrt{(n - 1)(2R - 1)} + 1 \leq \sqrt{2nR - 1}.
\]
But the lower bounds (2) and (3) are incomparable since
\[
\begin{align*}
2R - 1 & \leq \sqrt{2R - 1} - 1 + 2|1 - R| + 1 = 2 \quad \text{if } R \leq 1; \\
2R - 1 & > \sqrt{2R - 1} - 1 + 2|1 - R| + 1 > 2 \quad \text{if } R > 1.
\end{align*}
\]
Remark 7. It should be pointed out that when \( G = K_n \), then \(|\rho_2| = \cdots = |\rho_n| = \frac{1}{n-1} \) 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 \( x, y \in \mathbb{R}^n \) and let \( A(x) = \frac{1}{n} \sum_{i=1}^{n} x_i, A(y) = \frac{1}{n} \sum_{i=1}^{n} y_i \). If \( \phi \leq x_i \leq \Phi \) and \( \gamma \leq y_i \leq \Gamma \), then
\[
\left| \frac{1}{n} \sum_{i=1}^{n} x_i y_i - \frac{1}{n^2} \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i \right| \leq \sqrt{(\Phi - A(x))(A(x) - \phi)(\Gamma - A(y))(A(y) - \gamma)}.
\]

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

Theorem 9. Let \( G \) be a connected graph of order \( n \) with Randić eigenvalues \( \rho_1 \geq \rho_2 \geq \cdots \geq \rho_n \). Then
\[
RE \geq \frac{2R - 1 + (n - 1)\alpha\beta - 1}{\alpha + \beta} + 1,
\]
where \( \alpha = \min_{1 \leq i \leq n} \{|\rho_i|\} \) and \( \beta = \max\{\rho_2, |\rho_n|\} \).

Proof. Note that
\[
RE^2 = \left(1 + \sum_{i=2}^{n} |\rho_i|\right)^2 = 1 + \sum_{i=2}^{n} |\rho_i|^2 + \sum_{2 \leq i \neq j}^{n} |\rho_i||\rho_j| + 2 \sum_{i=2}^{n} |\rho_i|.
\]
That is
\[
RE^2 - 2RE + 2 = 2R - 1 + \sum_{2 \leq i \neq j}^{n} |\rho_i||\rho_j|, \quad \text{as } \sum_{i=1}^{n} |\rho_i|^2 = 2R - 1.
\]
Let $P = \sum_{2 \leq i \neq j} |\rho_i| |\rho_j|$, $x_i = |\rho_i|$ and $y_i = RE - 1 - |\rho_i|$ for $i = 2, \ldots, n$. 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

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

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 $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. Then

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

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

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

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

where $\alpha^* = \min \{|\rho_i| \mid \rho_i \neq 0, i = 1, 2, \ldots, n\}$ 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 \( \rho_1^* \geq \rho_2^* \geq \cdots \geq \rho_r^* \) be \( r \) non-zero Randić eigenvalues of \( G \). Clearly, \( \rho_1^* = 1 \). Hence
\[
RE^2 = \left( 1 + \sum_{i=2}^{r} |\rho_i^*|^2 \right) = 1 + \sum_{i=2}^{r} |\rho_i^*|^2 + \sum_{2 \leq i \neq j}^{r} |\rho_i^*| |\rho_j^*| + 2 \sum_{i=2}^{r} |\rho_i^*|.
\]
\[
= 2R_{-1} + 2RE - 2 + \sum_{2 \leq i \neq j}^{r} |\rho_i^*| |\rho_j^*|.
\]
Then similar argument as the proof of Theorem 9 leads to
\[
RE \geq 2 \left( \frac{R_{-1} + (\lfloor \frac{n}{2} \rfloor - 1) \alpha \rho_2 - 1}{\alpha + \rho_2} + 1 \right),
\]
where \( \alpha = \min_{2 \leq i \leq \lfloor \frac{n}{2} \rfloor} \{|\rho_i^*|\} \).

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 \( \rho_1 \geq \rho_2 \geq \cdots \geq \rho_n \). If \( G \) is not a complete bipartite graph, then
\[
RE \geq 2 \left( \frac{R_{-1} + (\lfloor \frac{n}{2} \rfloor - 1) \alpha \rho_2 - 1}{\alpha + \rho_2} + 1 \right),
\]
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 \( i = 1, \ldots, \lfloor \frac{n}{2} \rfloor \). In particular, \( \rho_1 = -\rho_n = 1 \). Therefore,
\[
RE^2 = \left( 2 + \sum_{i=2}^{\lfloor \frac{n}{2} \rfloor} \rho_i \right)^2 = 4 + 4 \sum_{i=2}^{\lfloor \frac{n}{2} \rfloor} \rho_i^2 + 4 \sum_{2 \leq i \neq j}^{\lfloor \frac{n}{2} \rfloor} \rho_i \rho_j + 8 \sum_{i=2}^{\lfloor \frac{n}{2} \rfloor} \rho_i.
\]
That is
\[
(RE - 2)^2 = 4R_{-1} - 4 + 4 \sum_{2 \leq i \neq j}^{\lfloor \frac{n}{2} \rfloor} \rho_i \rho_j.
\]

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 \( i = 2, \ldots, \lfloor \frac{n}{2} \rfloor \) 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 \( \rho_1 \geq \rho_2 \geq \cdots \geq \rho_n \). 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 \( \rho_1 \geq \rho_2 \geq \cdots \geq \rho_n \). 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 \( \alpha^* = \min \{ |\rho_i| \mid \rho_i \neq 0, i = 1, 2, \ldots, n \} \).

**Proof.** Note that \( G \) is a bipartite graph with \( \text{rank}(A) = r \). Then there are \( r \) non-zero Randić eigenvalues in \( G \). Let \( \rho^*_1 \geq \rho^*_2 \geq \cdots \geq \rho^*_r \) be \( r \) non-zero Randić eigenvalues of \( G \). Clearly, \( \rho_i^* = -\rho_{r-i+1}^* \) for \( i = 1, 2, \ldots, \frac{r}{2} \). Hence

\[
RE^2 = \left( 2 + 2 \sum_{i=2}^{\frac{r}{2}} \rho_i^* \right)^2 = 4 + 4 \sum_{i=2}^{\frac{r}{2}} (\rho_i^*)^2 + 4 \sum_{2 \leq i \neq j} \rho_i^* \rho_j^* + 8 \sum_{i=2}^{\frac{r}{2}} \rho_i^*
\]

\[
= 4R_{-1} + 4(RE - 2) + 4 \sum_{2 \leq i \neq j} \rho_i^* \rho_j^*.
\]

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.

**Acknowledgements:** The authors would like to thank the anonymous referees for their constructive corrections and valuable comments, which lead to an improvement of the original manuscript.
References


