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On Randić Energy of Graphs

Kinkar Ch. Das[a], Sezer Sorgun[a,b]

[a]*Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea*
e-mail: kinkardas2003@googlemail.com

[b]*Department of Mathematics, Nevsehir Haci Bektas Veli University, Nevsehir, Turkey*
e-mail: srgnrzs@gmail.com

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Abstract

Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The Randić matrix $R = (r_{ij})$ of a graph G whose vertex v_i has degree d_i is defined by $r_{ij} = 1/\sqrt{d_i d_j}$ if the vertices v_i and v_j are adjacent and $r_{ij} = 0$ otherwise. The Randić energy RE is the sum of absolute values of the eigenvalues of R. We provide lower and upper bounds for RE in terms of no. of vertices, maximum degree, minimum degree and the determinant of the adjacency matrix of graphs G.

1 Introduction

Throughout the paper we consider only simple graphs, herein called just graphs. Let $G = (V, E)$ be a graph on vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G)$. Also let d_i be the degree of vertex v_i for $i = 1, 2, \ldots, n$. The minimum vertex degree is denoted by $\delta = \delta(G)$ and the maximum by $\Delta = \Delta(G)$. Let N_i be the neighbor set of the vertex $v_i \in V(G)$. If the vertices v_i and v_j are adjacent, we denote that by $v_iv_j \in E(G)$. The adjacency matrix $A(G)$ of G is defined by its entries $a_{ij} = 1$ if $v_iv_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n$ denote the eigenvalues of $A(G)$. λ_1 is called the spectral radius of graph G. When more than one graph is under consideration, then we write $\lambda_i(G)$ instead of λ_i. Some well known results are the following:

$$\sum_{i=1}^{n} \lambda_i = 0 \tag{1}$$

$$\text{and} \qquad \prod_{i=1}^{n} \lambda_i = \det A. \tag{2}$$

The Randić matrix $R(G) = (r_{ij})_{n\times n}$ is defined as [1, 2, 9]

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

Denote the eigenvalues of the Randić matrix $R = R(G)$ by $\rho_1,\, \rho_2, \ldots,\, \rho_n$ and label them in non-increasing order. The multi set $Sp_R = Sp_R(G) = \{\rho_1,\, \rho_2, \ldots,\, \rho_n\}$ will be called the R-spectrum of the graph G.

The (ordinary) energy of a graph G is [10]

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

For recent papers on lower and upper bounds on $E(G)$, see [4, 5, 8].

The Randić energy [1, 2, 9] of G is defined as

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

For several lower and upper bounds on Randić energy, see [1, 2, 9].

Let $p \geq 0$. The tree Su_p of order $n = 2p+1$, containing p pendent vertices, each attached to a vertex of degree 2, and a vertex of degree p, will be called the p-sun (see Fig. 2 in [9]). Let $p,\, q \geq 0$. The tree $DSu_{p,\,q}$ of order $n = 2(p+q+1)$, obtained from a p-sun and a q-sun, by connecting their central vertices, will be called a $(p,\, q)$-double sun (see Fig. 2 in [9]). Recently, Gutman et al. [9] gave the following conjecture on Randić energy:

Conjecture 1. [9] Let T be a tree of order n. If n is odd, then the maximum $RE(T)$ is achieved for T being the $\left(\frac{n-1}{2}\right)$-sun. If n is even, then the maximum $RE(T)$ is achieved for T being the $\left(\lceil\frac{n-2}{4}\rceil, \lfloor\frac{n-2}{4}\rfloor\right)$-double sun.

The paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we obtain some upper bounds on $RE(G)$ of graph G. In Section 4, we present some lower bounds on $RE(G)$ of graph G.

2 Preliminaries

In this section, we shall list some previously known results that will be needed in the next two sections.

Lemma 2.1. [13] *Let* $\mathbf{B}$ *be a* $p \times p$ *symmetric matrix and let* $\mathbf{B}_k$ *be its leading* $k \times k$ *submatrix. Then, for* $i = 1, 2, \ldots, k$,

$$\lambda_{p-i+1}(\mathbf{B}) \leq \lambda_{k-i+1}(\mathbf{B}_k) \leq \lambda_{k-i+1}(\mathbf{B}) \tag{3}$$

where $\lambda_i(\mathbf{B})$ *is the* i*-th greatest eigenvalue of* $\mathbf{B}$.

Lemma 2.2. [15] *Let* G *be a simple graph of order* n. *Then*

$$\lambda_1 \geq \sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2}\,.$$

Moreover, the above equality holds if and only if G *is a regular graph or* G *is a bipartite semiregular graph.*

Lemma 2.3. [11] *Let* G *be a graph of order* n. *Then*

$$\rho_1 = 1.$$

Lemma 2.4. [6] *Let* G *be a bipartite graph of order* n. *Then*

$$\rho_i = -\rho_{n-i+1}\,,\ i = 1,\, 2, \ldots,\, \left\lceil\frac{n}{2}\right\rceil.$$

Lemma 2.5. [12] *Let G be a connected r-regular graph of order n. Then*

$$\mu_i = r - \lambda_{n-i+1}\,, i = 1,\, 2, \ldots,\, n,$$

where λ_i and μ_i are the largest i-th eigenvalue of the adjacency and the Laplacian matrix of graph G, respectively.

Lemma 2.6. [9] *Let G be a graph of order n. Then*

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

3 Upper bounds on the Randić energy of graphs

In this section we give some upper bounds on the Randić energy of graph G in terms of n and δ. For this we need the following result.

Lemma 3.1. [3] *Let T be a tree of order n. Then*

$$\sum_{v_i v_j \in E(T)} \frac{1}{d_i d_j} \leq \frac{5n+8}{18}\,.$$

Now we give an upper bound on Randić energy of trees T in terms of n.

Theorem 3.2. *Let T be a tree of order n. Then*

$$RE(T) \leq 2\sqrt{\left\lfloor \frac{n}{2} \right\rfloor \cdot \frac{5n+8}{18}}\,.$$

Proof: We have

$$\sum_{i=1}^{n} \rho_i^2 = 2 \sum_{v_i v_j \in E(G)} \frac{1}{d_i d_j}\,.$$

By Lemma 2.4, from the above, we get

$$\sum_{i=1}^{\lfloor n/2 \rfloor} \rho_i^2 = \sum_{v_i v_j \in E(G)} \frac{1}{d_i d_j}\,.$$

By Lemma 3.1, we get

$$\sum_{i=1}^{\lfloor n/2 \rfloor} \rho_i^2 \leq \frac{5n+8}{18}\,. \tag{4}$$

Now,

$$\begin{aligned} RE(G) &= \sum_{i=1}^{n} |\rho_i| = 2\sum_{i=1}^{\lfloor n/2 \rfloor} |\rho_i| \quad \text{by Lemma 2.4} \\ &= 2\sqrt{\left\lfloor \frac{n}{2} \right\rfloor \sum_{i=1}^{\lfloor n/2 \rfloor} \rho_i^2} \quad \text{by Cauchy–Schwarz inequality} \\ &\leq 2\sqrt{\left\lfloor \frac{n}{2} \right\rfloor \cdot \frac{5n+8}{18}} \quad \text{by (4)}\,. \end{aligned}$$

□

Remark 3.3. *Our result in Theorem 3.2 is very close to the the Randić energy of* $\left(\frac{n-1}{2}\right)$*-sun and* $\left(\lceil \frac{n-2}{4} \rceil, \lfloor \frac{n-2}{4} \rfloor\right)$*-double sun. But still the Conjecture 1 is open.*

Now we present some well known results needed in the following theorem. The results can be found in [7]. A strongly regular graph with parameters (n, r, λ, μ), denoted $SRG(n, r, \lambda, \mu)$, is a r-regular graph on n vertices such that for every pair of adjacent vertices there are λ vertices adjacent to both, and for every pair of non-adjacent vertices there are μ vertices adjacent to both. We assume throughout that a strongly regular graph G is connected and that G is not a complete graph. Consequently, r is an eigenvalue of the adjacency matrix of G with multiplicity 1 and the remaining eigenvalues must satisfy the equation

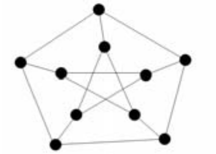
$$x^2 - (\lambda - \mu)x - (r - \mu) = 0.$$

Thus the eigenvalues of G are

$$r \quad \text{and} \quad x_1,\, x_2 = \frac{\lambda - \mu \pm \sqrt{(\lambda-\mu)^2 + 4(r-\mu)}}{2}\,. \tag{5}$$

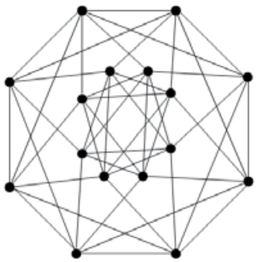
It is well known that the eigenvalues of G are

- r of multiplicity 1,
- $\dfrac{\lambda - \mu + \sqrt{(\lambda-\mu)^2 + 4(r-\mu)}}{2}$ of multiplicity $\dfrac{1}{2}\left[n - 1 - \dfrac{2r + (n-1)(\lambda-\mu)}{\sqrt{(\lambda-\mu)^2 + 4(r-\mu)}}\right]$,
- $\dfrac{\lambda - \mu - \sqrt{(\lambda-\mu)^2 + 4(r-\mu)}}{2}$ of multiplicity $\dfrac{1}{2}\left[n - 1 + \dfrac{2r + (n-1)(\lambda-\mu)}{\sqrt{(\lambda-\mu)^2 + 4(r-\mu)}}\right]$.



G_1

Fig. 1. Petersen Graph G_1.



G_2

Fig. 2. Graph G_2.

Two strongly regular graphs G_1 and G_2 have been shown in Fig. 1 and Fig. 2. Particularly, G_1 is well known Petersen graph.

Lemma 3.4. [14] *Let G be a connected d-regular graph on n vertices with three distinct Laplacian eigenvalues 0, r and s $(r \neq s)$. Then G is strongly regular graph with parameters $(n,\, d,\, rs/n + 2d - (r+s),\, rs/n)$.*

Now we are ready to give an upper bound on Randić energy $RE(G)$ of graphs G in terms of n and δ.

Theorem 3.5. *Let G be a connected graph of order n with minimum degree δ. Then*

$$RE(G) \leq 1 + \sqrt{\frac{(n-1)(n-\delta)}{\delta}} \tag{6}$$

with equality holding if and only if $G \cong K_n$ or $G \cong SRG\left(n,\, r,\, \frac{r(r-1)}{n-1},\, \frac{r(r-1)}{n-1}\right)$.

Proof: We have

$$\sum_{i=1}^{n} \rho_i^2 = 2 \sum_{v_iv_j \in E(G)} \frac{1}{d_i\, d_j} = \sum_{i=1}^{n} \frac{1}{d_i} \sum_{v_iv_j \in E(G)} \frac{1}{d_j}$$

$$\leq \sum_{i=1}^{n} \frac{1}{\delta} \sum_{v_iv_j \in E(G)} \frac{1}{d_j} \quad \text{as } d_i \geq \delta$$

$$= \frac{n}{\delta}\,. \tag{7}$$

Now,

$$RE(G) = \sum_{i=1}^{n} |\rho_i| = 1 + \sum_{i=2}^{n} |\rho_i| \quad \text{by Lemma 2.4}$$

$$\leq 1 + \sqrt{(n-1)\left(\sum_{i=1}^{n} \rho_i^2 - 1\right)} \quad \text{by Cauchy–Schwarz inequality} \tag{8}$$

$$\leq 1 + \sqrt{\frac{(n-1)(n-\delta)}{\delta}} \quad \text{by (7).}$$

The first part of the proof is done.

Now suppose that the equality holds in (6). Then all the above inequalities must be equalities. From the equality in (7), we get $d_1 = d_2 = \cdots = d_n = \delta$. Therefore G is isomorphic to an r-regular graph, (say).

From the equality in (8), we get $|\rho_2| = |\rho_3| = \cdots = |\rho_n|$. Moreover, we have

$$1 + (n-1)|\rho_2| = 1 + \sqrt{\frac{(n-1)(n-r)}{r}}\,,$$

that is,

$$|\rho_2| = \sqrt{\frac{n-r}{r(n-1)}}\,.$$

We consider two cases (i) $\rho_2 = \rho_n$, (ii) $\rho_2 = -\rho_n$.

Case (i) : $\rho_2 = \rho_n$. In this case $\rho_1 = 1$ and $\rho_i = -\frac{1}{n-1}$, $i = 2, 3, \ldots, n$ as $\sum_{i=1}^{n} \rho_i = 0$. Hence $G \cong K_n$.

Case (ii) : $\rho_2 = -\rho_n$. We have $\rho_2 > 0$. In this case the three distinct Randić eigenvalues of graph G are $(1, \rho_2, -\rho_2)$ with eigenvalue 1 of multiplicity 1. Since G is r-regular, we have $A(G) = r\,R(G)$. Therefore the three distinct adjacency eigenvalues of G are $(r,\, r\rho_2,\, -r\rho_2)$ with eigenvalue r of multiplicity 1. By Lemma 2.5, the three distinct Laplacian eigenvalues of graph G are $(0,\, r - r\rho_2,\, r + r\rho_2)$, that is,

$$\left(0,\, r - \sqrt{\frac{r(n-r)}{n-1}},\, r + \sqrt{\frac{r(n-r)}{n-1}}\right) \quad \text{as} \quad \rho_2 = \sqrt{\frac{n-r}{r(n-1)}}\,.$$

Moreover, G is connected. By Lemma 3.4, we get $G \cong SRG\left(n,\, r,\, \frac{r(r-1)}{n-1}\,,\, \frac{r(r-1)}{n-1}\right)$.

Conversely, let $G \cong K_n$. Then $S(G) = \left(1,\, -\frac{1}{n-1},\, -\frac{1}{n-1}, \ldots,\, -\frac{1}{n-1}\right)$. Hence $RE(G) = 2$.

Let G be isomorphic to strongly regular graph with parameters $\left(n,\, r,\, \frac{r(r-1)}{n-1}\,,\, \frac{r(r-1)}{n-1}\right)$. By (5), the distinct eigenvalues of the adjacency matrix are

$$r,\, \sqrt{\frac{r(n-r)}{n-1}}\,, -\sqrt{\frac{r(n-r)}{n-1}}\,,$$

that is, the distinct eigenvalues of the Randić matrix are

$$1,\, \sqrt{\frac{n-r}{(n-1)r}}\,, -\sqrt{\frac{n-r}{(n-1)r}}\,.$$

Hence

$$RE(G) = 1 + (n-1)\sqrt{\frac{n-r}{(n-1)r}} = 1 + \sqrt{\frac{(n-1)(n-r)}{r}}\,.$$

□

Remark 3.6. *Two strongly regular graphs G_1 and G_2 have been shown in Fig. 1 and Fig. 2. For G_1, we have $r = 3$, $n = 10$ and $\frac{r(r-1)}{n-1}$ is not an integer. Hence $G_1 \ncong SRG\left(n,\, r,\, \frac{r(r-1)}{n-1}\,,\, \frac{r(r-1)}{n-1}\right)$. For G_2, we have $n = 16$, $r = 6$ and $\frac{r(r-1)}{n-1} = 1$. Hence $G_2 \cong SRG\left(n,\, r,\, \frac{r(r-1)}{n-1}\,,\, \frac{r(r-1)}{n-1}\right)$.*

Remark 3.7. *Using Theorem 3.5, we obtain an upper bound on $RE(G) + RE(\overline{G})$ in terms of n, Δ and δ:*

$$\begin{aligned} RE(G) + RE(\overline{G}) &\le 2 + \sqrt{\frac{(n-1)(n-\delta)}{\delta}} + \sqrt{\frac{(n-1)(\Delta+1)}{n-\Delta-1}} \\ &= 2 + \sqrt{n-1}\left(\sqrt{\frac{n-\delta}{\delta}} + \sqrt{\frac{\Delta+1}{n-\Delta-1}}\right). \end{aligned}$$

4 Lower bounds on the Randić energy of graphs

Now we give a lower bound on Randić energy $RE(G)$ of graphs G in terms of n, Δ and the determinant of the adjacency matrix of graph G.

Theorem 4.1. *Let G be a connected graph of order n with maximum degree Δ and degree sequence $\pi(G) = (d_1, d_2, \ldots, d_n)$. Then*

$$RE(G) \geq 1 + \sqrt{\frac{n}{\Delta} - 1 + (n-1)(n-2)\left(\frac{|\det A|}{\prod_{i=1}^{n} d_i}\right)^{2/(n-1)}}\,, \tag{9}$$

where $\det A$ *is the determinant of the adjacency matrix of graph G. Moreover, the equality holds in* (9) *if and only if $G \cong K_n$ or $G \cong SRG\left(n,\, r,\, \frac{r(r-1)}{n-1},\, \frac{r(r-1)}{n-1}\right)$.*

Proof: Similarly as in Theorem 3.5, we get

$$\begin{aligned} \sum_{i=1}^{n} \rho_i^2 &= 2 \sum_{v_i v_j \in E(G)} \frac{1}{d_i\, d_j} \geq \sum_{i=1}^{n} \frac{1}{\Delta} \sum_{v_i v_j \in E(G)} \frac{1}{d_j} \quad \text{as } d_i \geq \delta \\ &= \frac{n}{\Delta}\,. \end{aligned} \tag{10}$$

By Arithmetic-Geometric mean inequality, we have

$$\begin{aligned} 2 \sum_{2 \leq i < j \leq n} |\rho_i||\rho_j| &\geq (n-1)(n-2)\left(\prod_{1=2}^{n} |\rho_i|\right)^{2/(n-1)} \\ &= (n-1)(n-2)\,(|\det\, R|)^{2/(n-1)} \\ &= (n-1)(n-2)\left(\frac{|\det\, A|}{\prod_{i=1}^{n} d_i}\right)^{2/(n-1)} \quad \text{by Lemma 2.6}\,. \end{aligned}$$

Using the above two results, we get

$$\left(\sum_{i=2}^{n} |\rho_i|\right)^2 = \sum_{i=2}^{n} \rho_i^2 + 2 \sum_{2 \leq i < j \leq n} |\rho_i||\rho_j|,$$

that is,

$$\sum_{i=2}^{n} |\rho_i| \geq \sqrt{\frac{n}{\Delta} - 1 + (n-1)(n-2) \left(\frac{|\det A|}{\prod_{i=1}^{n} d_i} \right)^{2/(n-1)}} \,.$$

Using the above result, we get

$$RE(G) = \sum_{i=1}^{n} |\rho_i| \geq 1 + \sqrt{\frac{n}{\Delta} - 1 + (n-1)(n-2) \left(\frac{|\det A|}{\prod_{i=1}^{n} d_i} \right)^{2/(n-1)}} \,.$$

The first part of the proof is done.

Now suppose that the equality holds in (9). Then all the above inequalities must be equalities. Then we must have $d_1 = d_2 = \cdots = d_n = \delta$ and $|\rho_2| = |\rho_3| = \cdots = |\rho_n|$. Similarly as in Theorem 3.5, one can see easily that $G \cong K_n$ or $G \cong SRG\left(n,\, r,\, \frac{r(r-1)}{n-1}\,,\, \frac{r(r-1)}{n-1}\right)$.

Conversely, let $G \cong K_n$. Then $S(G) = \left(1,\, -\frac{1}{n-1},\, -\frac{1}{n-1}, \ldots,\, -\frac{1}{n-1}\right)^T$. Hence $RE(G) = 2$.

Let G be isomorphic to strongly regular graph with parameters $\left(n,\, r,\, \frac{r(r-1)}{n-1}\,,\, \frac{r(r-1)}{n-1}\right)$. By (5), the distinct eigenvalues of the adjacency matrix are

$$r,\, \sqrt{\frac{r(n-r)}{n-1}}\,, -\sqrt{\frac{r(n-r)}{n-1}}\,.$$

Using some results before Lemma 3.4, we have

$$|\det A| = r \left(\frac{r(n-r)}{n-1} \right)^{\frac{n-1}{2}} \,.$$

Now,

$$1 + \sqrt{\frac{n}{\Delta} - 1 + (n-1)(n-2) \left(\frac{|\det A|}{\prod_{i=1}^{n} d_i} \right)^{2/(n-1)}} = 1 + \sqrt{\frac{(n-1)(n-r)}{r}} = RE(G)$$

as $d_i = r$, $i = 1, 2, \ldots, n$. □

Now we give another lower bound on Randić energy $RE(G)$ of graphs G in terms of n, the degree sequence, and the determinant of the adjacency matrix of graph G.

Theorem 4.2. *Let G be a connected graph of order n with degree sequence $\pi(G) = (d_1, d_2, \ldots, d_n)$. Then*

$$RE(G) \geq 1 + (n-1) \left(\frac{|\det A|}{\prod_{i=1}^{n} d_i} \right)^{1/(n-1)}, \tag{11}$$

where $\det A$ *is the determinant of the adjacency matrix of graph G.*

Proof: Using Lemmas 2.3 and 2.6 with arithmetic–geometric mean inequality, we get

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

This completes the proof. □

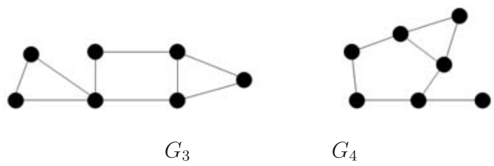


Fig. 3. Graphs G_3 and G_4.

Remark 4.3. *The lower bounds on the Randić energy given in* (9) *and* (11) *are incomparable. Two graphs G_3 and G_4 have been shown in Fig. 3. For graph G_3, the lower bounds in* (9) *and* (11) *are 3.302 and 3.335, respectively. On the other hand, for graph G_4, the lower bounds in* (9) *and* (11) *are 3.763 and 3.749, respectively.*

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