MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **73** (2015) 81-92

ISSN 0340 - 6253

On Randić Energy

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(Received February 17, 2014)

Abstract

Let G be a simple graph with n vertices and m edges. Let d_i be the degree of the i-th vertex of G. The Randić matrix $\mathbf{R} = (r_{ij})$ is defined by $r_{ij} = 1/\sqrt{d_i\, d_j}$ if the i-th and j-th vertices are adjacent and $r_{ij} = 0$ otherwise. The Randić energy RE is the sum of absolute values of the eigenvalues of $\mathbf{R}$. Cavers et al. [On the normalized Laplacian energy and general Randić index $R_1(G)$ of graphs, *Lin. Algebra Appl.* **433** (2010) 172–190] obtained some bounds on RE, but did not characterize the extremal graphs. We now find these extremal graphs. Additional lower and upper bounds for RE are obtained, in terms of n, m, maximum degree Δ, minimum degree δ, and the determinant of the adjacency matrix.

1 Introduction

In this paper we are concerned with simple finite graphs, without directed, multiple, or weighted edges, without self–loops, and without isolated vertices. Let $G = (V, E)$ be such a graph, with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G)$ such that $|E(G)| = m$. If the vertices v_i and v_j are adjacent, then we write $v_iv_j \in E(G)$.

For $i = 1, 2, \ldots, n$, let d_i be the degree of the vertex v_i. The minimum and maximum vertex degrees will be denoted by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. A vertex of degree zero is said to be isolated. In this work we assume that such vertices are not present in the graphs considered, i.e., that $\delta \geq 1$.

The adjacency matrix $\mathbf{A}(G)$ of G is defined by its entries $a_{ij} = 1$ if $v_i v_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ denote the eigenvalues of $\mathbf{A}(G)$. These form the (ordinary) spectrum of G [6]. The greatest graph eigenvalue λ_1 is referred to as the spectral radius of graph G.

For what follows we shall need the well known results [6]:

$$\det \mathbf{A} = \prod_{i=1}^{n} \lambda_i \ .$$

The (ordinary) energy of a graph G is [16]

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

For recent papers on lower and upper bounds on $\mathcal{E}(G)$ see [8,9,13].

The Randić matrix $\mathbf{R} = \mathbf{R}(G) = (r_{ij})_{n \times n}$ is defined as [1,2,14]

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

Denote its eigenvalues by $\rho_1, \rho_2, \ldots, \rho_n$ and label them in non-increasing order. Then, in analogy to Eq. (1), the Randić energy is defined as [2]:

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i| \ . \tag{2}$$

For several lower and upper bounds on RE, see [1,2,10,14]. For comparing energy and Randić energy, see [11].

Denote by $\mathbf{D} = \mathbf{D}(G)$ the diagonal matrix of vertex degrees of the graph G. If the graph G has no isolated vertices, then the matrix $\mathbf{D}^{-1/2}$ is well defined; this is just the diagonal matrix whose i-th diagonal element is $1/\sqrt{d_i}$.

The Laplacian matrix of the graph G is $\mathbf{L} := \mathbf{D} - \mathbf{A}$. The normalized Laplacian matrix is then defined as [5]

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

The eigenvalues of $\mathbf{L}$ and $\tilde{\mathbf{L}}$ will be denoted by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ and $\tilde{\mu}_1 \geq \tilde{\mu}_2 \geq \cdots \geq \tilde{\mu}_n$, respectively.

Recall that $\mathbf{D}^{-1/2}\,\mathbf{A}\,\mathbf{D}^{-1/2} = \mathbf{R}$. Therefore, $\tilde{\mathbf{L}} = \mathbf{I} - \mathbf{R}$ and $\tilde{\mu}_i = 1 - \rho_i$ for all $i = 1, 2, \ldots, n$ and for all graphs [14].

The normalized Laplacian energy of G is defined as [4]

$$\mathcal{E}_{\tilde{\mathbf{L}}} = \mathcal{E}_{\tilde{\mathbf{L}}}(G) = \sum_{i=1}^{n} |\tilde{\mu}_i - 1| \ .$$

It immediately follows [14] that the normalized Laplacian energy and the Randić energy coincide.

Recently, two of the present authors [10] reported the following bounds for Randić energy:

$$RE \ \geq \ 1 + (n-1)\left(\frac{|det\,\mathbf{A}|}{\prod\limits_{i=1}^{n} d_i}\right)^{1/(n-1)} \tag{3}$$

$$RE \ \geq \ 1 + \sqrt{\frac{n}{\Delta} - 1 + (n-1)(n-2)\left(\frac{|det\,\mathbf{A}|}{\prod\limits_{i=1}^{n} d_i}\right)^{2/(n-1)}} \tag{4}$$

$$RE \ \leq \ 1 + \sqrt{\frac{(n-1)(n-\delta)}{\delta}} \ . \tag{5}$$

The present paper is organized as follows. In Section 2, we state some previously known results, needed for the subsequent considerations. In Section 3, we characterize graphs extremal w.r.t. Randić energy. In Section 4, we obtain some novel lower and upper bounds on RE.

2 Preliminaries

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

Lemma 1. [18] *Let* $\mathbf{B}$ *be a* $p \times p$ *symmetric matrix and let* $\mathbf{B}_k$ *be its leading* $k \times k$ *submatrix. Then, for* $i = 1, 2, \ldots, k$,

$$\xi_{p-i+1}(\mathbf{B}) \leq \xi_{k-i+1}(\mathbf{B}_k) \leq \xi_{k-i+1}(\mathbf{B}) \tag{6}$$

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

Lemma 2. [15] *Let* $\mathbf{M}$ *be a real symmetric matrix of order* n *and* $\mathbf{S}$ *a nonsingular matrix of order* n. *For each* $k = 1, 2, \ldots, n$, *there exists a positive real number* θ_k *such that*

$$\xi_n(\mathbf{S}\,\mathbf{S}^t) \leq \theta_k \leq \xi_1(\mathbf{S}\,\mathbf{S}^t) \qquad \text{and} \qquad \xi_k(\mathbf{S}\,\mathbf{M}\,\mathbf{S}^t) = \theta_k\,\xi_k(\mathbf{M})$$

where by ξ_i *is denoted the i-th greatest eigenvalue of the underlying matrix.*

Lemma 3. [19] *Let* G *be a simple graph of order* n, *and* λ_1 *its spectral radius. Then*

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

Equality holds if and only if G *is either a regular or a bipartite semiregular graph.*

Lemma 4. [7] *Let* G *be a simple graph of order* n *with* m *edges. Then*

$$M_1(G) = \sum_{i=1}^{n} d_i^2 \geq \Delta^2 + \delta^2 + \frac{(2m - \Delta - \delta)^2}{n-2}\ .$$

Equality holds if and only if $d_2 = d_3 = \cdots = d_{n-1}$.

Lemma 5. [6, 14, 17] *Let* G *be a graph of order* n. *Then* $\rho_1 = 1$.

Lemma 6. [14] *If* G *possesses isolated vertices, then* $\det\,\mathbf{R} = \det\,\mathbf{A} = 0$. *If* G *does not possess isolated vertices, then*

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

Lemma 7. [3] *Let* G *be a graph of order* n *with no isolated vertices. Then*

$$\frac{\mu_2}{\Delta} \leq \tilde{\mu}_2 \leq \frac{\mu_2}{\delta}$$

where μ_2 *is the second largest Laplacian eigenvalue.*

3 Characterization of graphs extremal with regard to Randić energy

In [4], Cavers et al. obtained a lower bound on Randić energy $RE(G)$, but they did not characterize the extremal graphs. Here we determine these extremal graphs.

Lemma 8. [4] *Let G be a graph of order n with no isolated vertices. Then*

$$\mathcal{E}_{\tilde{\mathbf{L}}} \geq \sqrt{2R_{-1} + n(n-1)\ \det(\mathbf{I} - \tilde{\mathbf{L}})^{2/n}}$$

where

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

Evidently [14], $\det(\mathbf{I} - \tilde{\mathbf{L}}) = \det \mathbf{R}$, and Lemma 6 is applicable. We now can reformulate and strengthen Lemma 8 as follows:

Theorem 1. *Let G be a connected graph of order n. Then*

$$RE \geq \sqrt{2R_{-1} + n(n-1) \left(\frac{|\det \mathbf{A}|}{\prod_{i=1}^{n} d_i} \right)^{2/n}}\ . \tag{7}$$

Equality holds in (7) *if and only if $G \cong K_2$.*

Remark 1. *Inequality (7) holds also if the graph is not connected, but has no isolated vertices. Equality in (7) is then attained whenever G is regular of degree 1.*

Proof. We have

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

By the arithmetic–geometric mean inequality,

$$\sum_{1 \leq i < j \leq n} |\rho_i||\rho_j| \geq \frac{n(n-1)}{2} \left(\prod_{i=1}^{n} |\rho_i| \right)^{2/n}$$

with equality holding if and only if $|\rho_1| = |\rho_2| = \cdots = |\rho_n|$. This implies

$$\begin{aligned} \left(\sum_{i=1}^{n} |\rho_i| \right)^2 &= \sum_{i=1}^{n} \rho_i^2 + 2 \sum_{1 \leq i < j \leq n} |\rho_i||\rho_j| \\ &\geq 2R_{-1} + n(n-1) \left(\prod_{i=1}^{n} |\rho_i| \right)^{2/n} \qquad (8) \\ &= 2R_{-1} + n(n-1) \left(\frac{|\det \mathbf{A}|}{\prod_{i=1}^{n} d_i} \right)^{2/n}\ . \end{aligned}$$

The first part of the proof is done.

Suppose now that the equality holds in (7). Then all the above inequalities must be equalities. From equality in (8), we get $|\rho_1| = |\rho_2| = \cdots = |\rho_n|$. Since by Lemma 5, $\rho_1 = 1$, all Randić eigenvalues must be equal to $+1$ or -1. If $G \cong K_2$, then $\rho_1 = 1$, $\rho_2 = -1$, and thus the equality holds in (7).

Assume thus that $n \geq 3$. If $G \cong K_n$, then by direct calculations we can check that equality in (7) does not hold. Otherwise, if $G \ncong K_n$, then by Lemma 1, $\rho_2 \geq 0$. From Lemma 7 and $\mu_2 > 0$, we get

$$\tilde{\mu}_2 = 1 - \rho_2 \geq \frac{\mu_2}{\Delta} \qquad \text{that is,} \qquad \rho_2 \leq \frac{\Delta - \mu_2}{\Delta} < 1 \,.$$

Thus, $0 \leq \rho_2 < 1$, which shows that the condition $|\rho_1| = |\rho_2| = \cdots = |\rho_n|$ cannot be satisfied. □

In [4], Cavers et al. obtained the following relation between the ordinary graph energy $\mathcal{E}$ and the Randić energy RE.

Lemma 9. [4] *Let G be a graph of order n with no isolated vertices. Then*

$$\delta\, RE(G) \leq \mathcal{E}(G) \leq \Delta\, RE(G) \tag{9}$$

where Δ and δ are, respectively, the maximum and minimum vertex degree of G.

We now offer another relation between $\mathcal{E}$ and RE.

Theorem 2. *Let G be a graph of order n with no isolated vertices and spectral radius λ_1. Then*

$$\delta\, RE(G) + \lambda_1 - \delta \leq \mathcal{E}(G) \leq \Delta\, RE(G) + \lambda_1 - \Delta \,. \tag{10}$$

Proof. Setting in Lemma 2, $\mathbf{S} = \mathbf{D}^{1/2}$ and $\mathbf{M} = \mathbf{R}$, we get

$$\mathbf{S}\,\mathbf{M}\,\mathbf{S}^t = \mathbf{D}^{1/2}\,\mathbf{R}\,\mathbf{D}^{1/2} = \mathbf{A}$$

$$\xi_n(\mathbf{D}) \leq \theta_k \leq \xi_1(\mathbf{D}) \qquad \text{i.e.,} \qquad \delta \leq \theta_k \leq \Delta$$

$$\xi_k(\mathbf{A}) = \theta_k\, \xi_k(\mathbf{R}) \qquad \text{i.e.,} \qquad \lambda_k = \theta_k\, \rho_k$$

for $k = 1, 2, \ldots, n$. Thus

$$\delta\, |\rho_k| \leq \theta_k\, |\rho_k| \leq \Delta\, |\, \rho_k|$$

that is,

$$\delta\, |\rho_k| \leq |\lambda_k| \leq \Delta\, |\, \rho_k| \,. \tag{11}$$

By summing (11) over all k , $k = 1, 2, \ldots, n$, and by taking into account Eqs. (1) and (2) we arrive at (9). By summing (11) over $k = 2, \ldots, n$ and recalling that $\rho_1 = 1$, we obtain

$$\delta\,(RE - 1) \leq \mathcal{E} - \lambda_1 \leq \Delta\,(RE - 1)$$

from which (10) straightforwardly follows. □

Remark 2. *Because $\delta \leq \lambda_1 \leq \Delta$ [6], the inequalities (10) improve the result of Lemma 9. If the graph G is regular, then (10) reduces to (9).*

In Lemma 9, Cavers et al. did not characterize the extremal graphs. We now note that both equalities in (9) hold if and only if G regular.

4 Bounds for the Randić energy of graphs

A graph is nonsingular if all its eigenvalues are different from zero. For non-singular graphs, $|\det \mathbf{A}| > 0$. We now give some lower and upper bounds on the Randić energy in terms of n, maximum degree Δ, and the determinant of the adjacency matrix.

Theorem 3. *Let G be a connected non-singular graph of order n with maximum degree Δ. Then*

$$RE \geq 1 + \frac{n - 1 + \ln\left(\dfrac{|\det \mathbf{A}|}{\Delta}\right)}{\Delta} \tag{12}$$

with equality holding if and only if $G \cong K_n$.

Proof. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the adjacency matrix of graph G. In [9], it was shown that $x \geq 1 + \ln x$ for $x > 0$, with equality if and only if $x = 1$. Using this result, we get

$$\begin{aligned} \mathcal{E}(G) - \lambda_1 &= \sum_{i=2}^{n} |\lambda_i| \geq n - 1 + \sum_{i=2}^{n} \ln|\lambda_i| && (13) \\ &= n - 1 + \ln|\det \mathbf{A}| - \ln \lambda_1 \\ &\geq n - 1 + \ln|\det \mathbf{A}| - \ln \Delta\,. && (14) \end{aligned}$$

Combining above result with Theorem 2, we get

$$RE(G) \geq 1 + \frac{\mathcal{E}(G) - \lambda_1}{\Delta} \geq 1 + \frac{n - 1 + \ln|\det \mathbf{A}| - \ln \Delta}{\Delta}$$

which completes the first part of the proof.

One can easily check that equality in (12) holds for $G \cong K_n$.

Suppose now that the equality holds in (12). Then all the above inequalities must be equalities. The equality in (13) implies $|\lambda_2| = |\lambda_3| = \cdots = |\lambda_n| = 1$ and therefore $\lambda_n = -1$.

From the equality in (14), we get $\lambda_1 = \Delta$. Thus G must be a regular graph. If $\Delta = n-1$, then $G \cong K_n$ and the above equality holds. Therefore, it remains to consider the case $\Delta \leq n-2$. Then $K_{1,2}$ is an induced subgraph of G. By Lemma 1,

$$\lambda_n \leq \lambda_3(K_{1,2}) = -\sqrt{2}$$

which contradicts to the requirement $\lambda_n = -1$. □

Remark 3. *The lower bounds (3) and (4) from* [10] *and the presently deduced lower bounds (7) and (12) are incomparable. This is seen from the data given in Table 1, pertaining to the graphs depicted in Fig. 1.*

graph	Eq. (3)	Eq. (4)	Eq. (7)	Eq. (12)
G_1	1.82	2.11	2.89	1.71
G_2	1.998	1.999	1.908	2
G_3	3.941	3.923	3.921	3.095
G_4	3.749	3.762	3.737	2.864

Table 1. The values of the lower bounds (3), (4), (7), and (12) for the graphs depicted in Fig. 1. These show that the four bounds are mutually incomparable.

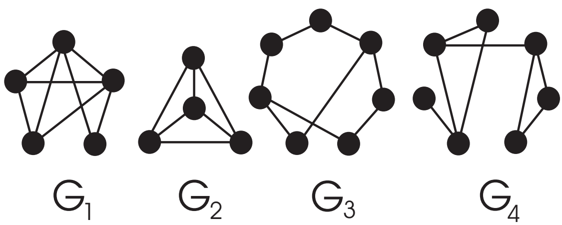

Fig. 1. Graphs used to illustrated the fact that the four lower bounds (3), (4), (7), and (12) are incomparable; see Table 1.

A strongly regular graph with parameters (n, r, λ, μ), denoted $SRG(n, r, \lambda, \mu)$, is an 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 [12].

Theorem 4. *Let G be a simple graph of order n , $n>2$. Then*

$$RE(G) \leq 1+\frac{1}{\delta}\sqrt{\frac{n-1}{n(n-2)}\left[2mn(n-2)-(2m-\Delta-\delta)^2-(n-2)(\Delta^2+\delta^2)\right]} \quad (15)$$

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. By Lemma 3,

$$\lambda_1 \geq \frac{1}{n}\sqrt{\sum_{i=1}^{n} d_i^2} \geq \sqrt{\frac{(n-2)(\Delta^2+\delta^2)+(2m-\Delta-\delta)^2}{n(n-2)}} \quad (16)$$

because by Lemma 4,

$$\sum_{i=1}^{n} d_i^2 \geq \Delta^2+\delta^2+\frac{(2m-\Delta-\delta)^2}{n-2} .$$

Now,

$$\begin{aligned} \mathcal{E}(G)-\lambda_1 &= \sum_{i=2}^{n}|\lambda_i| \leq \sqrt{(n-1)\sum_{i=2}^{n}\lambda_i^2} \quad (17) \\ &= \sqrt{(n-1)(2m-\lambda_1^2)} . \end{aligned}$$

Since $f(x)=2m-x^2$ is a decreasing function on any x, by (16),

$$\mathcal{E}(G)-\lambda_1 \leq \sqrt{(n-1)\left[2m-\frac{(n-2)(\Delta^2+\delta^2)+(2m-\Delta-\delta)^2}{n(n-2)}\right]} .$$

Using the above in (10), we get

$$\begin{aligned} RE(G) &\leq 1+\frac{\mathcal{E}(G)-\lambda_1}{\delta} \\ &\leq 1+\frac{1}{\delta}\sqrt{(n-1)\left[2m-\frac{(n-2)(\Delta^2+\delta^2)+(2m-\Delta-\delta)^2}{n(n-2)}\right]} . \quad (18) \end{aligned}$$

The first part of the proof is done.

One can easily check (see [10]), that equality in (15) holds in the case when $G \cong K_n$ and $G \cong SRG\left(n, r, \frac{r(r-1)}{n-1}, \frac{r(r-1)}{n-1}\right)$.

Suppose now that the equality holds in (15). Then all the above inequalities must be equalities. By Lemma 3, G must be either a regular graph or a bipartite semiregular graph. By Lemma 4, $d_2=d_3=\cdots=d_{n-1}$. From this we conclude that $G \cong K_{1,n-1}$ or that G is a regular graph. From equality in (17), it follows $|\lambda_2|=|\lambda_3|=\cdots=|\lambda_n|$.

Since

$$|\lambda_2(K_{1,n-1})| = 0 \neq \sqrt{n-1} = |\lambda_n(K_{1,n-1})|$$

G must be a regular graph of degree r. Thus, $\lambda_i = r\,\rho_i$, $i = 1, 2, \ldots, n$.

From the above results, we conclude that $|\rho_2| = |\rho_3| = \cdots = |\rho_n|$. In view of $\rho_1 = 1$, we have

$$|\rho_2| = |\rho_3| = \cdots = |\rho_n| = \sqrt{\frac{n-r}{r(n-1)}} \,.$$

From the equality in (18), it follows

$$RE(G) = 1 + \frac{1}{\delta}\sqrt{(n-1)\left[2m - \frac{(n-2)(\Delta^2+\delta^2) + (2m-\Delta-\delta)^2}{n(n-2)}\right]} \,.$$

Employing the same arguments as in the proof of Theorem 3.5 in [10], we arrive at $G \cong K_n$ or $G \cong SRG\left(n, r, \frac{r(r-1)}{n-1}, \frac{r(r-1)}{n-1}\right)$, as the graphs for which equality in (15) is attained. □

Remark 4. *The upper bound (5) from* [10] *and the presently deduced upper bounds (15) are incomparable. This is seen from the data given in Table 2, pertaining to the graphs depicted in Fig. 2.*

graph	Eq. (5)	Eq. (15)
G_5	3.828	3.725
G_6	6	6.845

Table 2. The values of the upper bounds (5) and (15) for the graphs depicted in Fig. 2. These show that the two bounds are mutually incomparable.

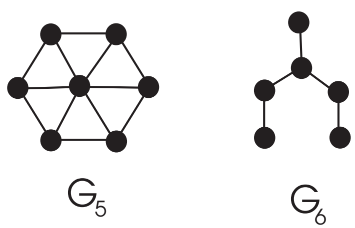

Fig. 2. Graphs used to illustrated the fact that the two upper bounds (5) and (15) are incomparable; see Table 2.

Acknowledgement. This work is supported by the Faculty research Fund, Sungkyunkwan University, 2012, and the National Research Foundation funded by the Korean government with the grant no. 2013R1A1A2009341. The second author is grateful to the Scientific and Technological Council of Turkey (TUBITAK) for supporting his Postdoctoral studies through their fellowship programmes.

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