EUROPEAN JOURNAL OF PURE AND APPLIED MATHEMATICS
Vol. 5, No. 1, 2012, 88-96
ISSN 1307-5543 – www.ejpam.com

SPECIAL ISSUE FOR THE INTERNATIONAL CONFERENCE ON APPLIED ANALYSIS AND ALGEBRA
29 JUNE - 02 JULY 2011, ISTANBUL TURKEY

Randić Energy and Randić Estrada Index of a Graph

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Abstract. Let G be a simple connected graph with n vertices and let d_i be the degree of its i-th vertex. The Randić matrix of G is the square matrix of order n whose (i,j)-entry is equal to $1/\sqrt{d_i d_j}$ if the i-th and j-th vertex of G are adjacent, and zero otherwise. The Randić eigenvalues are the eigenvalues of the Randić matrix. The Randić energy is the sum of the absolute values of the Randić eigenvalues. In this paper, we introduce a new index of the graph G which is called Randić Estrada index. In addition, we obtain lower and upper bounds for the Randić energy and the Randić Estrada index of G.

2000 Mathematics Subject Classifications: 05C50,15A18

Key Words and Phrases: Randić Matrix, Randić Eigenvalue, Randić Energy, Randić Estrada Index

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1. Introduction

Let G be a simple connected graph with n vertices and m edges. Throughout this paper, such a graph will be refered to as connected (n,m)-graph. Let $V(G) = \{v_1, v_2, \dots, v_n\}$ be the vertex set of G. If any two vetices v_i and v_j of G are adjacent, then we use the notation $v_i \sim v_j$. For $v_i \in V(G)$, the degree of the vertex v_i, denoted by d_i, is the number of the vertices adjacent to v_i.

Let $A(G)$ be the $(0,1)$-adjacency matrix of G and $\lambda_1, \lambda_2, \dots, \lambda_n$ be its eigenvalues. These are said to be eigenvalues of the graph G and to form its spectrum [3]. The Randić matrix of G is the $n \times n$ matrix $\mathbf{R} = \mathbf{R}(G) = \left[\mathbf{R}_{ij}\right]$ as the following

$$\mathbf{R}_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}}, & v_i \sim v_j \\ 0, & otherwise \end{cases}$$

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The Randić eigenvalues $\rho_1, \rho_2, \ldots, \rho_n$ of the graph G are the eigenvalues of its Randić matrix. Since $A(G)$ and $\mathbf{R}(G)$ are real symmetric matrices, their eigenvalues are real numbers. So we can order them so that $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ and $\rho_1 \geq \rho_2 \geq \ldots \geq \rho_n$.

The energy of the graph G is defined in [11,12,13] as:

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

The Randić energy of the graph G is defined in [1,2] as:

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

The Estrada index of the graph G is defined in [7,8,9,10] as:

$$EE = EE(G) = \sum_{i=1}^{n} e^{\lambda_i} \tag{3}$$

Denoting by $M_k = M_k(G)$ the k-th moment of the graph G

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k.$$

Recalling the power series expansion of e^x, we have

$$EE = \sum_{k=0}^{\infty} \frac{M_k}{k!}. \tag{4}$$

It is well known that [3] M_k is equal to the number of closed walks of length k in the graph G. Estrada index of graphs has an important role in Chemistry and Physics. For more information we refer to the reader [7,8,9,10]. In addition, there exist a vast literature that studies Estrada index and its bounds. For detailed information we may also refer to the reader [4,5,6,14].

Now we introduce the Randić Estrada index of the graph G.

Definition 1. *If G is a connected (n,m)-graph, then the Randić Estrada index of G, denoted by $REE(G)$, is equal to*

$$REE = REE(G) = \sum_{i=1}^{n} e^{\rho_i}. \tag{5}$$

where $\rho_1, \rho_2, \ldots, \rho_n$ are the Randić eigenvalues of G.

Let

$$N_k = N_k(G) = \sum_{i=1}^{n} (\rho_i)^k.$$

Recalling the power series expansion of e^x we have another expression of Randić Estrada index as the following

$$REE(G) = \sum_{k=0}^{\infty} \frac{N_k}{k!}. \tag{6}$$

In this paper, we obtain lower and upper bounds for the Randić energy and the Randić Estrada index of G. Firstly, we give some definitions and lemmas which will be needed then.

Definition 2. *[2] Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and Randić matrix* $\mathbf{R}$*. Then the Randić degree of v_i, denoted by R_i is given by*

$$R_i = \sum_{j=1}^{n} \mathbf{R}_{ij}.$$

Definition 3. *[2] Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and Randić matrix* $\mathbf{R}$*. Let the Randić degree sequence be $\{R_1, R_2, \ldots, R_n\}$. Then for each $i = 1, 2, \ldots, n$ the sequence $L_i^{(1)}, L_i^{(2)}, \ldots, L_i^{(p)}, \ldots$ is defined as follows: Fix $\alpha \in \mathbb{R}$, let*

$$L_i^{(1)} = R_i^{\alpha}$$

and for each $p \geq 2$, let

$$L_i^{(p)} = \sum_{i \sim j} \frac{1}{\sqrt{d_i d_j}} L_j^{(p-1)}.$$

Definition 4. *[15] Let G be a graph with Randić matrix* $\mathbf{R}$ *. Then the Randić index of G, denoted by $R(G)$ is given by*

$$R(G) = \frac{1}{2} \sum_{i=1}^{n} R_i.$$

Lemma 1. *[1] Let G be a graph with n vertices and Randić matrix* $\mathbf{R}$*. Then*

$$tr(\mathbf{R}) = \sum_{i=1}^{n} \rho_i = 0$$

and

$$tr\left(\mathbf{R}^2\right) = \sum_{i=1}^{n} \rho_i^2 = 2 \sum_{i \sim j} \frac{1}{d_i d_j}.$$

Lemma 2. *[2] Let G be a connected graph α be a real number and p be an integer. Then*

$$\rho_1 \geq \sqrt{\frac{S_{p+1}}{S_p}}.$$

where $S_p = \sum_{i=1}^{n} \left(L_i^{(p)}\right)^2$. Moreover, the equality holds for particular values of α and p if and only if

$$\frac{L_1^{(p+1)}}{L_1^{(p)}} = \frac{L_2^{(p+1)}}{L_2^{(p)}} = \cdots = \frac{L_n^{(p+1)}}{L_n^{(p)}}.$$

Lemma 3. *[2] A simple connected graph G has two distinct Randić eigenvalues if and only if G is complete.*

2. Bounds for the Randić Energy of a Graph

In this section, we obtain lower and upper bounds for the Randić energy of connected (n,m)-graph G.

Let N and M be two positive integers. We first consider the following auxiliary quantity Q as

$$Q = Q(G) = \sum_{i=1}^{N} q_i \tag{7}$$

where q_i, $i = 1,2,\ldots,N$ are some numbers which some how can be computed from the graph G. For which we only need to know that they satisfy the conditions

$$q_i \geq 0, \text{ for all } i = 1,2,\ldots,N$$

and

$$\sum_{i=1}^{N} (q_i)^2 = 2M \tag{8}$$

or, the conditions (7), (8) and

$$P = P(G) = \prod_{i=1}^{N} q_i \tag{9}$$

if all the conditions (7)-(9) are taken into account then [11]

$$\sqrt{2MN - (N-1)D} \leq Q \leq \sqrt{2MN - D} \tag{10}$$

where

$$D = 2M - NP^{2/N}. \tag{11}$$

For the graph energy (namely by setting into (10) and (11) $N = n$, $M = m$ and $P = |\det A|$), this yields [11]

$$\sqrt{2m + n(n-1)|\det A|^{2/n}} \leq E(G) \leq \sqrt{2m(n-1) + n|\det A|^{2/n}}.$$

The Randić energy-counterpart of the estimates (10) and (11) is obtained as the following result.

Theorem 1. *Let G be a connected (n,m)-graph and Δ be the absolute value of the determinant of the Randić matrix* **R**. *Then*

$$RE(G) \geq \sqrt{2\sum_{i\sim j} \frac{1}{d_i d_j} + n(n-1)\Delta^{2/n}} \tag{12}$$

and

$$RE(G) \leq \sqrt{2(n-1)\sum_{i\sim j}\frac{1}{d_i d_j} + n\Delta^{2/n}}. \tag{13}$$

Proof. The result is easily obtained using the estimates (10), (11) and Lemma 1.

In [1] the following result for $RE(G)$ was obtained

$$RE(G) \leq \sqrt{2n\sum_{i\sim j}\frac{1}{d_i d_j}} \tag{14}$$

Remark 1. *The upper bound (13) is sharper than the upper bound (14). Using arithmetic-geometric mean inequality, we obtain*

$$2\sum_{i\sim j}\frac{1}{d_i d_j} \geq n\Delta^{2/n}$$

and considering the upper bound (13) we arrive at

$$RE(G) \leq \sqrt{2n\sum_{i\sim j}\frac{1}{d_i d_j}}$$

which is the upper bound (14).

3. Bounds for the Randić Estrada Index of a Graph

In this section, we consider the Randić Estrada index of connected (n,m)-graph G. We also adapt the some results in [4] and [14] on the Randić Estrada index to give lower and upper bounds for it.

Theorem 2. *Let G be a connected (n,m)-graph. Then*

$$REE(G) \geq e^{\sqrt{\frac{S_{p+1}}{S_p}}} + \frac{n-1}{e^{\frac{1}{n-1}\sqrt{\frac{S_{p+1}}{S_p}}}}. \tag{15}$$

where α is a real number, p is an integer and $S_p = \sum_{i=1}^{n}\left(L_i^{(p)}\right)^2$. Moreover, the equality holds in (15) if and only if G is the complete graph K_n.

Proof. Starting with the equation (5) and using arithmetic-geometric mean inequality, we obtain

$$REE(G) = e^{\rho_1} + e^{\rho_2} + \cdots + e^{\rho_n}$$

$$\geq \quad e^{\rho_1} + (n-1)\left(\prod_{i=2}^{n} e^{\rho_i}\right)^{\frac{1}{n-1}} \tag{16}$$

$$= \quad e^{\rho_1} + (n-1)\left(e^{-\rho_1}\right)^{\frac{1}{n-1}}, \text{ since } \sum_{i=1}^{n}\rho_i = 0. \tag{17}$$

Now we consider the following function

$$f(x) = e^x + \frac{n-1}{e^{\frac{x}{n-1}}}$$

for $x > 0$. We have

$$f(x) = e^x - e^{-\frac{x}{n-1}} > 0$$

for $x > 0$. It is easy to see that f is an increasing function for $x > 0$. From the equation (17) and Lemma 2, we obtain

$$REE(G) \geq e^{\sqrt{\frac{S_{p+1}}{S_p}}} + \frac{n-1}{e^{\frac{1}{n-1}\sqrt{\frac{S_{p+1}}{S_p}}}}. \tag{18}$$

Now we assume that the equality holds in (15). Then all inequalities in the above argument must be equalities. From (18) we have

$$\rho_1 = \sqrt{\frac{S_{p+1}}{S_p}}$$

which implies $\frac{L_1^{(p+1)}}{L_1^{(p)}} = \frac{L_2^{(p+1)}}{L_2^{(p)}} = \cdots = \frac{L_n^{(p+1)}}{L_n^{(p)}}$. From (16) and arithmetic-geometric mean inequality we get $\rho_2 = \rho_3 = \cdots = \rho_n$. Therefore G has exactly two distinct Randić eigenvalues, by Lemma 3, G is the complete graph K_n.

Conversely, one can easily see that the equality holds in (15) for the complete graph K_n. This completes the proof of theorem.

Now we give a result which states a lower bound for the Randić Estrada index involving Randić index.

Corollary 1. *Let G be a connected (n,m)-graph. Then*

$$REE(G) \geq e^{\frac{2R(G)}{n}} + \frac{n-1}{e^{\frac{2R(G)}{n(n-1)}}} \tag{19}$$

where $R(G)$ denotes the Randić index of the graph G. Moreover the equality holds in (19) if and only if G is the complete graph K_n.

Proof. In [2], the authors showed that the folllowing inequality (see Theorem 4)

$$\rho_1 \geq \sqrt{\frac{S_{p+1}}{S_p}} \geq \sqrt{\frac{\sum_{i=1}^{n} R_i^2}{n}} \geq \frac{2R(G)}{n} \tag{20}$$

where $S_p = \sum_{i=1}^{n} \left(L_i^{(p)}\right)^2$. Combining Theorem 2 and (20) we get the inequality (19).

Also, the equality holds in (19) if and only if G is the complete graph K_n.

Theorem 3. *Let G be a connected (n,m)-graph.Then the Randić Estrada index $REE(G)$ and the Randić energy $RE(G)$ satisfy the following inequality*

$$\frac{1}{2}RE(G)(e-1)+n-n_+ \le REE(G) \le n-1+e^{\frac{RE(G)}{2}}. \tag{21}$$

where n_+ denotes the number of positive Randić eigenvalues of G. Moreover, the equality holds on both sides of (21) if and only if $G = K_1$.

Proof. **Lower bound:** Since $e^x \ge ex$, equality holds if and only if $x = 1$ and $e^x \ge 1 + x$, equality holds if and only if $x = 0$, we get

$$\begin{aligned} REE(G) &= \sum_{i=1}^{n} e^{\rho_i} = \sum_{\rho_i>0} e^{\rho_i} + \sum_{\rho_i\le 0} e^{\rho_i} \\ &\ge \sum_{\rho_i>0} e\rho_i + \sum_{\rho_i\le 0} (1+\rho_i) \\ &= e\left(\rho_1+\rho_2+\cdots+\rho_{n_+}\right) + (n-n_+) + \left(\rho_{n_++1}+\cdots+\rho_n\right) \\ &= (e-1)\left(\rho_1+\rho_2+\cdots+\rho_{n_+}\right) + (n-n_+) + \sum_{i=1}^{n}\rho_i \\ &= \frac{1}{2}RE(G)(e-1)+n-n_+. \end{aligned}$$

Upper bound: Since $f(x) = e^x$ monotonically increases in the interval $(-\infty, +\infty)$, we get

$$REE(G) = \sum_{i=1}^{n} e^{\rho_i} \le n - n_+ + \sum_{i=1}^{n_+} e^{\rho_i}$$

Therefore

$$\begin{aligned} REE(G) &= n - n_+ + \sum_{i=1}^{n_+}\sum_{k\ge 0} \frac{(\rho_i)^k}{k!} \\ &= n + \sum_{k\ge 1}\frac{1}{k!}\sum_{i=1}^{n_+}(\rho_i)^k \\ &\le n + \sum_{k\ge 1}\frac{1}{k!}\left[\sum_{i=1}^{n_+}\rho_i\right]^k = n-1+e^{\frac{RE(G)}{2}}. \end{aligned}$$

It is easy to see that the equality holds on both sides of (21) if and only if $RE(G) = 0$. Since G is a connected graph this only happens in the case of $G = K_1$.

4. Concluding Remarks

In this paper, the Randić Estrada index of a graph is introduced. Also the Randić energy and the Randić Estrada index are studied. In section 2, a sharper upper bound and a new lower bound for the Randić energy are obtained. In section 3, some bounds for the Randić Estrada index involving Randić index, Randić energy and some other graph invariants are also put forward.

ACKNOWLEDGEMENTS: The authors thank the referees for their helpful suggestions concerning the presentation of this paper.

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