Kragujevac Journal of Mathematics
Volume 42(2) (2018), Pages 209–215.

NOTE ON THE RANDIĆ ENERGY OF GRAPHS

JUN HE[1], YAN-MIN LIU[1], AND JUN-KANG TIAN[1]

Abstract. If G is a graph on n vertices, and d_i is the degree of its i-th vertex, then 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. In this note, we obtain some new lower and upper bounds for the Randić energy.

1. Introduction

Let G be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. Let d_i denote the degree of vertex v_i, where $i = 1, 2, \dots, n$. The maximum vertex degree is denoted by Δ. Use the notation $v_i \sim v_j$, if two vertices v_i and v_j of G are adjacent.

The Randić matrix $R = R(G)$ of G is defined as

$$r_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}}, & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent,} \\ 0, & \text{if the vertices } v_i \text{ and } v_j \text{ are not adjacent,} \\ 0, & \text{if } i = j. \end{cases}$$

The Randić matrix is real symmetric, so we can order the eigenvalues of its Randić matrix so that $\rho_1 \geq \rho_2 \geq \ldots \geq \rho_n$. The Randić energy of the graph G is defined in [2, 3, 6, 7] as:

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

As usual, the adjacency matrix $A = A(G)$ of the graph G is defined so that its (i,j)-element is equal to unity if the vertices v_i and v_j are adjacent, and is equal to

Key words and phrases. Randić energy, Randić matrix, bounds.
2010 *Mathematics Subject Classification.* Primary: 05C50. Secondary: 15A18.
Received: May 10, 2016.
Accepted: February 02, 2017.

zero otherwise. Let $L = D - A$ and $Q = D + A$ be, respectively, the Laplacian and the signless Laplacian matrix of the graph G [9, 10, 12]. If we define

$$\mathcal{L} = D^{-1/2} L D^{-1/2} \quad \text{and} \quad \mathcal{Q} = D^{-1/2} Q D^{-1/2},$$

where D is the diagonal matrix of vertex degrees, are the normalized Laplacian and normalized signless Laplacian matrix. Then, evidently,

$$\mathcal{L} = I_n - R \quad \text{and} \quad \mathcal{Q} = I_n + R. \tag{1.1}$$

The paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we present some lower and upper bounds on the Randić energy.

2. Preliminary Lemmas

In order to obtain bounds for the Randić energy of G, we need some lemmas.

Lemma 2.1. [1] *Let G be a graph with n vertices and Randić matrix R. Then*

$$tr(R) = 0, \quad tr(R^2) = 2\sum_{i\sim j} \frac{1}{d_i d_j},$$

$$tr(R^4) = \sum_{i=1}^{n} \left(\sum_{i\sim j} \frac{1}{d_i d_j} \right)^2 + \sum_{i\neq j} \frac{1}{d_i d_j} \left(\sum_{k\sim i, k\sim j} \frac{1}{d_k} \right)^2.$$

Lemma 2.2. [1] *A simple connected graph G has two distinct Randić eigenvalues if and only if G is complete.*

Lemma 2.3. [13] *Let $a_1, a_2, \ldots, a_n$ be non-negative numbers. Then*

$$n\left[\frac{1}{n}\sum_{j=1}^{n} a_j - \left(\prod_{j=1}^{n} a_j\right)^{1/n}\right] \leq n\sum_{j=1}^{n} a_j - \left(\sum_{j=1}^{n}\sqrt{a_j}\right)^2$$

$$\leq n(n-1)\left[\frac{1}{n}\sum_{j=1}^{n} a_j - \left(\prod_{j=1}^{n} a_j\right)^{1/n}\right].$$

Lemma 2.4. [11] *Let G be a graph on n vertices which has at least one edge, $\upsilon_1 \geq \ldots \geq \upsilon_n$ be the eigenvalues of the Laplacian L. Then*

$$\upsilon_1 \geq \Delta + 1.$$

Moreover, if G is connected, then the equality holds if and only if $\Delta = n - 1$.

3. Main results

It has been proved that $\rho_1 = 1$ is the largest R-eigenvalues with the Perron-Frobenius vector $\alpha^T = (\sqrt{d_1}, \dots, \sqrt{d_n})$ (see [4, 6, 8]).

Theorem 3.1. *Let G be a graph with n vertices and at least one edge. Then*

$$RE(G) \geq 1 + \left(2\sum_{i\sim j}\frac{1}{d_id_j} - 1\right)\sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_id_j} - 1}{\sum\limits_{i=1}^{n}\left(\sum\limits_{i\sim j}\frac{1}{d_id_j}\right)^2 + \sum\limits_{i\neq j}\frac{1}{d_id_j}\left(\sum\limits_{k\sim i, k\sim j}\frac{1}{d_k}\right)^2 - 1}}.$$

Proof. Using Hölder inequality, we have

$$\sum_{i=2}^{n} a_ib_i \leq \left(\sum_{i=2}^{n} a_i^p\right)^{1/p}\left(\sum_{i=2}^{n} b_i^q\right)^{1/q},$$

which holds for any non-negative real numbers a_i, b_i, $i = 2, 3, \dots, n$. Setting $a_i = |\rho|^{2/3}$, $b_i = |\rho|^{4/3}$, $p = 3/2$ and $q = 3$, we obtain

$$\sum_{i=2}^{n}|\rho_i|^2 = \sum_{i=2}^{n}|\rho_i|^{2/3}\sum_{i=2}^{n}|\rho_i|^{4/3} \leq \left(\sum_{i=2}^{n}|\rho_i|\right)^{2/3}\left(\sum_{i=2}^{n}|\rho_i|^4\right)^{1/3},$$

that is

$$RE(G) - 1 = \sum_{i=2}^{n}|\rho_i| \geq \sqrt{\frac{\left(\sum\limits_{i=2}^{n}|\rho_i|^2\right)^3}{\sum\limits_{i=2}^{n}|\rho_i|^4}} = \sqrt{\frac{(tr(R^2) - 1)^3}{tr(R^4) - 1}}.$$

Hence we get the result. ☐

We next derive a lower bound of the Randić energy in terms of the order n and $\det(R)$.

Theorem 3.2. *Let G be a graph with n vertices. Then*

$$RE(G) \geq 1 + (n-1)|\det(R)|^{\frac{1}{n-1}}, \tag{3.1}$$

and the equality holds in (3.1) *if and only if G is a complete graph or a non-bipartite connected graph with three distinct Randić eigenvalues*

$$\left(1, \sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_id_j}}{n-1}}, -\sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_id_j}}{n-1}}\right).$$

Proof. Using the arithmetic-geometric mean inequality, we obtain that

$$RE(G) = \rho_1 + \sum_{i=2}^{n}|\rho_i| \geq 1 + (n-1)\left(\prod_{i=2}^{n}|\rho_i|\right)^{\frac{1}{n-1}} = 1 + (n-1)|\det(R)|^{\frac{1}{n-1}},$$

and equality holds if and only if $\rho_1 = 1$ and $|\rho_2| = \ldots = |\rho_n| = \sqrt{\frac{2\sum_{i\sim j}\frac{1}{d_i d_j}}{n-1}}$, which is discussed in the proof of Theorem 4 in [4].

Now the proof is complete. □

Theorem 3.3. *Let G be a graph with n vertices. Then*

$$RE(G) \geq 1 + \sqrt{2\sum_{i\sim j}\frac{1}{d_i d_j} - 1 + (n-1)(n-2)\left(\det(R)\right)^{\frac{2}{n-1}}},$$

and

$$RE(G) \leq 1 + \sqrt{(n-2)\left(2\sum_{i\sim j}\frac{1}{d_i d_j} - 1\right) + (n-1)\left(\det(R)\right)^{\frac{2}{n-1}}}. \tag{3.2}$$

Proof. Let $a_i = \rho_i^2$, $i = 2, \ldots, n$. Then by Lemma 2.1 and Lemma 2.3 we obtain

$$K \leq (n-1)\sum_{i=2}^{n}\rho_i^2 - \left(\sum_{i=2}^{n}|\rho_i|\right)^2 \leq (n-2)K,$$

that is,

$$K \leq (n-1)\left(2\sum_{i\sim j}\frac{1}{d_i d_j} - 1\right) - \left(RE(G)-1\right)^2 \leq (n-2)K,$$

where

$$\begin{aligned}
K &= (n-1)\left[\frac{1}{n-1}\sum_{i=2}^{n}\rho_i^2 - \left(\prod_{i=2}^{n}\rho_i^2\right)^{\frac{1}{n-1}}\right] \\
&= (n-1)\left[\frac{1}{n-1}\left(2\sum_{i\sim j}\frac{1}{d_i d_j} - 1\right) - \left(\prod_{i=2}^{n}|\rho_i|\right)^{\frac{2}{n-1}}\right] \\
&= 2\sum_{i\sim j}\frac{1}{d_i d_j} - 1 - (n-1)\left(\det(R)\right)^{\frac{2}{n-1}}.
\end{aligned}$$

Hence we get the result. □

Remark 3.1. Using the relation between the arithmetic and geometric means,

$$\left(\det(R)\right)^2 \leq \left(\frac{2\sum_{i\sim j}\frac{1}{d_i d_j} - 1}{n-1}\right)^{n-1},$$

and bearing in mind the upper bound in (3.2), we arrive at

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

which is same as the result in [4, 8].

Lemma 3.1. *Let G be a graph with n vertices. Then*

$$|\rho_n| \geq \frac{1}{\Delta}.$$

Proof. Let $u_1 \geq \ldots \geq u_n$ be the eigenvalues of the normalized Laplacian $\mathcal{L}$, by equality (1.1), we have

$$\rho_n = 1 - u_1. \tag{3.3}$$

Let $\|A\|$ be the spectral norm of a matrix A, by $\mathcal{L} = D^{-1/2}LD^{-1/2}$ and Lemma 2.4, we can get

$$\Delta + 1 \leq \|L\| \leq \|D\|\|\mathcal{L}\| = \Delta u_1,$$

therefore,

$$u_1 \geq 1 + \frac{1}{\Delta}.$$

Then, by equality (3.3), we obtain

$$|\rho_n| \geq \frac{1}{\Delta}.$$

Now the proof is complete. □

Theorem 3.4. *Let G be a graph with $n \geq 2$ vertices. Then*

$$RE(G) \leq 1 + \sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_id_j} - 1}{n-1}} + \sqrt{(n-2)\left(2\sum_{i\sim j}\frac{1}{d_id_j} - 1 - \frac{2\sum\limits_{i\sim j}\frac{1}{d_id_j} - 1}{n-1}\right)}. \tag{3.4}$$

More, if $\frac{1}{\Delta} \geq \sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_id_j}-1}{n-1}}$, *then*

$$RE(G) \leq 1 + \frac{1}{\Delta} + \sqrt{(n-2)\left(2\sum_{i\sim j}\frac{1}{d_id_j} - 1 - \frac{1}{\Delta^2}\right)}. \tag{3.5}$$

Proof. Using Cauchy-Schwarz inequality, we obtain

$$\begin{aligned} RE(G) &= \rho_1 + \sum_{i=2}^{n-1}|\rho_i| + |\rho_n| \leq 1 + |\rho_n| + \sqrt{(n-2)\sum_{i=2}^{n-1}\rho_i^2} \\ &\leq 1 + |\rho_n| + \sqrt{(n-2)\left(2\sum_{i\sim j}\frac{1}{d_id_j} - 1 - \rho_n^2\right)}. \end{aligned}$$

Define a function $f(x) = 1 + x + \sqrt{(n-2)\left(2\sum\limits_{i\sim j}\frac{1}{d_id_j} - 1 - x^2\right)}$, it is easy to see that the function $f(x)$ is monotonously decreasing in $x \geq \sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_id_j}-1}{n-1}}$, which implies that the inequality (3.4) holds.

By Lemma 3.1, if we have $|\rho_n| \geq \frac{1}{\Delta} \geq \sqrt{\frac{2\sum\limits_{i\sim j}\frac{1}{d_i d_j}-1}{n-1}}$, then

$$f(|\rho_n|) \leq f\left(\frac{1}{\Delta}\right),$$

which implies that the inequality (3.5) holds. Now the proof is complete. □

Acknowledgements. He is supported by Science and technology Foundation of Guizhou province (Qian ke he Ji Chu [2016]1161); Guizhou province natural science foundation in China (Qian Jiao He KY [2016]255); The doctoral scientific research foundation of Zunyi Normal College (BS [2015]09). Liu is supported by National Natural Science Foundations of China (71461027); Science and technology talent training object of Guizhou province outstanding youth (Qian ke he ren zi [2015]06); Guizhou province natural science foundation in China (Qian Jiao He KY [2014]295); 2013, 2014 and 2015 Zunyi 15851 talents elite project funding; Zhunyi innovative talent team (Zunyi KH [2015]38). Tian is supported by the Science and Technology fund Project of GZ (Qian ke he J Zi [2015]2147, Qian jiao he KY [2015]451).

References

[1] Ş. B. Bozkurt, A. D. Güngör, I. Gutman and A. S. Çevik, *Randić matrix and Randić energy*, MATCH Commun. Math. Comput. Chem. **64** (2010), 239–250.

[2] Ş. B. Bozkurt, A. D. Güngör and I. Gutman, *Randić spectral radius and Randić energy*, MATCH Commun. Math. Comput. Chem. **64** (2010), 321–334.

[3] Ş. B. Bozkurt and D. Bozkurt, *Randić energy and Randić Estrada index of a graph*, Eur. J. Pure Appl. Math. **5** (2012), 88–96.

[4] Ş. B. Bozkurt and D. Bozkurt, *Sharp upper bounds for energy and randić energy*, MATCH Commun. Math. Comput. Chem. **70** (2013), 669–680.

[5] I. Gutman, *Bounds for total π-electron energy*, Chem. Phys. Lett. **24** (1974), 283–285.

[6] I. Gutman, B. Furtula and Ş. B. Bozkurt, *On Randić Energy*, Linear Algebra Appl. **442** (2014), 50–57.

[7] X. Li and Y. Shi, *A survey on the Randić index*, MATCH Commun. Math. Comput. Chem. **59** (2008), 127–156.

[8] B. Liu, Y. Huang and J. Feng, *A note on the Randić spectral radius*, MATCH Commun. Math. Comput. Chem. **68** (2012), 913–916.

[9] J. H. Koolen, V. Moulton and I. Gutman, *Improving the McClelland inequality for total π-electron energy*, Chem. Phys. Lett. **320** (2000), 213–216.

[10] J. H. Koolen and V. Moulton, *Maximal energy graphs*, Adv. Appl. Math. **26** (2001), 47–52.

[11] R. Merris, *Laplacian matrices of graphs: a survey*, Linear Algebra Appl. 197-198 (1994), 143–176.

[12] B. Zhou, *Energy of a graph*, MATCH Commun. Math. Comput. Chem. **51** (2004), 111–118.

[13] B. Zhou, I. Gutman and T. Aleksić, *A note on the Laplacian energy of graphs*, MATCH Commun. Math. Comput. Chem. **60** (2008), 441–446.

[1]School of mathematics,
Zunyi Normal College,
Zunyi, Guizhou, 563002, P.R. China
E-mail address: hejunfan1@163.com
E-mail address: 546692653@qq.com
E-mail address: 17261717@qq.com