Research Article

Bounds on graph energy and Randić energy

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Abstract
In the present paper, new lower and upper bounds on energy and Randić energy of non-singular (bipartite) graphs are reported. Additionally, it is shown that the obtained lower bounds are stronger than two previously known lower bounds in the literature.

Keywords: graph energy; Randić energy; bound.

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1. Introduction

Let $G$ be a simple connected graph. Denote by $n$ and $m$ the number of vertices and edges of $G$, respectively. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ be the set of the vertices of $G$ and $d_i$ be the degree of the vertex $v_i \in V(G)$, $i = 1, 2, \ldots, n$. If $v_i$ and $v_j$ are two adjacent vertices of $G$, then it is denoted by $i \sim j$. Let $\Delta$ and $\delta$ be the maximum and minimum vertex degrees of $G$, respectively.

Let us denote by $A = A(G)$ the adjacency matrix of a graph $G$. The eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ of $A$ represent the eigenvalues of $G$ [6]. As well known in spectral graph theory, $\lambda_1$ is the spectral radius of $G$ and

$$\sum_{i=1}^{n} \lambda_i = 0, \quad \sum_{i=1}^{n} \lambda_i^2 = 2m \quad \text{and} \quad \prod_{i=1}^{n} \lambda_i = \det A.$$  

(1)

A graph $G$ is called as non-singular if no eigenvalue of $G$ is equal to zero. For non-singular graphs, it is obvious that $\det A \neq 0$. A graph $G$ is singular if at least one of its eigenvalue is equal to zero. Then, $\det A = 0$.

The energy of a graph $G$ was defined in [12] as

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

(2)

This graph invariant is utilized to estimate the total $\pi$-electron energy of a molecule represented by a (molecular) graph. [13,22]. A vast literature exists on $E(G)$, for survey and comprehensive information, see [2,11,14,19,23].

Recently, energy of non-singular graphs has also been studied in the literature. In [8], Das et al. obtained a lower bound on energy of non-singular graphs that improves the lower bounds in [3,22], under certain conditions. Gutman and Das [15] established upper bounds on energy of non-singular (bipartite) molecular graphs. In [15], it was also stated that the upper bound obtained on energy of non-singular molecular graphs improves the upper bound in [3].

The following upper bound on $E(G)$ was found in [11]

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

(3)

The Randić matrix $R = R(G)$ of a graph $G$ is defined so that its $(i,j)$-th entry is equal to $1/\sqrt{d_id_j}$ if $i \sim j$ and is equal to 0 otherwise [1]. The eigenvalues $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$ of $R$ are called as the Randić eigenvalues of $G$ [1]. Some well known results concerning the Randić eigenvalues are [1,16]

$$\sum_{i=1}^{n} \rho_i = 0, \quad \sum_{i=1}^{n} \rho_i^2 = 2R_{-1} \quad \text{and} \quad \prod_{i=1}^{n} \rho_i = \det R.$$  

(4)

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where

\[ R_{-1} = R_{-1}(G) = \sum_{i=j}^{1} \frac{1}{d_i d_j} \]

is the general Randić index of the graph \( G \) [4, 18].

In full analogous manner with the graph energy [12], the Randić energy of \( G \) was introduced in [1]. It was defined as [1]

\[ RE = RE(G) = \sum_{i=1}^{n} |\rho_i|. \tag{5} \]

For details on the properties and bounds of \( RE \), see the recent works [1, 9, 10, 16, 17, 20, 21, 23].

The following upper bound on \( RE(G) \) was obtained in [17, 21]

\[ RE(G) \leq 1 + \sqrt{(n - 2)(2R_{-1} - 1) + (n - 1) |\text{det } R|^{2/(n-1)}}. \tag{6} \]

In the present paper, we find new lower and upper bounds on energy and Randić energy of non-singular (bipartite) graphs. We also show that our lower bounds are stronger than two previously known lower bounds given in [7, 9, 14, 17].

2. Lemmas

We now list some lemmas that will be needed for our main results.

**Lemma 2.1.** [5] Let \( x_i > -1 \) for \( 1 \leq i \leq n \). If \( \sum_{i=1}^{n} x_i = 0 \) and \( \sum_{i=1}^{n} x_i^2 \geq a^2 (1 - n^{-1}) \), then

\[ \sum_{i=1}^{n} \ln (1 + x_i) \leq \ln (1 + a - an^{-1}) + (n - 1) \ln (1 - an^{-1}). \]

**Lemma 2.2.** [6, 27] Let \( G \) be a graph with \( n \) vertices and maximum vertex degree \( \Delta \). Then, for each \( i = 1, 2, \ldots, n \)

\[ |\lambda_i| \leq \Delta. \]

**Lemma 2.3.** [10] Let \( G \) be a graph with \( n \) vertices and without isolated vertices. Then, for each \( i = 1, 2, \ldots, n \)

\[ \delta |\rho_i| \leq |\lambda_i| \leq \Delta |\rho_i|. \tag{7} \]

where \( \Delta \) and \( \delta \) denote, respectively, the maximum and minimum vertex degrees of \( G \).

**Lemma 2.4.** [10] Let \( G \) be a graph with \( n \) vertices and without isolated vertices and let \( \lambda_1 \) be its spectral radius. Then

\[ \delta (RE(G) - 1) \leq E(G) - \lambda_1 \leq \Delta (RE(G) - 1) \]

where \( \Delta \) and \( \delta \) denote, respectively, the maximum and minimum vertex degrees of \( G \).

**Lemma 2.5.** [6, 20] For a graph \( G \), the Randić spectral radius \( \rho_1 = 1 \).

**Lemma 2.6.** Let \( G \) be a bipartite graph with \( n \) vertices and without isolated vertices and let \( \lambda_1 \) be its spectral radius. Then

\[ \delta (RE(G) - 2) \leq E(G) - 2\lambda_1 \leq \Delta (RE(G) - 2) \]

where \( \Delta \) and \( \delta \) denote, respectively, the maximum and minimum vertex degrees of \( G \).

**Proof.** Note that \( \lambda_1 = -\lambda_n \) and \( \rho_1 = -\rho_n \), for bipartite graphs [6]. Then, by taking summation (7) over \( i = 2, 3, \ldots, n - 1 \) and considering Lemma 2.5 and Equations (2) and (5), one can get the required result. \( \square \)

**Lemma 2.7.** [16] Let \( G \) be a graph with \( n \) vertices, adjacency matrix \( A \) and Randić matrix \( R \). If \( A \) has \( n_+ \), \( n_0 \) and \( n_- \) positive, zero and negative eigenvalues, respectively \( (n_+ + n_0 + n_- = n) \), then \( R \) has \( n_+ \), \( n_0 \) and \( n_- \) positive, zero and negative eigenvalues, respectively.

For a graph \( G \) with \( n \) vertices, the following relation between the determinants of its adjacency and Randić matrices was also given in [16].

**Lemma 2.8.** [16] If \( G \) is a graph with isolated vertices, then \( \det R = \det A = 0 \). If \( G \) is a graph without isolated vertices, then

\[ \det R = \frac{\det A}{\prod_{i=1}^{n} d_i}. \]
3. Main results

**Theorem 3.1.** Let $G$ be a connected non-singular graph with $n \geq 2$ vertices and $m$ edges. Then

$$E(G) \geq n \left( \frac{|\text{det } A|}{(1 + (n - 1) b) (1 - b)^{n-1}} \right)^{1/n}$$

where

$$b = \left[ \frac{2mn - \left(2m(n-1) + n|\text{det } A|^{2/|r|} \right)}{(n-1) \left(2m(n-1) + n|\text{det } A|^{2/|r|} \right)} \right]^{1/2}.$$  

**Proof.** We first recall that $|\lambda_i| > 0$, $1 \leq i \leq n$, for a non-singular graph $G$. Let $r = \frac{E(G)}{n}$ and $x_i = \frac{|\lambda_i|}{r} - 1$, for $1 \leq i \leq n$. Observe that $x_i > -1$. By means of Equations (1)–(3), we also have

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} \left( \frac{|\lambda_i|}{r} - 1 \right) = \frac{\sum_{i=1}^{n} |\lambda_i|}{r} - n = 0$$

and

$$\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} \left( \frac{|\lambda_i|}{r} - 1 \right)^2 = \frac{\sum_{i=1}^{n} \lambda_i^2}{r^2} - 2 \sum_{i=1}^{n} \frac{|\lambda_i|}{r} + 2 n$$

$$\geq \frac{2mn^2}{(E(G))^2} - n$$

$$= \frac{2mn^2}{2m(n-1) + n|\text{det } A|^{2/|r|}} - n$$

$$= \left( \frac{2mn^3}{(n-1) \left(2m(n-1) + n|\text{det } A|^{2/|r|} \right)} - \frac{n^2}{n-1} + 1 \right) \left( 1 - \frac{1}{n} \right)$$

$$= \left( nb \right)^2 \left( 1 - \frac{1}{n} \right).$$

From Lemma 2.1, we get that

$$\sum_{i=1}^{n} \ln \left( \frac{|\lambda_i|}{r} \right) \leq \ln (1 + (n - 1) b) + (n-1) \ln (1 - b).$$

Hence,

$$\prod_{i=1}^{n} |\lambda_i| \leq r^n (1 + (n - 1) b) (1 - b)^{n-1}$$

that is,

$$|\text{det } A| \leq \left( \frac{E(G)}{n} \right)^n (1 + (n - 1) b) (1 - b)^{n-1}.$$  

This leads to the lower bound (8). \hfill \Box

For a non-singular graph $G$ of order $n$, the following lower bound on $E(G)$ was found in [7, 14]

$$E(G) \geq n \left( |\text{det } A| \right)^{1/n}.$$  

**Remark 3.1.** Let $b$ be given by Equation (9). Note that $0 \leq b < 1$, since $G$ is connected non-singular graph with $n \geq 2$ vertices and the fact that [11, 22]

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

Let

$$f(x) = (1 + (n - 1) x) (1 - x)^{n-1}.$$  

Note that $f$ is decreasing for $0 \leq x < 1$ [25]. Thus, $f(b) \leq f(0) = 1$, this implies that the lower bound (8) is stronger than the lower bound (10) for connected non-singular graphs. Further, if $G$ is the graph $K_2$, then the equality in (8) holds.
Theorem 3.2. Let $G$ be a connected non-singular graph with $n \geq 2$ vertices, $m$ edges and maximum vertex degree $\Delta$. Then

$$E(G) \leq \frac{2m}{n} + n - 1 + \Delta \ln \left( \frac{n|\det A|}{2m} \right).$$

(11)

The equality in (11) is achieved for $G \cong K_n$.

Proof. At first, recall that the following inequality

$$x \leq 1 + x \ln x,$$

for $x > 0 \ [24]$. Obviously, $|\lambda_i| > 0$, $1 \leq i \leq n$, for a non-singular graph $G$. Considering these facts with Equation (2), we have

$$E(G) = \lambda_1 + \sum_{i=2}^{n} |\lambda_i| \leq \lambda_1 + \sum_{i=2}^{n} (1 + |\lambda_i| \ln |\lambda_i|) \leq \lambda_1 + n - 1 + \Delta \sum_{i=2}^{n} \ln |\lambda_i|, \text{ by Lemma 2.2}$$

$$= \lambda_1 + n - 1 + \Delta \ln |\det A| - \Delta \ln \lambda_1.$$ 

(12)

Let us consider the function $f(x)$, defined by

$$f(x) = x - \Delta \ln x.$$ 

It is not difficult to see that $f$ is a decreasing function in the interval $1 \leq x \leq \Delta$. Notice that $\lambda_1 \geq \frac{2m}{n} [6]$ and $\frac{2m}{n}$ is the average of the vertex degrees that is inevitably greater than unity for connected (molecular) graphs [15]. These together with Lemma 2.2 imply that $1 \leq \frac{2m}{n} \leq \lambda_1 \leq \Delta$. Therefore, we have

$$f(\lambda_1) \leq f\left(\frac{2m}{n}\right) = \frac{2m}{n} - \Delta \ln \left(\frac{2m}{n}\right).$$

Based on this inequality and Equation (12), we obtain the upper bound in (11). Moreover, one can readily check that the equality in (11) is achieved for $G \cong K_n$. \qed

Theorem 3.3. Let $G$ be a connected non-singular bipartite graph with $n \geq 2$ vertices, $m$ edges and maximum vertex degree $\Delta$. Then

$$E(G) \leq \frac{4m}{n} + n - 2 + \Delta \ln \left( \frac{n^2|\det A|}{4m^2} \right).$$

(13)

Proof. Notice that $x \leq 1 + x \ln x$, for $x > 0 \ [24]$. Further, $|\lambda_i| > 0$, $1 \leq i \leq n$, for non-singular graphs and $\lambda_1 = -\lambda_n$, for bipartite graphs [6]. Taking into account these with Equation (2), we obtain

$$E(G) = 2\lambda_1 + \sum_{i=2}^{n-1} |\lambda_i| \leq 2\lambda_1 + \sum_{i=2}^{n-1} (1 + |\lambda_i| \ln |\lambda_i|) \leq 2\lambda_1 + n - 2 + \Delta \sum_{i=2}^{n-1} \ln |\lambda_i|, \text{ by Lemma 2.2}$$

$$= 2\lambda_1 + n - 2 + \Delta \ln |\det A| - \Delta \ln \lambda_1^2.$$ 

(14)

Let

$$f(x) = 2x - \Delta \ln x^2.$$ 

It can be readily seen that $f$ is a decreasing function in the interval $1 \leq x \leq \Delta$. Recall from Theorem 3.2 that both $\frac{2m}{n}$ and $\lambda_1$ belong to this interval and $\lambda_1 \geq \frac{2m}{n} [6]$. Thus,

$$f(\lambda_1) \leq f\left(\frac{2m}{n}\right) = \frac{4m}{n} - \Delta \ln \left( \frac{4m^2}{n^2} \right).$$

Combining this with Equation (14), we get the required result in (13). \qed
In the next theorem, we give a lower bound on Randić energy of non-singular graphs considering the similar techniques in Theorem 3.1 together with Equations (4)–(6) and Lemmas 2.1, 2.5 and 2.7. Therefore, its proof is omitted.

**Theorem 3.4.** Let $G$ be a connected non-singular graph with $n \geq 3$ vertices. Then

$$RE(G) \geq 1 + (n-1) \left( \frac{\det A}{\prod_{i=1}^{n} d_i} \right)^{1/(n-1)}$$ (15)

where

$$c = \left[ \frac{(n-1)(2R_{-1} - 1) - \left( (n-2)(2R_{-1} - 1) + (n-1)(\det R)^{2/(n-1)} \right)}{(n-2)(2R_{-1} - 1) + (n-1)(\det R)^{2/(n-1)}} \right]^{1/2}.\quad (16)$$

For a (connected) graph $G$ of order $n$, the authors derived that $[9,17]

$$RE(G) \geq 1 + (n-1)(\det R)^{1/(n-1)} = 1 + (n-1) \left( \frac{\det A}{\prod_{i=1}^{n} d_i} \right)^{1/(n-1)}.$$ (17)

**Remark 3.2.** Let $c$ be defined by Equation (16). Observe that $0 \leq c < 1$, since $G$ is connected non-singular graph with $n \geq 3$ vertices and the fact that $[17,20,21]$

$$RE(G) \leq 1 + \sqrt{(n-2)(2R_{-1} - 1) + (n-1)(\det R)^{2/(n-1)}}$$

Consider the function $f(x)$ defined as follows

$$f(x) = (1 + (n-2)x)(1-x)^{n-2}.$$ Notice that $f$ is decreasing for $0 \leq x < 1$ [26]. Then $f(c) \leq f(0) = 1$. Combining this with Lemma 2.8, we deduce that the lower bound (15) is stronger than the lower bound (17) for connected non-singular graphs. Furthermore, if $G$ is the complete graph $K_n$, then the equality in (15) is attained.

**Theorem 3.5.** Let $G$ be a connected non-singular graph with $n \geq 2$ vertices, $m$ edges, maximum vertex degree $\Delta$ and minimum vertex degree $\delta$. Then

$$RE(G) \leq 1 + \frac{n-1 + \Delta \ln \left( \frac{n^2(\det A)}{2m} \right)}{\delta}.$$ (18)

The equality in (18) is achieved for $G \cong K_n.$

**Proof.** According to Lemma 2.4 and Equation (12), we have

$$RE(G) \leq 1 + \frac{E(G) - \lambda_1}{\delta} \leq 1 + \frac{n-1 + \Delta (\ln |\det A| - \ln \lambda_1)}{\delta}.$$ From the above and the fact that $\lambda_1 \geq \frac{2m}{n}$ [6], we arrive at

$$RE(G) \leq 1 + \frac{n-1 + \Delta (\ln |\det A| - \ln \frac{2m}{n})}{\delta}.$$ Hence the upper bound in (18) holds. Moreover, it is elementary to check that the equality in (18) is achieved for $G \cong K_n.$

**Theorem 3.6.** Let $G$ be a connected non-singular bipartite graph with $n \geq 2$ vertices, $m$ edges, maximum vertex degree $\Delta$ and minimum vertex degree $\delta$. Then

$$RE(G) \leq 2 + \frac{n-2 + \Delta \ln \left( \frac{n^2(\det A)}{4m^2} \right)}{\delta}.$$ (19)

**Proof.** From Lemma 2.6 and Equation (14), we directly get

$$RE(G) \leq 2 + \frac{E(G) - 2\lambda_1}{\delta}.$$
\[ \leq 2 + \frac{n - 2 + \Delta \left( \ln |\text{det} A| - \ln \lambda_1^2 \right)}{\delta}. \]

Considering this with the lower bound \( \lambda_1 \geq \frac{2m}{n} \) [6], we obtain

\[ RE (G) \leq 2 + \frac{n - 2 + \Delta \left( \ln |\text{det} A| - \ln \frac{4m^2}{n^2} \right)}{\delta} \]

which is the upper bound in (19).

**Remark 3.3.** We finally note that the upper bounds in Equations (11), (13), (18) and (19) can be improved using a lower bound such that \( \lambda_1 \geq \gamma \geq \frac{2m}{n} \) in Theorems 3.2, 3.3, 3.5 and 3.6, respectively.

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