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Randić degree-based energy of graphs

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Abstract: Let $G = (V,E)$, $V = \{1,2,\ldots,n\}$, be a simple graph of order n and size m, without isolated vertices. Denote by $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(i)$, a sequence of its vertex degrees. If vertices i and j are adjacent, we write $i \sim j$. With TI we denote a topological index that can be represented as $TI = TI(G) = \sum_{i \sim j} F(d_i,d_j)$, where F is an appropriately chosen function with the property $F(x,y) = F(y,x)$. Randić degree–based adjacency matrix $RA = (r_{ij})$ is defined as $r_{ij} = \frac{F(d_i,d_j)}{\sqrt{d_i d_j}}$ if $i \sim j$, and 0 otherwise. Denote by f_i, $i = 1,2,\ldots,n$, the eigenvalues of RA. The Randić degree-based energy of graph could be defined as $RE_{TI} = RE_{TI}(G) = \sum_{i=1}^{n} |f_i|$. Upper and lower bounds for RE_{TI} are obtained.
Keywords: Topological indices, vertex degree, Randić degree-based energy (of graph)

1 Introduction

Let $G = (V,E)$, $V = \{1,2,\ldots,n\}$, be a simple graph of order n and size m, without isolated vertices. Denote by $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(i)$, a sequence of its vertex degrees. If vertices i and j are adjacent, we write $i \sim j$.

In chemistry, a variety of graph invariants, so-called ”topological indices”, is currently being considered (see [5]), that can be represented in the form

$$TI = TI(G) = \sum_{i \sim j} F(d_i,d_j)\,,$$

where F is an appropriately chosen function with the property $F(x,y) = F(y,x)$.

To each topological index TI, we can associate Randć vertex degree adjacency matrix $RA = (r_{ij})$, defined as

$$r_{ij} = \begin{cases} \frac{F(d_i,d_j)}{\sqrt{d_i d_j}}\,, & \text{if } i \sim j \\ 0\,, & \text{otherwise} \end{cases}$$

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Let $f_1 \geq f_2 \geq \cdots \geq f_n$ be the eigenvalues of the matrix RA, and $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_n$ the absolute values of eigenvalues f_i, $i = 1, 2, \ldots, n$ given in a decreasing order. It is elementary to show that

$$\mathrm{tr}(RA) = \sum_{i=1}^{n} f_i = 0\,, \tag{1}$$

and

$$\mathrm{tr}\big((RA)^2\big) = \sum_{i=1}^{n} f_i^2 = \sum_{i=1}^{n} \gamma_i^2 = 2\sum_{i\sim j} \frac{F(d_i,d_j)^2}{d_i d_j}\,, \tag{2}$$

where $\mathrm{tr}(RA)$ and $\mathrm{tr}((RA)^2)$ are traces of matrices RA and $(RA)^2$, respectively.

Randić degree-based energy, RE_{TI} can be defined as

$$RE_{TI} = RE_{TI}(G) = \sum_{i=1}^{n} |f_i| = \sum_{i=1}^{n} \gamma_i\,.$$

In what follows, we list some particular vertex-degree-based topological indices and the corresponding Randić degree-based energy of graph.

- For $F(d_i,d_j) = 1$, the Randić energy, $RE_{TI} = RE$, defined in [1, 2] is obtained.
- For $F(d_i,d_j) = \sqrt{d_i d_j}$, $TI = RR$ is the reciprocal Randić index [7]. In this case the ordinary energy $RE_{TI} = E$, defined in [6] is obtained.
- For $F(d_i,d_j) = d_i + d_j$, $TI = M_1$ is the first Zagreb index [8]. The corresponding Randić first Zagreb energy, $RE_{TI} = RZ_1E$ could be defined.
- For $F(d_i,d_j) = d_i d_j$, $TI = M_2$ is the second Zagreb index [9]. The corresponding Randić second Zagreb energy, $RE_{TI} = RZ_2E$ could be defined.

The general Randić index R_{-1} is defined as [16]

$$R_{-1} = R_{-1}(G) = \sum_{i\sim j} \frac{1}{d_i d_j}\,.$$

The symmetric division deg index, SDD is defined as [18]

$$SDD = SDD(G) = \sum_{i\sim j} \frac{d_i^2 + d_j^2}{2 d_i d_j}\,.$$

In this paper we are concerned with the lower and upper bounds for the Randić degree-based energy RE_{TI}.

2 Preliminaries

In this section, we recall some analytical inequalities for real number sequences which will be used subsequently.

Let $a = (a_i)$, $i = 1, 2, \ldots, n$ be a sequence of positive real numbers. Then, for any real r, $r \geq 1$ or $r \leq 0$, the Jensen's inequality (see e.g. [15]) is valid

$$n^{r-1} \sum_{i=1}^{n} a_i^r \geq \left(\sum_{i=1}^{n} a_i \right)^r . \tag{3}$$

If $0 \leq r \leq 1$, then the sense of (3) reverses.

Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \ldots, n$, are positive real numbers with the properties $p_1 + p_2 + \cdots + p_n = 1$ and $0 < a \leq a_i \leq A < +\infty$. The following inequality was proved in [17]

$$\sum_{i=1}^{n} p_i a_i + aA \sum_{i=1}^{n} \frac{p_i}{a_i} \leq a + A \tag{4}$$

3 Main result

In this section we determine upper and lower bounds for the Randić degree-based energy, RE_{TI}.

Theorem 3.1. *Let G be a simple graph of order $n \geq 2$, without isolated vertices. Then*

$$RE_{TI} \leq \sqrt{n \operatorname{tr}((RA)^2) - \frac{n}{2} (\gamma_1 - \gamma_n)^2} \tag{5}$$

with equality if and only if $\gamma_2 = \gamma_3 = \cdots = \gamma_{n-1} = \frac{\gamma_1 + \gamma_n}{2}$.

Proof. Based on the Lagrange's identity we have that

$$n \sum_{i=1}^{n} \gamma_i^2 - \left(\sum_{i=1}^{n} \gamma_i \right)^2 = \sum_{1 \leq i < j \leq n} (\gamma_i - \gamma_j)^2 \geq \sum_{i=2}^{n-1} ((\gamma_1 - \gamma_i)^2 + (\gamma_i - \gamma_n)^2) + (\gamma_1 - \gamma_n)^2 . \tag{6}$$

For $r = 2$, $n = 2$, $a_1 = \gamma_1 - \gamma_i$ and $a_2 = \gamma_i - \gamma_n$, according to (3) we have that

$$(\gamma_1 - \gamma_i)^2 + (\gamma_i - \gamma_n)^2 \geq \frac{1}{2} (\gamma_1 - \gamma_n)^2 . \tag{7}$$

From (6) and (7) we get

$$n \sum_{i=1}^{n} \gamma_i^2 - \left(\sum_{i=1}^{n} \gamma_i \right)^2 \geq \frac{1}{2} \sum_{i=2}^{n-1} (\gamma_1 - \gamma_n)^2 + (\gamma_1 - \gamma_n)^2 = \frac{n}{2} (\gamma_1 - \gamma_n)^2 ,$$

that is

$$n\,\mathrm{tr}((RA)^2) - \frac{n}{2}(\gamma_1 - \gamma_n)^2 \geq (RE_{TI})^2 .$$

From the above we arrive at (5).

Since equality in (6) holds if and only if $\gamma_1 = \gamma_2 = \cdots = \gamma_{n-1}$ and $\gamma_2 = \gamma_3 = \cdots = \gamma_n$, therefore equality in (5) holds if and only if $\gamma_2 = \gamma_3 = \cdots = \gamma_{n-1} = \frac{\gamma_1+\gamma_n}{2}$.

□

Remark 3.2. *For $F(d_i,d_j) = 1$, $F(d_i,d_j) = \sqrt{d_i d_j}$, $F(d_i,d_j) = d_i + d_j$ and $F(d_i,d_j) = d_i d_j$, from* (5)*, respectively, the following inequalities are obtained:*

$$RE \leq \sqrt{2nR_{-1} - \frac{n}{2}(\gamma_1 - \gamma_n)^2}\,, \tag{8}$$

$$E \leq \sqrt{2mn - \frac{n}{2}(\gamma_1 - \gamma_n)^2}\,, \tag{9}$$

$$RZ_1E \leq \sqrt{4n(SDD+m) - \frac{n}{2}(\gamma_1 - \gamma_n)^2}\,,$$

$$RZ_2E \leq \sqrt{2nM_2 - \frac{n}{2}(\gamma_1 - \gamma_n)^2}\,.$$

The inequality (8) *was proved in [12], whereas* (9) *in [13].*

Since $(\gamma_1 - \gamma_n)^2 \geq 0$, we have the following corollary of Theorem 3.1.

Corollary 3.3. *Let G be a simple graph of order $n \geq 2$, without isolated vertices. Then*

$$RE_{TI} \leq \sqrt{n\,\mathrm{tr}((RA)^2)}\,, \tag{10}$$

with equality if and only if $\gamma_1 = \gamma_2 = \cdots = \gamma_n$.

Remark 3.4. *For $F(d_i,d_j) = 1$, $F(d_i,d_j) = \sqrt{d_i d_j}$, $F(d_i,d_j) = d_i + d_j$ and $F(d_i,d_j) = d_i d_j$, from* (10)*, respectively, the following inequalities are obtained:*

$$RE \leq \sqrt{2nR_{-1}}\,, \tag{11}$$

$$E \leq \sqrt{2mn}\,, \tag{12}$$

$$RZ_1E \leq 2\sqrt{n(SDD+m)}\,,$$

$$RZ_2E \leq \sqrt{2nM_2}\,.$$

The inequality (11) *was proven in [2], and* (12) *in [11].*

Theorem 3.5. *Let G be a simple, non-empty graph, of order $n \geq 2$, without isolated vertices. Then*

$$RE_{TI} \geq \frac{\mathrm{tr}((RA)^2) + \gamma_1 \gamma_n}{\gamma_1 + \gamma_n}, \tag{13}$$

with equality if and only if $\gamma_i = \gamma_1$ or $\gamma_i = \gamma_n$, for $i = 1, 2, \ldots, n$.

Proof. For $p_i = \frac{\gamma_i}{RE_{TI}}$, $a_i = \gamma_i$, $a = \gamma_n$, $A = \gamma_1$, $i = 1, 2, \ldots, n$, the inequality (4) transforms into

$$\frac{\sum_{i=1}^{n} \gamma_i^2}{RE_{TI}} + \frac{\gamma_1 \gamma_n \sum_{i=1}^{n} 1}{RE_{TI}} \leq \gamma_1 + \gamma_n,$$

that is

$$\mathrm{tr}((RA)^2) + n\gamma_1 \gamma_n \leq (\gamma_1 + \gamma_n) RE_{TI},$$

wherefrom we obtain (13). □

Remark 3.6. *For $F(d_i, d_j) = 1$, $F(d_i, d_j) = \sqrt{d_i d_j}$, $F(d_i, d_j) = d_i + d_j$ and $F(d_i, d_j) = d_i d_j$, from (13), respectively, the following inequalities are obtained:*

$$\begin{aligned} RE &\geq \frac{2R_{-1} + n\gamma_1 \gamma_n}{\gamma_1 + \gamma_n}, \\ E &\geq \frac{2m + n\gamma_1 \gamma_n}{\gamma_1 + \gamma_n}, \\ RZ_1E &\geq \frac{4(SDD + m) + n\gamma_1 \gamma_n}{\gamma_1 + \gamma_n} \\ RZ_2E &\geq \frac{2M_2 + n\gamma_1 \gamma_n}{\gamma_1 + \gamma_n} \end{aligned} \tag{14}$$

The inequality (14) was proved in [14].

Theorem 3.7. *Let G be a simple non-singular graph with $n \geq 2$ vertices. Then*

$$RE_{TI} \geq \frac{2\mathrm{tr}((RA)^2)}{f_i - f_n}. \tag{15}$$

Equality holds if and only if $f_1 = f_2 = \cdots = f_p = -f_{p+1} = \cdots = -f_n$, $(n = 2p)$.

Proof. According to the inequality (4) we have that

$$\begin{aligned} \mathrm{tr}((RA)^2) = \sum_{i=1}^{n} \gamma_i^2 = \sum_{i=1}^{n} f_i^2 = \frac{1}{2} \left| \sum_{i=1}^{n} \left(2f_i - f_1 - f_n\right) f_i \right| \leq \\ \leq \frac{1}{2} \sum_{i=1}^{n} \left(|2f_i - f_1 - f_n| \, |f_i| \right). \end{aligned} \tag{16}$$

Since $f_1 \geq f_i \geq f_n$, for $i = 1, 2, \ldots, n$,

$$-(f_1 - f_n) \leq 2f_i - f_1 - f_n \leq f_1 - f_n\,,$$

that is

$$|2f_i - f_1 - f_n| \leq f_1 - f_n\,. \tag{17}$$

Now, based on (16) and (17) we get

$$\operatorname{tr}((RA)^2) \leq \frac{1}{2}(f_1 - f_n) RE_{TI}\,,$$

which gives the required result (15). □

Remark 3.8. *For $F(d_i, d_j) = 1$, $F(d_i, d_j) = \sqrt{d_i d_j}$, $F(d_i, d_j) = d_i + d_j$ and $F(d_i, d_j) = d_i d_j$, from* (15)*, respectively, the following inequalities are obtained:*

$$RE \geq \frac{4R_{-1}}{f_1 - f_n}\,, \tag{18}$$

$$E \geq \frac{4m}{f_1 - f_n}\,,$$

$$RZ_1E \geq \frac{8(SDD + m)}{f_1 - f_n}\,,$$

$$RZ_2E \geq \frac{4M_2}{f_1 - f_n}\,.$$

The inequality (18) *was proven in [4]. Since, in this case, $f_1 - f_n \leq 2$, this inequality is stronger then*

$$RE \geq 2R_{-1}\,,$$

which was proved in [3].

Theorem 3.9. *Let G be a simple non-empty graph with $n \geq 2$ vertices. Then*

$$RE_{TI} \geq \sqrt{2\operatorname{tr}((RA)^2)}\,, \tag{19}$$

with equality if and only if $f_1 = -f_n$, $f_2 = f_3 = \cdots = f_{n-1} = 0$.

Proof. Bearing in mind the inequality (1), we have that

$$0 = \left(\sum_{i=1}^{n} f_i\right)^2 = \sum_{i=1}^{n} f_i^2 + 2\sum_{i<j} f_i f_j\,.$$

Accordingly

$$\sum_{i=1}^{n} f_i^2 = -2\sum_{i<j} f_i f_j\,,$$

that is

$$\sum_{i=1}^{n} f_i^2 = 2\left|\sum_{i<j} f_i f_j\right|.$$

Now, we have that

$$\begin{aligned}(RE_{TI})^2 \quad &= \left(\sum_{i=1}^{n} |f_i|\right)^2 = \sum_{i=1}^{n} |f_i|^2 + 2\sum_{i<j} |f_i|\,|f_j| \geq \\ &\geq \sum_{i=1}^{n} |f_i|^2 + 2\left|\sum_{i<j} f_i f_j\right| = 2\sum_{i=1}^{n} |f_i|^2 = 2\mathrm{tr}((RA)^2)\,.\end{aligned}$$

which gives the required result in (19). □

Remark 3.10. *For $F(d_i,d_j) = 1$, from* (19) *we obtain*

$$E \geq 2\sqrt{m}\,,$$

which was proved in [10].

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