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 Randić 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

\[
\text{tr}(RA) = \sum_{i=1}^{n} f_i = 0, \tag{1}
\]

and

\[
\text{tr}((RA)^2) = \sum_{i=1}^{n} f_i^2 = \sum_{i=1}^{n} \gamma_i^2 = 2 \sum_{i<j} \frac{F(d_i,d_j)^2}{d_id_j}, \tag{2}
\]

where \( \text{tr}(RA) \) and \( \text{tr}((RA)^2) \) 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 \( F(d_i,d_j) = \sqrt{d_id_j} \), \( TI = RR \) 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 \( F(d_i,d_j) = d_id_j \), \( TI = M_2 \) 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]

\[
R_{-1} = R_{-1}(G) = \sum_{i<j} \frac{1}{d_id_j}.
\]

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

\[
SDD = SDD(G) = \sum_{i<j} \frac{d_i^2 + d_j^2}{2d_id_j}.
\]

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

\[
n^{r-1} \sum_{i=1}^{n} a_i^r \geq \left( \sum_{i=1}^{n} a_i \right)^r.
\]

(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

\[
p_1 + p_2 + \cdots + p_n = 1 \quad \text{and} \quad 0 < a_i \leq A < +\infty.
\]

The following inequality was proved in [17]

\[
\sum_{i=1}^{n} p_i a_i + aA \sum_{i=1}^{n} \frac{p_i}{a_i} \leq a + A
\]

(4)

3 Main result

In this section we determine upper and lower bounds for the Randić degree-based energy, \( \text{RE}_{T1} \).

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

\[
\text{RE}_{T1} \leq \sqrt{n \text{tr} \left( (RA)^2 - \frac{n}{2} (\gamma_1 - \gamma_n)^2 \right)}
\]

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

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

(6)

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

\[
(\gamma_1 - \gamma)^2 + (\gamma - \gamma_n)^2 \geq \frac{1}{2} (\gamma_1 - \gamma_n)^2.
\]

(7)

From (6) and (7) we get

\[
n \sum_{i=1}^{n} \gamma_i^2 - \left( \sum_{i=1}^{n} \gamma_i \right)^2 \geq \frac{1}{2} \sum_{i=2}^{n-1} (\gamma_i - \gamma_1)^2 + (\gamma_i - \gamma_n)^2 = \frac{n}{2} (\gamma_1 - \gamma_n)^2.
\]
that is
\[ n \text{tr}((RA)^2) - \frac{n}{2} (\gamma_1 - \gamma_0)^2 \geq (RE_{TI})^2. \]

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 \( \gamma_2 = \gamma_3 = \cdots = \gamma_{n-1} = \frac{n+\gamma_0}{2} \).

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

\[
\begin{align*}
RE & \leq \sqrt{2nR_{-1} - \frac{n}{2} (\gamma_1 - \gamma_0)^2}, \\
E & \leq \sqrt{2mn - \frac{n}{2} (\gamma_1 - \gamma_0)^2}, \\
RZ_1E & \leq \sqrt{4n(SDD + m) - \frac{n}{2} (\gamma_1 - \gamma_0)^2}, \\
RZ_2E & \leq \sqrt{2nM_2 - \frac{n}{2} (\gamma_1 - \gamma_0)^2}.
\end{align*}
\]

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

Since \( (\gamma_1 - \gamma_0)^2 \geq 0 \), 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

\[ RE_{TI} \leq \sqrt{n \text{tr}((RA)^2)}, \quad (10) \]

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

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

\[
\begin{align*}
RE & \leq \sqrt{2nR_{-1}}, \\
E & \leq \sqrt{2mn}, \\
RZ_1E & \leq 2 \sqrt{n(SDD + m)}, \\
RZ_2E & \leq \sqrt{2nM_2}.
\end{align*}
\]

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
\[
RT_{TI} \geq \frac{\text{tr}((RA)^2) + \gamma_1 \gamma_n}{\gamma_1 + \gamma_n},
\]  
(13)
with equality if and only if $\gamma_i = \gamma_1$ or $\gamma_i = \gamma_n$, for $i = 1, 2, \ldots, n$.

Proof. For $p_i = \frac{\gamma_i}{RT_{TI}}$, $a_i = \gamma_i$, $A = \gamma_1$, $i = 1, 2, \ldots, n$, the inequality (4) transforms into
\[
\sum_{i=1}^{n} \gamma_i^2 \frac{\gamma_1 \gamma_n}{RT_{TI}} + \frac{n \gamma_1 \gamma_n}{RT_{TI}} \leq \gamma_1 + \gamma_n,
\]
that is
\[
\text{tr}((RA)^2) + n \gamma_1 \gamma_n \leq (\gamma_1 + \gamma_n)RT_{TI},
\]
wherefrom we obtain (13).

Remark 3.6. For $F(d_i, d_j) = 1, F(d_i, d_j) = \sqrt{d_id_j}, F(d_i, d_j) = d_i + d_j$ and $F(d_i, d_j) = d_id_j$, from (13), respectively, the following inequalities are obtained:
\[
\begin{align*}
RE & \geq \frac{2R - 1 + n \gamma_1 \gamma_n}{\gamma_1 + \gamma_n}, \\
E & \geq \frac{2m + n \gamma_1 \gamma_n}{\gamma_1 + \gamma_n}, \\
RZ_1E & \geq \frac{4(SDD + m) + n \gamma_1 \gamma_n}{\gamma_1 + \gamma_n}, \\
RZ_2E & \geq \frac{2M_2 + n \gamma_1 \gamma_n}{\gamma_1 + \gamma_n}
\end{align*}
\]
(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
\[
RT_{TI} \geq \frac{2\text{tr}((RA)^2)}{f_1 - f_n}.
\]
(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
\[
\text{tr}((RA)^2) = \sum_{i=1}^{n} \gamma_i^2 = \sum_{i=1}^{n} f_i^2 = \frac{1}{2} \left| \sum_{i=1}^{n} (2f_i - f_1 - f_n) f_i \right| \leq \frac{1}{2} \sum_{i=1}^{n} (|2f_i - f_1 - f_n| |f_i|).
\]
(16)
Since $f_i \geq f_i \geq f_n$, for $i = 1, 2, \ldots, n$,

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

that is

$$|2f_i - f_1 - f_n| \leq f_1 - f_n.$$  \hspace{1cm} (17)

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

$$\text{tr}((RA)^2) \leq \frac{1}{2} (f_1 - f_n) R_{ETI},$$

which gives the required result (15). \hfill \Box

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

\begin{align*}
RE & \geq \frac{4R_{-1}}{f_1 - f_n}, \\
E & \geq \frac{4R_{2}}{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}.
\end{align*}

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

$$R_{ETI} \geq \sqrt{2\text{tr}((RA)^2)},$$

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

$$0 = \left( \sum_{i=1}^{n} f_i \right)^2 = \sum_{i=1}^{n} f_i^2 + 2 \sum_{i<j} f_if_j.$$
Accordingly
\[ \sum_{i=1}^{n} f_i^2 = -2 \sum_{i<j} f_if_j, \]
that is
\[ \sum_{i=1}^{n} f_i^2 = 2 \left| \sum_{i<j} f_if_j \right|. \]
Now, we have that
\[ (RE_{T1})^2 = \left( \sum_{i=1}^{n} |f_i| \right)^2 = \sum_{i=1}^{n} |f_i|^2 + 2 \sum_{i<j} |f_i||f_j| \geq \]
\[ \geq \sum_{i=1}^{n} |f_i|^2 + 2 \left| \sum_{i<j} f_if_j \right| = 2 \sum_{i=1}^{n} |f_i|^2 = 2tr((RA)^2). \]
which gives the required result in (19).

\[ \square \]

**Remark 3.10.** For \( F(d_i,d_j) = 1 \), from (19) we obtain
\[ E \geq 2\sqrt{m}, \]
which was proved in [10].

**References**


