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Improvement of some bounds for the Randić Estrada index of graphs

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Abstract: Let G be a graph with n vertices and m edges, and let $\rho_1, \rho_2, \ldots, \rho_n$ be the eigenvalues of the Randić matrix. The Randić Estrada index of G is $REE(G) = \sum_{i=1}^{n} e^{\rho_i}$. In this paper, we establish bounds for the Randić Estrada index in terms of graph invariants such as the number of vertices and some Randić eigenvalues of graphs and improve some previously published lower bounds.

Keywords: Randić eigenvalues of a graph, Estrada index, Randić Estrada index, bounds, graph invariants

1 Introduction

Let G be a simple undirected graph with n vertices and m edges. Its vertex and edge sets are $V(G)$ and $E(G)$, respectively. We denote the complete graph on n vertices by K_n, the complete bipartite graph whose parts are of orders m, n by $K_{n,m}$.

The adjacency matrix $A(G)$ is defined by its entries as $a_{ij} = 1$ if $v_i v_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ denote the eigenvalues of $A(G)$. λ_1 is called the spectral radius of the graph G. The graph invariant EE defined by

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

was introduced by Estrada [6] in 2000, and it is called the Estrada index. This index was first used to quantify the degree of folding of a protein. It has also been used to measure the centrality of complex networks. The applications of the Estrada index in quantum chemistry [8], and in information theory [4] can also be found in the literature. In addition to this, in [8] a connection between EE and the concept of extended atomic branching was considered. An employment of the Estrada index in statistical thermodynamics has also been reported

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[7]. The mathematical properties of the Estrada index were studied in several recent works [9, 16, 11, 17, 18].
For any graph G of order n, the Randić matrix of G, $R = (r_{ij})$, is defined in [3] as follows:

$$r_{ij} = \begin{cases} \frac{1}{\sqrt{d_i \times d_j}} & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent} \\ 0 & \text{otherwise.} \end{cases}$$

The Randić eigenvalues $\rho_1, \rho_2, \ldots, \rho_n$ of the graph G are the eigenvalues of its Randić matrix. Since R is a real symmetric matrix, its eigenvalues are real numbers. Therefore, we can order them so that $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$.
The Randić Estrada index of the graph G is defined in [2] as following:

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

For some reason, this index has largely escaped the attention of researchers. Consequently, only limited results concerning this index are available (see [12, 15]).

Recall that the general Randić index of a graph G is defined in [1] as:

$$R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha.$$

The general Randić index when $\alpha = -1$ is simply the Randić index:

$$R_{-1} = R_{-1}(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

2 Preliminaries and known results

Here, we list some previously known results that will be needed in the next section.
In order to obtain bounds for the Randić Estrada index of G, we need some inequalities and lemmas.

Lemma 1. *[13] Let $a_1, a_2, ..., a_n \geq 0$ and $p_1, p_2, ..., p_n \geq 0$ such that $\sum_{i=1}^{n} p_i = 1$. Then*

$$\sum_{i=1}^{n} p_i a_i - \prod_{i=1}^{n} a_i^{p_i} \geq n\Upsilon \left(\frac{1}{n} \sum_{i=1}^{n} a_i - \prod_{i=1}^{n} a_i^{\frac{1}{n}} \right).$$

where $\Upsilon = \min\{p_1, \ldots, p_n\}$. Equality holds if and only if $a_1 = \cdots = a_n$.

Lemma 2. *[19] Let $a_1, a_2, ..., a_n > 0$. Then*

$$n \left(\frac{1}{n} \sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i \right)^{\frac{1}{n}} \right) \leq \Phi \leq n(n-1) \left(\frac{1}{n} \sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i \right)^{\frac{1}{n}} \right),$$

where $\Phi = n \sum_{i=1}^{n} a_i - \left(\sum_{i=1}^{n} \sqrt{a_i} \right)^2$.

Lemma 3. *[14] The Randić spectral radius* $\rho_1(G) = 1$.

Lemma 4. *For any real x,* $e^x \geqslant 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{4!} + \frac{x^5}{5!}$. *Equality holds if and only if* $x = 0$.

Proof. Applying Taylor theorem, for any $x \neq 0$, there is a real $\alpha \neq 0$ between x and 0 such that $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \frac{x^5}{5!} + \frac{\alpha^6}{6!}$. This proves the lemma. □

Let tr denotes the trace of a Randić matrix and $\rho_1, \rho_2, ..., \rho_n$ be the eigenvalues of the Randić matrix $R(G)$, recall that

$$N_k = tr(R^k) = \sum_{i=1}^{n} \rho_i^k$$

where N_k denotes the number of self-returning walks of length k [5], then

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

Lemma 5. *[12] Let G be a graph of order n and Randić matrix R. Then*

$$tr(R) = 0, \tag{1}$$

$$tr(R^2) = 2 \sum_{uv \in E(G)} \frac{1}{d_u d_v}, \tag{2}$$

$$tr(R^3) = 2 \sum_{uv \in E(G)} \frac{1}{d_u d_v} \sum_{\substack{z \in V(G) \\ z \sim u, z \sim v}} \frac{1}{d_z}, \tag{3}$$

$$tr(R^4) = \sum_{u \in V(G)} \left(\sum_{\substack{v \in V(G) \\ u \sim v}} \frac{1}{d_u d_v} \right)^2 + \sum_{\substack{u,v \in V(G) \\ u \neq v}} \frac{1}{d_u d_v} \left(\sum_{\substack{z \in V(G) \\ z \sim u, z \sim v}} \frac{1}{d_z} \right)^2. \tag{4}$$

Now, we obtain a lower bound for $tr(R^4)$.

Theorem 1. *Let G be a graph with minimum degree* δ *and maximum degree* Δ. *Then*

$$tr(R^4) \geq \frac{2\delta}{\Delta^3} R(G) + \frac{M_1(G) - 2m}{\Delta^4},$$

where $M_1(G)$ *is the first Zagreb index [10].*

Proof. Denote by CP_3 the cardinality of the set of paths of length 2 in G that are not cycles. For any fixed $z \in V(G)$, the set of paths of length 2 that are not cycles and have z as central vertex has cardinality $\frac{1}{2}z(z-1)$. Hence,

$$CP_3 = \sum_{z \in V(G)} \frac{1}{2} z(z-1) = \frac{1}{2} M_1(G) - m.$$

$$\sum_{\substack{u,v\in V(G)\\u\neq v}}\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1=2CP_3=M_1(G)-2m.$$

Note that if $N(u)\cap N(v)=\emptyset$, then

$$0=\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)=\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)=0$$

and otherwise

$$\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)=\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)|N(u)\cap N(v)|\geq\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right).$$

Hence, we have in both cases

$$\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)\geq\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1.$$

Therefore, by definitions, we have

$$\begin{aligned}\sum_{\substack{u,v\in V(G)\\u\neq v}}\frac{1}{d_ud_v}\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}\frac{1}{d_z}\right)^2&=\sum_{\substack{u,v\in V(G)\\u\neq v}}\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}\frac{1}{\sqrt{d_ud_z}\sqrt{d_vd_z}}\right)^2\\&\geq\frac{1}{\Delta^4}\sum_{\substack{u,v\in V(G)\\u\neq v}}\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)\\&\geq\frac{1}{\Delta^4}\sum_{\substack{u,v\in V(G)\\u\neq v}}\left(\sum_{\substack{z\in V(G)\\z\sim u,z\sim v}}1\right)\\&=\frac{M_1(G)-2m}{\Delta^4}.\end{aligned}\tag{5}$$

By Lemma 5 and Equality (5), we have

$$
\begin{aligned}
tr(R^4) &= \sum_{u\in V(G)} \left(\sum_{\substack{v\in V(G)\\ u\sim v}} \frac{1}{d_u d_v} \right)^2 + \sum_{\substack{u,v\in V(G)\\ u\neq v}} \frac{1}{d_u d_v} \left(\sum_{\substack{z\in V(G)\\ z\sim u, z\sim v}} \frac{1}{d_z} \right)^2 \\
&\geq \sum_{u\in V(G)} \left(\frac{1}{\sqrt{d_u d_v}} \sum_{\substack{v\in V(G)\\ u\sim v}} \frac{1}{\sqrt{d_u d_v}} \right)^2 + \frac{M_1(G)-2m}{\Delta^4} \\
&\geq \sum_{i=1}^{n} \left(\frac{1}{\Delta} \sum_{\substack{v\in V(G)\\ u\sim v}} \frac{1}{\sqrt{d_u d_v}} \right)^2 + \frac{M_1(G)-2m}{\Delta^4} \\
&\geq \frac{1}{\Delta^2} \sum_{u\in V(G)} \left(\sum_{\substack{v\in V(G)\\ u\sim v}} \frac{1}{\sqrt{d_u d_v}} \right)^2 + \frac{M_1(G)-2m}{\Delta^4} \\
&\geq \frac{1}{\Delta^2} \sum_{u\in V(G)} \left(\sum_{\substack{v\in V(G)\\ u\sim v}} \frac{1}{\sqrt{d_u d_v}} \right) \left(\sum_{\substack{v\in V(G)\\ u\sim v}} \frac{1}{\Delta} \right) + \\
&\geq \frac{1}{\Delta^3} \sum_{u\in V(G)} \sum_{\substack{v\in V(G)\\ u\sim v}} \frac{1}{\sqrt{d_u d_v}} d_u + \frac{M_1(G)-2m}{\Delta^4} \\
&\geq \frac{1}{\Delta^3}\, 2 \sum_{u,v\in E(G)} \frac{1}{\sqrt{d_u d_v}} \delta + \frac{M_1(G)-2m}{\Delta^4} \\
&= \frac{2\delta}{\Delta^3} R(G) + \frac{M_1(G)-2m}{\Delta^4}.
\end{aligned}
$$

□

For a sequence x of positive numbers defined as above, denoted by

$$A_n(x) := \frac{1}{n}\sum_{i=1}^{n} x_i, \ \ G_n(x) := \left(\prod_{i=1}^{n} x_i \right)^{\frac{1}{n}}$$

its arithmetic and geometric mean, respectively.

Theorem 2. *[20] Let $A_n(x)$ and $G_n(x)$ be the arithmetic and the geometric mean, respectively. Then*

$$A_n(x) - G_n(x) \geq \frac{1}{n} \left(\sqrt{b} - \sqrt{a} \right)^2$$

where $a = x_1 \leq x_2 \leq \cdots \leq x_n = b$.

3 Bounds for the Randić Estrada index

In this section, we establish some lower bounds for the Randić Estrada index in terms of graph invariants such as the number of vertices and eigenvalue of graphs.

We begin some previously published lower bounds for the Randić Estrada index.

Theorem 3. *[12] Let G be a connected graph of order n. Then*

$$REE(G) \geq e + \frac{n-1}{e^{\frac{1}{n-1}}},$$

the equality holds if and only if G is a complete graph.

Theorem 4. *[12] Let G be a connected bipartite graph of order n. Then*

$$REE(G) \geq e + \frac{1}{e},$$

the equality holds if and only if G is a complete bipartite graph.

Theorem 5. *[12] Let G be a connected bipartite graph with n vertices. Then*

$$REE(G) \geq e + \frac{1}{e} + \sqrt{(n-2)^2 + \frac{2(n-2\Delta)}{\Delta}},$$

the equality holds if and only if G is a complete bipartite regular graph.

Theorem 6. *[12] Let G be a graph of order n with maximum degree Δ. Then*

$$REE(G) \geq e + \sqrt{(n-1)\left(1 + \frac{n-2}{e^{\frac{2}{n-1}}}\right) + 2\left(\frac{2n}{\Delta} - 3\right)},$$

the equality holds if and only if G is a complete bipartite regular graph.

Now we present a lower bound for Randić Estrada index and this bound improves the bound in Theorem 4 for $n \geq 3$.

Theorem 7. *Let G be a connected non-empty graph of order n. Then*

$$REE(G) > e + (n-2).$$

Proof. Consider the following function $f_1(x) = (x-1) - \ln(x), x > 0$ that is is decreasing in $(0,1]$ and increasing in $[1,+1)$. Hence, $f(x) \geq f(1) = 0$, implying that

$$x \geq 1 + \ln x, x > 0, \tag{6}$$

the equality holds if and only if $x = 1$. By the definition of Randić Estrada index and Inequality (6), we get:

$$\begin{aligned} REE(G) \geq & e^{\rho_1} + (n-1) + \sum_{i=2}^{n} \ln e^{\rho_i} \\ & = e^{\rho_1} + (n-1) + \sum_{i=2}^{n} \rho_i \\ & = e^{\rho_1} + (n-1) + \sum_{i=1}^{n} \rho_i - \rho_1 \\ & = e^{\rho_1} + (n-1) - \rho_1. \end{aligned}$$

Define the function

$$g(x) = e^x + (n-1) - x. \tag{7}$$

Note that, this is a strictly increasing function on $D_g = [1, +\infty)$. Using Lemma 3 and Equality (7), the proof is complete. □

If G is bipartite, the property of R-eigenvalues of G is similar to that of A-eigenvalues of G, hence $\rho_1 = -\rho_n$.
In the following result, we obtain a sharp lower bound of the Randić Estrada index for a bipartite graph and improve bound in Theorem 4.

Theorem 8. *Let G be a connected bipartite graph of order n. Then*

$$REE(G) \geq e + \frac{1}{e} + (n-2). \tag{8}$$

Equality holds if and only if $G \cong K_{n,m}$.

Proof. Recall that for a bipartite graph $\rho_1 = -\rho_n$. By the definition of Randić Estrada index and Inequality (6), we have

$$\begin{aligned} REE(G) &= e^{\rho_1} + e^{-\rho_1} + \sum_{i=2}^{n-1} e^{\rho_i} \\ &\geq 2\cosh\rho_1 + (n-2) + \sum_{i=2}^{n-1} \rho_i \qquad (9) \\ &= 2\cosh\rho_1 + (n-2) + \sum_{i=1}^{n} \rho_i + \rho_1 - \rho_1 \\ &= 2\cosh\rho_1 + (n-2). \end{aligned}$$

Since,

$$f(x) = 2\cosh x + (n-2)$$

is an increasing function on $D_f = [0, +\infty)$, hence we get the result.

Suppose that the equality holds in (8). Then all the inequalities in the proof must be equalities. From the equality in (9) we have $\sum_{i=2}^{n-1} e^{\rho_i} = (n-2) + \sum_{i=2}^{n-1} \rho_i$, that is $\rho_2 = \rho_3 = \cdots = \rho_{n-1} = 0$. Note that $\sum_{i=1}^{n} \rho_i = 0$, since G is a connected bipartite graph, we have $\rho_1 = -\rho_n \neq 0$. Applying Lemma 3, we have $\rho_1 = 1$ and $\rho_n = -1$. Therefore, G is a complete bipartite graph.

Conversely, if $G \cong K_{n,m}$, then it is easy to check that the equality holds in (8). $\square$

Now by Lemmas 4 and 5 we will present a lower bound for Randić Estrada index of graphs.

Theorem 9. *Let G be a graph of order n. Then*

$$REE(G) \geqslant \sqrt{n^2 + nN_2 + \frac{nN_3}{3} + \frac{nN_4}{12} + \frac{nN_5}{60} + \frac{N_2N_3}{6} + \frac{N_2^2}{4}}.$$

Equality holds if and only if $G \cong \overline{K}_n$.

Proof. Suppose that $\rho_1, \rho_2, \ldots, \rho_n$ is the spectrum of G. Using Lemma 4 we have

$$\begin{aligned}
EE(G)^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n} e^{\rho_i+\rho_j} \\
&\geqslant \sum_{i=1}^{n}\sum_{j=1}^{n} \left(1 + \rho_i + \rho_j + \frac{(\rho_i+\rho_j)^2}{2} + \frac{(\rho_i+\rho_j)^3}{6} + \frac{(\rho_i+\rho_j)^4}{24} + \frac{(\rho_i+\rho_j)^5}{120}\right) \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} \left(1 + \rho_i + \rho_j + \frac{\rho_i^2}{2} + \frac{\rho_j^2}{2} + \rho_i\rho_j + \frac{\rho_i^3}{6} + \frac{\rho_j^3}{6} + \frac{\rho_i^2\rho_j}{2} + \frac{\rho_i\rho_j^2}{2} + \frac{\rho_i^4}{24} + \frac{\rho_j^4}{24} \right. \\
&\left. + \frac{\rho_i^2\rho_j^2}{4} + \frac{\rho_i^3\rho_j}{6} + \frac{\rho_i\rho_j^3}{6} + \frac{\rho_i^5}{120} + \frac{\rho_j^5}{120} + \frac{\rho_i^4\rho_j}{24} + \frac{\rho_i\rho_j^4}{24} + \frac{\rho_i^3\rho_j^2}{12} + \frac{\rho_i^2\rho_j^3}{12}\right).
\end{aligned}$$

By Equalities (1)-(4), we have the following equations:

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\rho_i+\rho_j)=n\sum_{i=1}^{n}\rho_i+n\sum_{j=1}^{n}\rho_j=0.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\rho_i\rho_j=(\sum_{i=1}^{n}\rho_i)^2=0.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\frac{\rho_i^2}{2}+\frac{\rho_j^2}{2})=\frac{n}{2}\sum_{i=1}^{n}\rho_i^2+\frac{n}{2}\sum_{j=1}^{n}\rho_j^2=nN_2.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\frac{\rho_i^3}{6}+\frac{\rho_j^3}{6})=\frac{n}{6}\sum_{i=1}^{n}\rho_i^3+\frac{n}{6}\sum_{j=1}^{n}\rho_j^3=\frac{nN_3}{3}.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\frac{\rho_i^4}{24}+\frac{\rho_j^4}{24})=\frac{n}{24}\sum_{i=1}^{n}\rho_i^4+\frac{n}{24}\sum_{j=1}^{n}\rho_j^4=\frac{nN_4}{12}.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\frac{\rho_i^5}{120}+\frac{\rho_j^5}{120})=\frac{n}{120}\sum_{i=1}^{n}\rho_i^5+\frac{n}{120}\sum_{j=1}^{n}\rho_j^5=\frac{nN_5}{60}.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{\rho_i^2\rho_j^3}{12}+\frac{\rho_i^3\rho_j^2}{12}\right)=\frac{1}{12}\sum_{i=1}^{n}\sum_{j=1}^{n}\rho_i^2\rho_j^3+\frac{1}{12}\sum_{i=1}^{n}\sum_{j=1}^{n}\rho_i^3\rho_j^2=\frac{N_2N_3}{6}.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\rho_i^4\rho_j}{24}=\frac{1}{24}\sum_{i=1}^{n}\rho_i^4\sum_{j=1}^{n}\rho_j=0.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\rho_i\rho_j^4}{24}=\frac{1}{24}\sum_{i=1}^{n}\rho_i\sum_{j=1}^{n}\rho_j^4=0.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\rho_i^2\rho_j^2}{4}=\frac{1}{4}\sum_{i=1}^{n}\rho_i^2\sum_{j=1}^{n}\rho_j^2=\frac{N_2^2}{4}.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\rho_i\rho_j^3}{6}=\frac{1}{6}\sum_{i=1}^{n}\rho_i\sum_{j=1}^{n}\rho_j^3=0.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\rho_i^3\rho_j}{6}=\frac{1}{6}\sum_{i=1}^{n}\rho_i^3\sum_{j=1}^{n}\rho_j=0.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\rho_i\rho_j^2}{2}=\frac{1}{2}\sum_{i=1}^{n}\rho_i\sum_{j=1}^{n}\rho_j^3=0.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\rho_i^2\rho_j}{2}=\frac{1}{2}\sum_{i=1}^{n}\rho_i^2\sum_{j=1}^{n}\rho_j=0.$$

Combining the above relations, we get

$$REE(G)\geqslant\sqrt{n^2+nN_2+\frac{nN_3}{3}+\frac{nN_4}{12}+\frac{nN_5}{60}+\frac{N_2N_3}{6}+\frac{N_2^2}{4}}.$$

□

Since N_k is equal to the number of self-returning walks of length k, consequently, $N_k \geq 0$ for all graphs and for all $k \geq 0$. If the graph G is bipartite, then it contains no odd-membered cycles and, consequently, it has no self-returning walks of odd length, i.e., $N_k(G) = 0$ for $k = 1,3,5,7,\ldots$.
Therefore, by Theorems 9 and 1, we have the following result.

Corollary 1. *Let G be a connected bipartite graph of order n. Then*

$$REE(G) \geqslant \sqrt{n^2 + R_{-1}(G)\,(2n + R_{-1}(G)) + \frac{n\,(2R(G)\Delta\delta + M_1(G) - 2m)}{12\Delta^4}}.$$

Next, we obtain a lower bound for the Randić Estrada index in terms of the order n and the eigenvalues of its Randić matrix.

Theorem 10. *Let G be a graph with $n \geq 2$ vertices. Then*

$$REE(G) \geq 2(n-1)e^{\frac{\rho_2+\cdots+\rho_n}{2(n-1)}} + e^{\rho_1} - n + 1.$$

Equality holds if and only if $G \cong \overline{K}_n$.

Proof. Consider $p_1 = \frac{1}{2n}$, $p_i = \frac{2n-1}{2n(n-1)}$ for $i = 2,\ldots,n$ and $a_j = e^{\rho_j}$ for $j = 1,\ldots,n$. Note that $\Upsilon = \min\{\frac{1}{2n}, \frac{2n-1}{2n(n-1)}\} = \frac{1}{2n}$.

$$\frac{e^{\rho_1}}{2n} + \frac{2n-1}{2n(n-1)}\sum_{i=2}^{n} e^{\rho_i} - \Psi \geq \frac{1}{2}\left(\frac{1}{n}\sum_{i=1}^{n} e^{\rho_i} - 1\right)$$

where

$$\Psi = e^{\frac{\rho_1}{2n}}\prod_{i=2}^{n} e^{\frac{\rho_i(2n-1)}{2n(n-1)}}.$$

It's straightforwardly verified that

$$\Psi = e^{\frac{\rho_1}{2n}}\prod_{i=2}^{n} e^{\frac{\rho_i(2n-1)}{2n(n-1)}} = e^{\frac{\rho_2+\cdots+\rho_n}{2(n-1)}}.$$

Hence,

$$\frac{e^{\rho_1}}{2n} + \frac{(2n-1)\left(\sum_{i=1}^{n} e^{\rho_i} - e^{\rho_1}\right)}{2n(n-1)} - \Psi \geq \frac{1}{2n}\sum_{i=1}^{n} e^{\rho_i} - \frac{1}{2}.$$

Therefore,

$$e^{\frac{\rho_2+\cdots+\rho_n}{2(n-1)}} + \frac{e^{\rho_1}}{2(n-1)} - \frac{1}{2} \leq \frac{1}{2(n-1)}REE(G).$$

□

Note that for non-empty graphs, we have $\rho_1 = 1$ and $\sum_{i=2}^{n}\rho_i = -1$, applying Theorem 10, we get the next result.

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

$$REE(G) > 2(n-1)e^{\frac{-1}{2(n-1)}} + e - n + 1.$$

Now we derive a lower bound and an upper bound of the Randić Estrada index in terms of the order n and the eigenvalues of its Randić matrix.

Theorem 11. *Let G be a graph of order n. Then*

$$\frac{\left(\sum_{i=1}^{n} e^{\frac{\rho_i}{2}}\right)^2 - n}{n-1} \leq REE(G) \leq \left(\sum_{i=1}^{n} e^{\frac{\rho_i}{2}}\right)^2 - n(n-1). \tag{10}$$

Equalities holds if and only if G is the empty graph $\overline{K}_n$.

Proof. Setting $a_i = e^{\rho_i}$ for $i = 1,2,...,n$. Applying Lemma 2 and the definition of the Estrada index, we have

$$n\left(\frac{1}{n}\sum_{i=1}^{n} e^{\rho_i} - \left(\prod_{i=1}^{n} e^{\rho_i}\right)^{\frac{1}{n}}\right) \leq n\sum_{i=1}^{n} e^{\rho_i} - \left(\sum_{i=1}^{n} e^{\frac{\rho_i}{2}}\right)^2.$$

We know that $\sum_{i=1}^{n} \rho_i = 0$. Hence,

$$\sum_{i=1}^{n} e^{\rho_i} - n \leq n\sum_{i=1}^{n} e^{\rho_i} - \left(\sum_{i=1}^{n} e^{\frac{\rho_i}{2}}\right)^2.$$

Therefore by the definition of Randić Estrada index, we have

$$REE(G) \geq \frac{\left(\sum_{i=1}^{n} e^{\frac{\rho_i}{2}}\right)^2 - n}{n-1}.$$

Also,

$$n\sum_{i=1}^{n} e^{\rho_i} - \left(\sum_{i=1}^{n} e^{\frac{\rho_i}{2}}\right)^2 \leq n(n-1)\left(\frac{1}{n}\sum_{i=1}^{n} e^{\rho_i} - \left(\prod_{i=1}^{n} e^{\rho_i}\right)^{\frac{1}{n}}\right).$$

Again, by the definition of Randić Estrada index, we have the following result:

$$REE(G) \leq \left(\sum_{i=1}^{n} e^{\frac{\rho_i}{2}}\right)^2 - n(n-1).$$

The equality holds if and only if all ρ_i is zero, that is G is $\overline{K}_n$. □

Theorem 12. *Let G be a graph of order n. Then*

$$REE(G) \geq \left(\sqrt{e^{\rho_1}} - \sqrt{e^{\rho_n}}\right)^2 + n.$$

Equalities holds if and only if G is the empty graph $\overline{K}_n$.

Proof. Setting $x_i = e^{\rho_i}$, $b = e^{\rho_1}$ and $a = e^{\rho_n}$ for $i = 1,2,...,n$. Applying Theorem 2 and the definition of the Estrada index, we have

$$\begin{aligned}\frac{REE(G)}{n} &= \frac{1}{n}\sum_{i=1}^{n} e^{\rho_i} \\ &\geq \frac{1}{n}\left(\sqrt{e^{\rho_1}} - \sqrt{e^{\rho_n}}\right)^2 + \left(\prod_{i=1}^{n} e^{\rho_i}\right)^{\frac{1}{n}} \\ &= \frac{1}{n}\left(\sqrt{e^{\rho_1}} - \sqrt{e^{\rho_n}}\right)^2 + 1.\end{aligned}$$

□

- Note that for all graphs that $\Delta > \frac{n}{2}$, our lower bound in Theorem 12 is better than the lower bound in Theorem 5.
- Because Theorem 12 is better than Theorem 5, therefore, it is also better than Theorem 4.
- Also, we know that

$$\begin{aligned}& e + \sqrt{(n-1) + \left(1 + \frac{n-2}{e^{\frac{2}{n-1}}}\right) + 2\left(\frac{2n}{\Delta} - 3\right)} \\ &\leq e + \sqrt{(n-1) + (1 + n - 2) + 2\left(\frac{2n}{2} - 3\right)} \\ &= e + \sqrt{4(n-1)} \\ &= e + 2\sqrt{n-1}.\end{aligned}$$

  Hence, for $n \geq 7$, we can see that

$$e + 2\sqrt{n-1} < \left(\sqrt{e^{\rho_1}} - \sqrt{e^{\rho_n}}\right)^2 + n.$$

  Therefore, our lower bound in Theorem 12 is better than the lower bound in Theorem 6, for $n \geq 7$.

- Note that for a bipartite graph $\rho_1 = -\rho_n$.
  It is not hard to see that for $n > 1$, $n + \frac{1}{e} + 2 > \sqrt[1-n]{e}(n-1)$. It follows that $\frac{en+2e+1}{e} - e^{\frac{-1}{n-1}}(n-1) > 0$. This is equivalent to

$$e^{\frac{-1}{n-1}-1}\left(ne^{\frac{1}{n-1}+1} - en + 2e^{\frac{1}{n-1}+1} + \sqrt[n-1]{e} + e\right) > 0.$$

  Thus, $n + 2 + \frac{1}{e} - ne^{\frac{-1}{n-1}} + e^{\frac{-1}{n-1}} > 0$. Therefore our lower bound in Theorem 12 is better than the lower bound in Theorem 3, for bipartite graphs.

4 Conclusion

In this paper, we studied the Randić Estrada index $REE(G)$ of a simple graph G and established several bounds in terms of classical graph invariants and the eigenvalues of the Randić matrix. In particular, new estimates were obtained that depend on the order, degree sequence, Randić index, and Zagreb index of the graph. For bipartite graphs, we presented a sharper lower bound improving earlier results.

The results enhance the understanding of the spectral properties of the Randić matrix and may serve as a basis for further research on extremal properties and applications of the Randić Estrada index in (chemical) graph theory and network analysis.

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