An increasing sequence of lower bounds for the Estrada index of graphs and matrices

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Abstract
Let $G$ be a graph on $n$ vertices and $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ its eigenvalues. The Estrada index of $G$ is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. In this work, we use an increasing sequence converging to the $\lambda_1$ to obtain an increasing sequence of lower bounds for $EE(G)$. In addition, we generalize this succession for the Estrada index of an arbitrary nonnegative Hermitian matrix.

Keywords:
Estrada Index; Adjacency matrix; Hermitian matrix; Lower bound; Graph.

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1. Introduction

In this paper, we consider undirected simple graphs $G$ with by edge set denoted by $\mathcal{E}(G)$ and its vertex set $V(G) = \{1, \ldots, n\}$ with cardinality $m$ and $n$, respectively. If $e \in \mathcal{E}(G)$ has end vertices $i$ and $j$, then we say that $i$ and $j$ are adjacent and this edge is denoted by $ij$. For a finite set $U$, $|U|$ denotes its cardinality. Let $K_n$ be the complete graph with $n$ vertices and $\overline{K}_n$ its complement. A graph $G$ is bipartite if there exists a partitioning of

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$V(G)$ into disjoint, nonempty sets $V_1$ and $V_2$ such that the end vertices of each edge in $G$ are in distinct sets $V_1$, $V_2$. A graph $G$ is a complete bipartite graph if $G$ is bipartite and each vertex in $V_1$ is connected to all the vertices in $V_2$. If $|V_1| = p$ and $|V_2| = q$, the complete bipartite graph is denoted by $K_{p,q}$. For more properties of bipartite graphs, see [19].

If $i \in V(G)$, then $NG(i)$ denoted the set of neighbors of the vertex $i$ in $G$, that is, $NG(i) = \{ j \in V(G) : ij \in E(G) \}$. For the $i$-th vertex of $G$, the cardinality of $NG(i)$ is called the degree of $i$ and it is denoted by $d(i)$. The number of walks of length $k$ of $G$ starting at $i$ is denoted by $d_k(i)$, is also called $k$-degree of the vertex $i$. Clearly, we define $d_0(i) = 1$, $d_1(i) = d(i)$ and for $k \geq 1$

$$d_{k+1}(i) = \sum_{j \in NG(i)} d_k(j).$$

A graph $G$ is called $r$-regular if $d(i) = r$, for all $i \in V(G)$. Further, a graph $G$ is called $(a, b)$-semiregular if $\{ d(i), d(j) \} = \{ a, b \}$ holds for all edges $ij \in E(G)$.

A semiregular graph that is not regular will henceforth be called strictly semiregular.

Clearly, a connected strictly semiregular graph must be bipartite. A graph $G$ is called harmonic [11] (in [28] is called pseudoregular) if there exist a constant $\mu$ such that $d_2(i) = \mu d(i)$ holds for all $i \in V(G)$; in which case $G$ is also called $\mu$-pseudoregular. A graph $G$ is called semipseudoregular [28], if there exist a constant $\mu$ such that $d_3(i) = \mu d(i)$ holds for all $i \in V(G)$; in which case $G$ is also called $\mu$-semiharmonic. Thus every $\mu$-pseudoregular graph is $\mu^2$-semipseudoregular. Also every $(a, b)$-semiregular graph is $ab$-semipseudoregular. A semipseudoregular graph that is not pseudoregular will henceforth be called strictly semipseudoregular. Finally, a graph $G$ is called $(a, b)$-pseudosemiregular if $\left\{ \frac{d_2(i)}{d(i)}, \frac{d_2(j)}{d(j)} \right\} = \{ a, b \}$ holds for all edges $ij \in E(G)$. A pseudosemiregular graph that is not pseudoregular will henceforth be called strictly pseudosemiregular. Clearly, a connected strictly pseudosemiregular graph must be bipartite.

The adjacency matrix $A(G)$ of the graph $G$ is a symmetric matrix of order $n$ with entries $a_{ij}$, such that $a_{ij} = 1$ if $ij \in E(G)$ and $a_{ij} = 0$ otherwise. Denoted by $\lambda_1 \geq \ldots \geq \lambda_n$ to the eigenvalues of $A(G)$, see [2, 3].
The Estrada index of the graph $G$ is defined as

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

This spectral quantity is put forward by E. Estrada [6] in the year 2000. There have been found a lot of chemical and physical applications, including quantifying the degree of folding of long-chain proteins, [6, 7, 8, 14, 15, 18], and complex networks [9, 10, 23, 24, 25, 26]. Mathematical properties of this invariant can be found in e.g. [12, 13, 16, 20, 27, 29, 30].

Denote by $M_k = M_k(G)$ to the $k$-th spectral moment of the graph $G$, i.e.,

$$M_k = \sum_{i=1}^{n} (\lambda_i)^k.$$ 

Then, we can write the Estrada index as

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k}{k!}.$$ 

In [2], for an $(n, m)$-graph $G$, the authors proved that

$$M_0 = n, \quad M_1 = 0, \quad M_2 = 2m, \quad M_3 = 6t,$$

where $t$ is the number of triangles in $G$.

In [1], the authors showed that for $G$ a $(n, m)$-graph:

$$EE(G) \geq e^{\left(\frac{2m}{n}\right)} + n - 1 - \frac{2m}{n}. \quad (2)$$

The equality holds in (2) if and only if $G$ is isomorphic to $\overline{K_n}$. To obtain the last lower bound, at first, the authors showed that the following relationship holds:

$$EE(G) \geq e^{\lambda_1} + n - 1 - \lambda_1. \quad (3)$$

Let $R$ be a Hermitian matrix of order $\ell$ with eigenvalues $\rho_1, \rho_2, \ldots, \rho_\ell$. The Estrada index of $R$ is denoted and defined as

$$\text{HEE}(R) = \sum_{i=1}^{\ell} e^{\rho_i - \frac{\text{Tr}(R)}{\ell}}.$$
where $\text{tr}(R)$ is the trace of $R$, \[^5\]. On the other hand, if we consider

$$EE(R) = \sum_{i=1}^{\ell} e^{\rho_i}$$

the Estrada index of Hermitian matrix $R$, we have that

$$HEE(R) = e^{\text{Tr}(R)} EE(R).$$

Therefore, both indexes are basically equivalent. In this paper, we will work with the definition given in \[^4\] of the Estrada index to obtain new boundaries for the invariant $HEE(G)$. Moreover, the equality in the previous definition occurs when we identify $R$ with the adjacency matrix of a graph. For details on the theory of the Hermitian Estrada index see the papers \[^1, 5, 22\] and the references cited therein.

In \[^1\], the authors showed that for a nonnegative Hermitian matrix $R$ of order $\ell$

$$EE(R) \geq e^{\rho_1} + (\ell - 1) + \text{Tr}(R) - \rho_1.$$  \[^5\]

In this work, we will use the increasing sequence of lower bounds for $\lambda_1$ given in \[^17\] to obtain an increasing sequence of lower bounds for the Estrada index of graphs, which converges to the lower bound \[^3\]. Moreover, applying this technique, we obtain an increasing sequence of lower bounds for the Estrada index of a Hermitian matrix $R$, which converges to the lower bound \[^5\].

2. Increasing sequence of lower bounds for the Estrada index of graphs

In this section, we obtain a sequence of lower bounds for Estrada index of graphs. For this, we need the following results.

**Theorem 1.** \[^2\] Let $G$ be a connected graph. Then

$$\lambda_1 \geq \sqrt{\frac{\sum_{i\in V(G)} d^2(i)}{n}}$$

with equality if and only if $G$ is regular or a semiregular.
Theorem 2. [28] Let \( G \) be a connected graph. Then

\[
\lambda_1 \geq \sqrt[\sum_{i \in V(G)} d_2^2(i)}{\sum_{i \in V(G)} d^2(i)}
\]

(7)

with equality if and only if \( G \) is a pseudo-regular graph or a strictly pseudo-semiregular graph.

Furthermore, we have to

\[
\sqrt[\sum_{i \in V(G)} d_2^2(i)}{\sum_{i \in V(G)} d^2(i)} \geq \sqrt[\sum_{i \in V(G)} d_2^2(i)}{\sum_{i \in V(G)} d^2(i)}.
\]

In [17], the authors generalized these results and built an increasing sequence of lower bounds for \( \lambda_1 \), as follows:

\[
\gamma^{(0)} = \sqrt[\sum_{i \in V(G)} d_2^2(i)}{n}
\]

\[
\gamma^{(1)} = \sqrt[\sum_{i \in V(G)} d_2^2(i)}{\sum_{i \in V(G)} d^2(i)}
\]

(8)

\[
\vdots
\]

\[
\gamma^{(k)} = \sqrt[\sum_{i \in V(G)} d_{k+1}^2(i)}{\sum_{i \in V(G)} d_k^2(i)}.
\]

Thereby, they obtain the following results.
Theorem 3. Let $G$ be a connected graph and $k \geq 1$. Then
\[ \lambda_1 \geq \gamma^{(k)} \]
with equality if and only if $G$ is pseudoregular or strictly pseudosemiregular.

Theorem 4. Let $G$ be a graph, then $\{\gamma^{(k)}\}_{k \geq 0}$ is an increasing sequence and
\[ \lim_{k \to \infty} \gamma^{(k)} = \lambda_1. \]

Remark 5. Consider the following function
\[ f(x) = (x - 1) - \ln(x), \quad x > 0. \] (9)
Clearly the function $f$ is decreasing in $(0, 1]$ and increasing in $[1, +\infty)$ Consequently, $f(x) \geq f(1) = 0$, implying that
\[ x \geq 1 + \ln x, \quad x > 0, \] (10)
the equality holds if and only if $x = 1$. Let $G$ be a graph of order $n$, using (11) and (12), we get:
\begin{align*}
EE(G) &\geq e^{\lambda_1} + (n - 1) + \sum_{k=2}^{n} \ln e^{\lambda_k} \\
&= e^{\lambda_1} + (n - 1) + \sum_{k=2}^{n} \lambda_k \\
&= e^{\lambda_1} + (n - 1) + M_1 - \lambda_1 \\
&= e^{\lambda_1} + (n - 1) - \lambda_1.
\end{align*} (11)

Define the function
\[ \phi(x) = e^x + (n - 1) - x, \quad x > 0. \] (12)
Note that, this is an increasing function on $D_\phi = [0, +\infty)$.

Considering this Remark, we have the following result.

Theorem 6. Let $G$ a connected graph of order $n$ and the sequence $\{\gamma^{(k)}\}_{k=0}^\infty$ as in (8). Then the sequence $\{\phi(\gamma^{(k)})\}_{k=0}^\infty$ is increasing and converges to $\phi(\lambda_1)$, moreover for all $k \geq 0$
\[ EE(G) > e^{\gamma^{(k)}} + n - 1 - \gamma^{(k)}. \] (13)
Proof. First, we observe that \( \gamma^{(k)} \in D_\phi \), for all \( k \geq 0 \). This is an immediate consequence of Theorem 4 and that \( \gamma^{(0)} = \sqrt{\sum_{i \in V(G)} d^2(i)} / n \geq \sqrt{2m/n} \geq 1 \).

Since \( \{\gamma^{(k)}\}_{k=0}^\infty \) is an increasing sequence and by Theorem 4 converges to \( \lambda_1 \). Then, by the continuity of \( \phi \) allows us to prove the first statement.

Remark 7. Suppose that the equality holds in (13). Then all the inequalities in (11) must be considered as equalities. From the equality (10), we get \( e^{\lambda_2} = \ldots = e^{\lambda_n} = 1 \), then \( \lambda_2 = \ldots = \lambda_n = 0 \) implying that \( \lambda_1 = \gamma^{(k)} = 0 \). Thus \( G \) is isomorphic to the \( K_n \).

The following result, we obtain a sharp increasing sequence of lower bounds for the Estrada index of a bipartite graph. Considering (11) and (10), we obtain

\[
EE(G) = e^{\lambda_1} + e^{-\lambda_1} + \sum_{k=2}^{n-1} e^{\lambda_k} \\
\geq 2 \cosh \lambda_1 + (n-2) + \sum_{k=2}^{n-1} \lambda_k \\
= 2 \cosh \lambda_1 + (n-2) + M_1 + \lambda_1 - \lambda_1 \\
= 2 \cosh \lambda_1 + n - 2. 
\]

(14)

Define the function, \( \Phi(x) = 2 \cosh x + n - 2 \). Note that, this is an increasing function on \( D_\Phi = [0, +\infty) \).

Theorem 8. Let \( G \) be a bipartite connected graph of order \( n \) with \( n > 2 \). Considering the sequence \( \{\gamma^{(k)}\}_{k=0}^\infty \) as in (8). Then

\[
EE(G) \geq 2 \cosh (\gamma^{(k)}) + n - 2. 
\]

(15)

Equality holds if and only if \( G \) is isomorphic to the complete bipartite graph.

Proof.

Analogous to the proof of Theorem 6, \( \gamma^{(k)} \in D_\phi \). Since \( \{\gamma^{(k)}\}_{k=0}^\infty \) is an increasing sequence and by Theorem 4 converges to \( \lambda_1 \). Then the continuity of \( \phi \) allows us to prove the first statement.

Moreover, we get

\[
EE(G) \geq 2 \cosh (\gamma^{(k)}) + n - 2. 
\]
Suppose now that the equality holds in (15). Then all the inequalities in (14) must be considered as equalities. From the equality (10), we get $e^{\lambda_2} = \ldots = e^{\lambda_{n-1}} = 1$, then $\lambda_2 = \ldots = \lambda_{n-1} = 0$ and $\lambda_1 = -\lambda_n = \gamma^{(k)}$, which implies that $G$ is a bipartite complete graph, $K_{p,q}$ such that $p + q = n$. \(\square\)

3. Lower bounds for the Estrada index of nonnegative Hermitian matrix

Recall that a Hermitian complex $\ell \times \ell$ matrix $R = (r_{ij})$, $r_{ij} \in \mathbb{C}$, is such that $R = R^*$ where $R^*$ denotes the conjugate transpose of $R$. For $x, y \in \mathbb{C}^\ell$, we denote by $<x, y> = x^* y$, the inner product in $\mathbb{C}^\ell$ and the norm, $\|x\| = \sqrt{<x, x>}$. Here, $|R| = \sqrt{\text{trace}(R^* R)}$ is the Frobenius norm of $R$. For Hermitian matrices it is possible find an orthonormal basis of $\mathbb{C}^\ell$, $x_1, x_2, \ldots, x_\ell$, of eigenvectors associated to $\rho_1, \rho_2, \ldots, \rho_\ell$ the eigenvalues of $R$ where $Rx_i = \rho_i x_i$, for $i = 1, 2, \ldots, \ell$. The spectral radius of a square matrix $R$ is the largest absolute value of its eigenvalues, it is denoted by $|\rho_1| = \max \{|\rho| : \rho_i \in \sigma(R)\}$. Let $f \in \mathbb{C}^\ell$ such that $<f, x_i> \neq 0$ for $i = 1, \ldots, \ell$. We define the vector sequence

\[
\begin{align*}
r^{(0)} &= f \\
r^{(1)} &= Rr^{(0)} = Rf \\
&\vdots \\
r^{(k)} &= Rr^{(k-1)} = R^{(k)}f
\end{align*}
\]

In view of the fact that for $k = 0, 1, \ldots, R^{(k)}f \neq 0$, in [4] the following numerical sequence was defined

\[
\begin{align*}
\xi^{(0)} &= \frac{\|r^{(1)}\|}{\|r^{(0)}\|} = \frac{\|Rr^{(0)}\|}{\|f\|} \\
\xi^{(1)} &= \frac{\|r^{(2)}\|}{\|r^{(1)}\|} = \frac{\|Rr^{(1)}\|}{\|Rr^{(0)}\|} \\
&\vdots \\
\xi^{(k)} &= \frac{\|r^{(k+1)}\|}{\|r^{(k)}\|} = \frac{\|Rr^{(k)}\|}{\|Rr^{(k-1)}\|}.
\end{align*}
\]

Thereby, the authors in [4], we obtain the following result.
Lemma 9. [4] Let \( \{\xi^{(k)}\}_{k \geq 0} \) be the sequence defined in (17), then \( \{\xi^{(k)}\}_{k \geq 0} \) is an increasing sequence. Furthermore
\[
\lim_{k \to \infty} \xi^{(k)} = |\rho_1|.
\]

The matrix \( R = (r_{ij}) \) is called nonnegative if \( r_{ij} \geq 0 \) for \( i, j = 1, 2, \ldots, \ell \), see [21]. The matrix \( R \) is an irreducible nonnegative matrix, then its spectral radius is simple with a positive eigenvector \( x_1 \). Let \( e \) be the \( n \)-dimensional all-one vector \( e = (1, \ldots, 1)^T \). Evidently, \( < e, x_1 > \neq 0 \).

Considering the argument used in (11) and the inequality (10), we have that
\[
EE(R) \geq e^{\rho_1} + \ell - 1 + \text{Tr}(R) - \rho_1.
\]
(18)
The equality holds if only if \( \rho_2 = \rho_3 = \ldots = \rho_\ell = 0 \).

Let
\[
\varphi(x) = e^x + \ell - 1 + \text{Tr}(R) - x.
\]
Note that \( \varphi \) is an increasing function on \( D_\varphi = [0, +\infty) \).

Theorem 10. Let \( R \) be a nonnegative symmetric \( \ell \times \ell \) matrix with spectral radius \( \rho_1 \). Define the sequence \( \{\xi^{(k)}\}_{k \geq 0} \) as in (17) with \( f \) replaced by \( e \). Then \( \xi^{(k)} \in D_\varphi \), for all \( k = 0, 1, 2, \ldots, \ell \), where \( \varphi \) is defined in (19).

Proof. Before starting the proof, it is worth noting that
\[
\rho_1 \leq \sqrt{\rho_1^2 + \rho_2^2 + \ldots + \rho_\ell^2} = |R|.
\]
For the Rayleigh quotient, we have that \( 0 < \xi^{(k)} \leq |\rho_1| \) for all \( k \geq 0 \), then \( 0 < \xi^{(k)} \leq |R| \). Since \( R \) is a nonnegative matrix,
\[
\text{trace}(R^*R) = \text{trace}(R^2) \leq e^*R^2e,
\]
implies that \( |R| \leq \|Re\| \). Consequently,
\[
0 \leq \frac{|R|}{\sqrt{\ell}} \leq \frac{\|Re\|}{\sqrt{\ell}} = \xi^{(0)}.
\]
(20)
Finally, by using Lemma 9, the result follows.

The following result of this section generalize the Theorem 6.
Theorem 11. Let $R$ be a nonnegative symmetric $\ell \times \ell$ matrix with spectral radius $\rho_1$. Define the sequence $\{\xi^{(k)}\}_{k \geq 0}$ as in (19) with $f$ replaced by $e$. Then the sequence $\{\varphi(\xi^{(k)})\}_{k=0}^{\infty}$ is increasing and converges to $\varphi(\rho_1)$, moreover for all $k \geq 0$

$$EE(R) \geq e^{\xi^{(k)}} + \ell - 1 + Tr(R) - \xi^{(k)}.$$  \hspace{1cm} (21)

Equality holds in (21) if and only if $\rho_2 = \rho_3 = \ldots = \rho_\ell = 0$.

Proof. Since $\xi^{(k)} \in D_\varphi$, for all $k \geq 0$, see Theorem 10. Since $\{\xi^{(k)}\}_{k=0}^{\infty}$ is an increasing sequence and converges to $\rho_1$, by Lemma 9. Then the continuity of $\varphi$ allows us to prove the statement. \qed
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