New Lower Bounds for the Estrada Index

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Abstract
Let $G$ be a graph on $n$ vertices and $\lambda_1, \lambda_2, \ldots, \lambda_n$ its eigenvalues. The Estrada index of $G$ is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. In this work, using a different demonstration technique, new lower bounds are obtained for the Estrada index, that depends on the number of vertices, the number of edges and the energy of the graph is given. Moreover, another lower bound for the Estrada index is obtained of an arbitrary Hermitian matrix are established.

Keywords:
Estrada Index; Energy; Adjacency matrix; Signless Laplacian matrix; Lower bound; Graph.

2000 MSC: 05C50, 15A18

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. We say that $G$ is an $(n,m)$ graph. 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 (edgeless) complement. A graph
G is bipartite if there exists a partitioning of \( V(G) \) 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 [25].

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 [3, 7]. A matrix is singular if it has zero as an eigenvalue, otherwise, it is called non-singular. A graph \( G \) will be said non-singular if its adjacency matrix is non-singular. The matrix \( Q(G) = D(G) + A(G) \) is called the signless Laplacian matrix of \( G \) [4, 5, 6], where \( D(G) \) is the diagonal matrix of vertex degrees of \( G \). It well know that the matrix \( Q(G) \) is positive semidefinite, see [34]. We denoted the eigenvalues of the signless Laplacian matrix by \( q_1(G) \geq \ldots \geq q_{n-1}(G) \geq q_n(G) \geq 0 \).

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 [10] 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, [10, 11, 12, 20, 21, 24], and complex networks [13, 14, 29, 30, 31, 32]. Mathematical properties of this invariant can be found in e.g. [16, 19, 22, 26, 33, 35, 36].

In [2], was introduced the innovative notion of the signless Laplacian Estrada index a

\[
EE(Q(G)) = SLEE(G) = \sum_{i=1}^{n} e^{q_i}.
\]

Also established lower and upper bounds for \( EE(Q(G)) \) in terms of the number of vertices and edges.
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 [3], for an $(n,m)$-graph $G$, the authors proved that

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

(1)

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

The energy of $G$ was defined by I. Gutman in 1978, [18], as

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

Similarly, the signless Laplacian energy of a graph $G$ with $n$ vertices and $m$ edges is defined in [23] by

$$QE(G) = \sum_{i=1}^{n} \left| q_i - \frac{2m}{n} \right|.$$ 

(2)

Nowadays studies on the signless Laplacian energy are still in course [1, 9].

In [27], Koolen and Moulton showed that the following relation holds for all graph $G$

$$E(G) \leq \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)}.$$ 

(3)

For all $(n,m)$-graph $G$ connected and nonsingular, Das et al. in [8], proved the following relation holds

$$E(G) \geq \lambda_1 + (n-1) + \ln |\det A| + \ln(\lambda_1),$$ 

(4)

then using the inequality $2m/n \leq \lambda_1$, they obtained the following upper bound

$$E(G) \geq \frac{2m}{n} + (n-1) + \ln |\det A| + \ln \left( \frac{2m}{n} \right).$$
With respect to Estrada index, for all \((n,m)\)-graph, De la Peña et al. in [15] proved that
\[
\sqrt{n^2 + 4m} \leq EE(G) \leq n - 1 + e^{\sqrt{2m}}.
\] (5)
Equality on both sides of (5) is attained if and only if \(G\) is isomorphic to \(K_n\).

In this work, under the motivation and the ideas of [8], we obtain new lower bounds for the Estrada index in terms of the number of vertices and edges of an arbitrary \(G\) graph. Furthermore, new lower bounds for \(EE(G)\) in relation with \(E(G)\) and considering an arbitrary Hermitian matrix are obtained.

2. Lower bound for the Estrada index

In this section, new lower bounds for Estrada index in relation to the number of vertices, edges and an arbitrary Hermitian matrix are established.

**Theorem 1.** Let \(G\) a \((n, m)\)-graph then,
\[
EE(G) \geq e^{\left(\frac{2m}{n}\right)} + (n - 1) - \frac{2m}{n}.
\] (6)
Equality holds in (6) if and only if \(G\) is isomorphic to \(K_n\).

**Proof.** Consider the following function
\[
f(x) = (x - 1) - \ln(x), \ x > 0.
\] (7)
Clearly the function \(f\) is decreasing in \((0, 1]\) and increasing in \([1, +\infty)\) Consequently, \(f(x) \geq f(1) = 0\), implying that
\[
x \geq 1 + \ln x, \ x > 0,
\] (8)
the equality holds if and only if \(x = 1\). Let \(G\) be a graph of order \(n\), using (1) and (8), we get:
\[
EE(G) \geq e^{\lambda_1} + (n - 1) + \sum_{k=2}^{n} \ln e^{\lambda_k}
= e^{\lambda_1} + (n - 1) + \sum_{k=2}^{n} \lambda_k
= e^{\lambda_1} + (n - 1) + M_1 - \lambda_1
= e^{\lambda_1} + (n - 1) - \lambda_1.
\] (9)
Define the function
\[ \phi(x) = e^x + (n - 1) - x, \quad x > 0. \]  
(10)

Note that, this is an increasing function on \( D_\phi = [0, +\infty) \).

On the other hand, we have inequality
\[ \lambda_1 \geq \frac{2m}{n} \geq 0, \]
therefore, we verify
\[ \phi(\lambda_1) \geq \phi\left(\frac{2m}{n}\right). \]

Finally, we get
\[ EE(G) \geq e^{\left(\frac{2m}{n}\right)} + (n - 1) - \left(\frac{2m}{n}\right). \]

Suppose now that the equality holds in (6). Then all the inequalities in (9) must be considered as equalities. From the equality \( e^{\lambda_2} = \ldots = e^{\lambda_n} = 1 \), then \( \lambda_2 = \ldots = \lambda_n = 0 \) and \( \lambda_1 = \frac{2m}{n} \). It follows that \( G \) is regular. Thus \( G \) is isomorphic to the \( K_n \).

A direct consequence is the following result.

**Corollary 2.** Let \( G \) be a connected \( \alpha \)-regular graph with \( n \) vertices. Then,
\[ EE(G) \geq e^\alpha + n - \alpha - 1. \]  
(11)

**Remark 3.** Let’s see some examples of families of graphs where Theorem 1 is verified, more than one, it is shown that the lower bound for the Estrada index obtained in this first main results is better than the Estrada index existing in the literature. Then, for our analysis we will use the following notation, from (9), \( EE(G) \geq e^{\left(\frac{2m}{n}\right)} + (n - 1) - \left(\frac{2m}{n}\right) = J(G) \) and from (5) \( EE(G) \geq \sqrt{n^2 + 4m} = CP(G) \). Therefore, we will claim that, for some kinds of graphs \( G \), \( J(G) \geq CP(G) \)

1. **Star graph.** Note that \( S_n \) denote a complete bipartite graph \( K_{1,k} \). It is well known that \( S_n \) hold the relation between its edges and vertices is given by \( m = n - 1 \). Then, replacing this condition, we have
\[ J(S_n) = e^{\left(2 - \frac{2}{n}\right)} + (n + \frac{2}{n}) - 3 \] and \[ CP(S_n) = \sqrt{n^2 + 4n - 4}, \] then it is easily demonstrated that \( J(S_n) \geq CP(S_n) \), for all \( n \neq 2 \). Therefore, we obtain that \( EE(S_n) \geq J(S_n) \geq CP(S_n) \), which shows that our lower bound is much better than the one proposed by [2] for the Estrada index.

2. **Path graph.** We will denote to \( P_n \) a path. Note that \( P_n \) satisfies the relation \( m = n - 1 \) which is the same relation that exists in \( S_n \) between \( n \) and \( m \), then we show \( EE(P_n) \geq J(P_n) \geq CP(P_n) \), for all \( n \neq 2 \).

3. **Complete graph.** For \( K_n \) is true that \( m = \frac{n(n-1)}{2} \). Then we have \( J(K_n) = e^{n-1} \) and \( CP(K_n) = \sqrt{3n^2 - 2n} \). Then it is readily demonstrated that \( J(K_n) \geq CP(K_n) \), for all \( n \neq 2 \). Therefore, we obtain that \( EE(K_n) \geq J(K_n) \geq CP(K_n) \), which shows that our lower bound is much better than the one proposed by [3] for the Estrada index.

4. **Cycle graph.** For a cycle graph \( C_n \), the condition \( m = n \) is verified. So we have \( J(C_n) = e^2 + n - 3 \) and \( CP(C_n) = \sqrt{n^2 + 4n} \), then we show that \( J(C_n) \geq CP(C_n) \) for all \( n \). Then, \( EE(C_n) \geq J(C_n) \geq CP(C_n) \), which shows that our lower bound is much better.

In the following result, we obtain a sharp lower bound of the Estrada index for a bipartite graph.

**Theorem 4.** Let \( G \) be a bipartite \((n,m)\)-graph, with \( n > 2 \), then
\[
EE(G) \geq 2 \cosh \left( \frac{2m}{n} \right) + (n-2). \quad (12)
\]
Equality holds in (12) if and only if \( G \) is isomorphic to \( K_{p,p} \) \((2p \leq n)\) with \( n - 2p \) isolated vertices.

**Proof.** Considering (11) and (8), we obtain
\[
EE(G) = e^{\lambda_1} + e^{-\lambda_1} + \sum_{k=2}^{n-1} e^{\lambda_k} \geq 2 \cosh \lambda_1 + (n-2) + \sum_{k=2}^{n-1} \lambda_k \quad (13)
\]
\[
= 2 \cosh \lambda_1 + (n-2) + M_1 + \lambda_1 - \lambda_1
\]
\[
= 2 \cosh \lambda_1 + (n-2).
\]
Since, $\Phi(x) = 2\cosh x + n - 2$, is an increasing function on $D_\Phi = [0, +\infty)$.

Analogous to Theorem 1, we have inequality

$$\lambda_1 \geq \frac{2m}{n} \geq 0,$$

therefore, we verify

$$\Phi(\lambda_1) \geq \Phi\left(\frac{2m}{n}\right).$$

Finally, we get

$$EE(G) \geq 2 \cosh\left(\frac{2m}{n}\right) + (n - 2).$$

Suppose now that the equality holds in (12). Then all the inequalities in (13) must be considered as equalities. From the equality (8), we get $e^{\lambda_2} = \ldots = e^{\lambda_{n-1}} = 1$, then $\lambda_2 = \ldots = \lambda_{n-1} = 0$ and $\lambda_1 = -\lambda_n = \frac{2m}{n}$, which implies that $G$ is isomorphic to a component $G' = K_{p,p}$ with $n - 2p$ isolated vertices. \(\square\)

The next result, is obtained applying the proof technique of the above Theorem to signless Laplacian matrix.

**Theorem 5.** Let $G$ a $(n, m)$-graph then,

$$EE(Q(G)) \geq e^{\left(\frac{4m}{n}\right)} + (n - 1) + 2m - \frac{4m}{n} \quad (14)$$

Equality holds in (14) if and only if $G$ is isomorphic to $\overline{K_n}$.

**Proof.** Using (8), we get:

$$EE(Q(G)) = e^{q_1} + \sum_{k=2}^{n} e^{q_k} \geq e^{q_1} + (n - 1) + \sum_{k=2}^{n} \ln(e^{q_k})$$

$$= e^{q_1} + (n - 1) + \sum_{k=2}^{n} q_k \quad (15)$$

$$= e^{q_1} + (n - 1) + \sum_{k=1}^{n} q_k - q_1$$

$$= e^{q_1} + (n - 1) + 2m - q_1.$$
Thereby, the function $\tau(x) = e^x + n - 1 + 2m - x, x > 0$, is an increasing function on $D_\tau = [0, +\infty)$.

In [17], is showed the inequality $q_1 \geq 2\lambda_1$ and join with $\lambda_1 \geq \frac{2m}{n}$, we verify $\tau(q_1) \geq \tau\left(\frac{4m}{n}\right)$.

Finally, we get

$$
EE(Q(G)) \geq e^{\left(\frac{4m}{n}\right)} + (n-1) + 2m - \left(\frac{4m}{n}\right).
$$

Suppose now that the equality holds in (15). From the equality in (8), we get $e^{q_2} = \ldots = e^{q_n} = 1$, then $q_2 = \ldots = q_n = 0$ and $q_1 = \frac{2m}{n}$. It follows that $G$ is regular. Thus $G$ is isomorphic to the $K_n$.

On the other hand, a Hermitian complex matrix $M = (m_{ij})$ of order $\iota$, is such that $M = M^*$ where $M^*$ denotes the conjugate transpose of $M$. Let $\rho_1, \rho_2, \ldots, \rho_\iota$ be the eigenvalues of $M$ and consider $|\rho_i| \leq \rho_1$, for all $i = 1, \ldots, \iota$.

The next result shows bounds for the greater eigenvalue of the matrix in relation with your rows, see [28].

**Theorem 6.** If $N$ is non-negative matrix with maximal eigenvalue $\lambda$ and row sums $s_1, \ldots, s_n$. Then

$$
r \leq \lambda \leq R
$$

where $r = \min\{s_i : i = 1, \ldots, n\}$ and $R = \max\{s_i : i = 1, \ldots, n\}$. If $N$ is irreducible, then equality can hold on either side of (17) if and only if all row sums of $N$ are equal.

Applying the above proof technique to the matrix $M$ and considering the inequality $x \geq 1 + \ln(x)$, we have
\[
EE(M) = e^{\rho_1} + \sum_{i=2}^{n} e^{\rho_i} \\
\geq e^{\rho_1} + (n - 1) + \sum_{i=2}^{n} \rho_i \\
= e^{\rho_1} + (n - 1) + \sum_{i=1}^{n} \rho_i - \rho_1 \\
= e^{\rho_1} + (n - 1) + Tr(M) - \rho_1,
\]
where \(Tr(M)\) is the trace of \(M\). Define the function
\[
\psi(x) = e^x + (n - 1) + Tr(M) - x.
\]
Its straightforward verified that \(\psi(x)\) is increasing in \([0, \infty)\). Then, by above Theorem \(\rho_1 \geq \min \{s_i : i = 1, \ldots, n\} = r\). Since \(\psi(\rho_1) \geq \psi(r)\), we proved the following result.

**Theorem 7.** Let \(M\) be a Hermitian matrix of order \(n\) with eigenvalues \(\rho_1, \rho_2, \ldots, \rho_n\). Then
\[
EE(G) \geq e^{r} + Tr(M) + (n - 1) - r.
\]

3. Estrada index and energy

In this section, new lower bounds for the Estrada index in relation to the energy of the graph \(G\) are established.

**Theorem 8.** Let \(G\) be a \((n, m)\)-graph with \(k\) non-negative eigenvalues. Then
\[
EE(G) \geq \frac{E(G)}{2} + e^{\lambda_1} + (k - 1) - \lambda_1. \tag{17}
\]

Equality holds in (17) if and only if \(G\) is isomorphic to \(K_n\).

**Proof.** Let \(x \geq 0\), consider the following function
\[
g(x) = -1 - x + e^x. \tag{18}
\]
the equality holds if and only if $x = 0$. Is straightforward show that function $g(x)$ is increasing in $[0, +\infty)$. Then $g(x) \geq g(0)$, implying that

$$x \leq e^x - 1, x \geq 0. \tag{19}$$

Note that, $A(G)$ is a symmetric matrix with zero trace, these eigenvalues are real with sum equal to zero, i.e,

$$\lambda_1 \geq \ldots \geq \lambda_n \tag{20}$$

and

$$\lambda_1 + \ldots + \lambda_n = 0. \tag{21}$$

Then by the definition of energy join to (20) and (21) we have

$$\frac{E(G)}{2} = \sum_{\lambda_i > 0} \lambda_i^+ = -\sum_{\lambda_i < 0} \lambda_i^- \tag{22}$$

Supposed that $A(G)$ have $k$ non-negative eigenvalues, then using (22) and (19) we obtain

$$\frac{E(G)}{2} = \sum_{i=1,\lambda_i \geq 0}^k \lambda_i$$

$$= \lambda_1 + \sum_{i=2,\lambda_i \geq 0}^k \lambda_i$$

$$\leq \lambda_1 + \sum_{i=2,\lambda_i \geq 0}^k (e^{\lambda_i} - 1)$$

$$= \lambda_1 - (k - 1) + \sum_{i=1,\lambda_i \geq 0}^k e^{\lambda_i} - e^{\lambda_1}$$

$$\leq \lambda_1 - (k - 1) + \sum_{i=1,\lambda_i \geq 0}^k e^{\lambda_i} + \sum_{i=k+1,\lambda_i < 0}^n e^{\lambda_i} - e^{\lambda_1}$$

$$= \lambda_1 - (k - 1) + \sum_{i=1}^n e^{\lambda_i} - e^{\lambda_1}.$$
Suppose now that the equality holds. From the equality in (18), we get $q_1 = \ldots = q_n = 0$. Then $k = n$. Therefore $G$ is isomorphic to the $K_n$. \hfill \Box

A direct consequence of the above Theorem is the following.

**Corollary 9.** Let $G$ be a $(n,m)$-graph with $k$ non-negative eigenvalues. Then

$$EE(G) \geq \frac{E(G)}{2} + e^{\left(\frac{2m}{n}\right)} + (k - 1) - \frac{2m}{n}. \tag{23}$$

Equality holds in (23) if and only if $G$ is isomorphic to $K_n$.

Considering the above Theorem and the lower bound due Das et al in [4], we obtain the following result.

**Corollary 10.** Let $G$ be a connected non-singular graph of order $n$ with $k$ strictly positive eigenvalues. Then

$$EE(G) \geq \frac{1}{2} \left( n - 1 + \ln \left( \det (A(G)) \right) + \ln (\lambda_1) \right) + e^{\lambda_1} + (k - 1) - \frac{\lambda_1}{2}. $$

Applying the technique used in above Theorem, to the signless Laplacian matrix, we obtain the following result.

**Theorem 11.** Let $(n,m)$ graph $G$. Then

$$EE(Q(G)) \geq QE(G) + e^{q_1} + (n - 1) - q_1. $$

The equality holds if and only if $G = K_n$.

**Proof.** By the definition of signless Laplacian energy, we have

$$QE((G)) = \sum_{i=1}^{n} \left| q_i - \frac{2m}{n} \right| \leq \sum_{i=1}^{n} q_i$$

$$= q_1 + \sum_{i=2}^{n} q_i$$

$$\leq q_1 + \sum_{i=2}^{n} (e^{q_i} - 1)$$

$$= q_1 + \sum_{i=1}^{n} e^{q_i} - (n - 1) - e^{q_1}$$

$$= q_1 + EE(Q(G)) - (n - 1) - e^{q_1}. $$

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Suppose now that the equality holds. From the equality in (18), we get $q_1 = \ldots = q_n = 0$. Therefore $G$ is isomorphic to the $K_n$. Therefore, we prove the result.

A direct consequence of the above Theorem is the following result.

**Corollary 12.** Let $G$ be a $(n,m)$-graph. Then

$$EE(Q(G)) \geq QE(G) + e(\frac{4m}{n}) + (n - 1) - \frac{4m}{n}. \quad (24)$$

Equality holds in (24) if and only if $G$ is isomorphic to $K_n$. 

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