A Note on Some Bounds of the $\alpha$-Estrada Index of Graphs

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1. Introduction

Let $G = (V(G), E(G))$ be a simple undirected graph with $n$ vertices, where $V(G)$ denotes the vertex set of $G$ and $E(G)$ denotes the edge set of $G$. Let $A(G)$ and $D(G)$ denote the adjacency matrix and degree matrix of $G$, respectively. The Laplacian (signless Laplacian) matrix of $G$ is $L(G) = D(G) - A(G)$, where $0 \leq \alpha \leq 1$ and $A(G)$ and $D(G)$ denote the adjacency matrix and degree matrix of $G$, respectively. The Laplacian (signless Laplacian) matrix of $G$ is $L(G) = D(G) - A(G)$, where $0 \leq \alpha \leq 1$ and $A(G)$ and $D(G)$ denote the adjacency matrix and degree matrix of $G$, respectively. The Laplacian (signless Laplacian) matrix of $G$ is $L(G) = D(G) - A(G)$, where $0 \leq \alpha \leq 1$ and $A(G)$ and $D(G)$ denote the adjacency matrix and degree matrix of $G$, respectively. The Laplacian (signless Laplacian) matrix of $G$ is $L(G) = D(G) - A(G)$, where $0 \leq \alpha \leq 1$ and $A(G)$ and $D(G)$ denote the adjacency matrix and degree matrix of $G$, respectively. The Laplacian (signless Laplacian) matrix of $G$ is $L(G) = D(G) - A(G)$, where $0 \leq \alpha \leq 1$ and $A(G)$ and $D(G)$ denote the adjacency matrix and degree matrix of $G$, respectively. The Laplacian (signless Laplacian) matrix of $G$ is $L(G) = D(G) - A(G)$, where $0 \leq \alpha \leq 1$ and $A(G)$ and $D(G)$ denote the adjacency matrix and degree matrix of $G$, respectively. The Laplacian (signless Laplacian) matrix of $G$ is $L(G) = D(G) - A(G)$, where $0 \leq \alpha \leq 1$ and $A(G)$ and $D(G)$ denote the adjacency matrix and degree matrix of $G$, respectively.

The Estrada index [7] of $G$ is defined as

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

where $\lambda_1, \ldots, \lambda_n$ are eigenvalues of $A(G)$. The Estrada index can be used to measure the folding degree of long-chain proteins [8, 9] and subgraph centrality in complex networks [10–13].

The Laplacian Estrada index and signless Laplacian Estrada index of $G$ are defined as $\text{LEE}(G) = \sum_{i=1}^{n} e^{\lambda_i}$ and $\text{SLEE}(G) = \sum_{i=1}^{n} e^{q_i}$, respectively, where $q_1, \ldots, q_n$ are eigenvalues of $L(G)$ and $Q(G)$, respectively [14, 15]. Some mathematical and chemical properties of $\text{EE}(G)$, $\text{LEE}(G)$, and $\text{SLEE}(G)$ are investigated extensively in mathematical chemistry [14, 16–25]. For other generalized Estrada index, see [26, 27].

In [28], Guo and Zhou proposed the $\alpha$-Estrada index as

$$\text{EE}_\alpha(G) = \sum_{i=1}^{n} e^{\lambda_i^\alpha} = \sum_{i=1}^{n} \sum_{k=0}^{\infty} \frac{\lambda_i^k}{k!}, \quad (2)$$

where $\lambda_1, \ldots, \lambda_n$ are eigenvalues of $\tilde{A}_\alpha(G)$. Obviously, $\text{EE}_\alpha(G)$ is the Estrada index; note that $\text{EE}_{1/2}$ is somewhat different from the signless Laplacian Estrada index, which is defined to be $\text{SLEE}(G) = \sum_{i=1}^{n} e^{2\lambda_i}$, where $\lambda_i$ are the eigenvalues of $\tilde{A}_{1/2}(G)$.

The paper is organized as follows: In Section 2, some bounds for $\text{EE}_\alpha(G)$ are obtained in terms of the number of vertices, edges, and triangles of $G$. We also give some new bounds for $\text{EE}_\alpha(G)$ through different numerical inequalities. Furthermore, some relations between the $\alpha$-Estrada index and $\alpha$-energy are established. In Section 3, we compare our new bounds to the existing results for the $\alpha$-Estrada index by certain graphs, benchmark graphs, and random graphs.
In Section 4, we summarize the results of the paper, and the future work is envisaged.

2. Some Bounds for the $\alpha$-Estrada Index

In what follows, let $\text{tr}(M)$ denote the trace of matrix $M$. Let $d_i$ denote the degree of vertex $i$.

**Lemma 1** (see [1, 5]). Let $G$ be a graph with $m$ edges and $t$ triangles. Then

$$\text{tr}(A_{\alpha}(G)) = 2am,$$

(3)

$$\text{tr}(A_{\alpha}^2(G)) = 2(1-\alpha)^2m + \alpha^2 \sum_{i \in V(G)} d_i^2,$$

(4)

$$\text{tr}(A_{\alpha}^3(G)) = \alpha^3 \sum_{i \in V(G)} d_i^4 + 3a(1-\alpha)^2 \sum_{i \in V(G)} d_i^2 + 6(1-\alpha)^3 t.$$  

(5)

In this section, let $\tau(G) = \{i,j,k\} \subseteq V(G)$: $i,j,k$ form a triangle of $G$; let $\beta$ and $\xi$ denote the numbers of subgraphs of $G$ which are isomorphic to path $P_3$ and cycle $C_4$, respectively.

**Proposition 2.** Let $G$ be a graph with $m$ edges. Then

$$\text{tr}(A_{\alpha}^4(G)) = \alpha^4 \sum_{i \in V(G)} d_i^4 + 4\alpha^2(1-\alpha)^2 \sum_{i \in V(G)} d_i^3$$

$$+ 8\alpha(1-\alpha)^3 \sum_{\{i,j,k\} \in \tau(G)} (d_i + d_j + d_k).$$

(6)

It is known that $\text{tr}(A_{\alpha}^4(G)) = 2m + 4\beta + 8\xi$ (see [29]). Let $\mathcal{A} = \alpha D(G)$ and $\mathcal{B} = (1-\alpha)A(G)$ Taking the trace of $A_{\alpha}^4(G)$, we have

$$\text{tr}((\mathcal{A} + \mathcal{B})^4) = \text{tr}(\mathcal{A}^2 + \mathcal{A} \mathcal{B} + \mathcal{B} \mathcal{A} + \mathcal{B}^2)$$

$$= \text{tr}(\mathcal{A}^2 + \mathcal{A} \mathcal{B} + \mathcal{B} \mathcal{A} + \mathcal{B}^2)$$

$$= \text{tr}(\mathcal{A}^4 + 4\mathcal{A}^3 \mathcal{B} + 6\mathcal{A}^2 \mathcal{B}^2 + 4\mathcal{A} \mathcal{B}^3 + 2(\mathcal{A} \mathcal{B} + \mathcal{B}^2))$$

$$= \alpha^4 \sum_{i \in V(G)} d_i^4 + 4\alpha^2(1-\alpha)^2 \sum_{i \in V(G)} d_i^3$$

$$+ 8\alpha(1-\alpha)^3 \sum_{\{i,j,k\} \in \tau(G)} (d_i + d_j + d_k)$$

$$+ 4\alpha^2(1-\alpha)^2 \sum_{\{i,j\} \in \mathcal{E}(G)} d_i d_j$$

$$+ (1-\alpha)^4(2m + 4\beta + 8\xi).$$

(8)

In the following, we give a lower bound for the $\alpha$-Estrada index of a graph by using the parameter $\alpha$, the vertex number, the edge number, and the numbers of subgraphs of $G$.

**Theorem 3.** Let $G$ be a graph with $n$ vertices, $m$ edges, and $t$ triangles. Then

$$\text{EE}_{\alpha}(G) \geq n + \left(2\alpha + (1-\alpha)^2 + \frac{1}{12}(1-\alpha)^4\right) m$$

$$+ (2\alpha^2 + 2\alpha(1-\alpha)^2) \sum_{\{i,j,k\} \in \tau(G)} d_i + d_j + d_k$$

$$+ \frac{m^3}{n^3} + \alpha^2 \sum_{\{i,j\} \in \mathcal{E}(G)} d_i d_j$$

$$+ 6(1-\alpha)^2 t + \frac{1}{6}(1-\alpha)^4(\beta + 2\xi).$$

(9)

where $\gamma = \sum_{\{i,j\} \in \mathcal{E}(G)} d_i + d_j$, $\xi = \sum_{\{i,j,k\} \in \tau(G)} d_i + d_j + d_k$.

**Proof.** By defining $\text{EE}_{\alpha}(G)$, we have

$$\text{EE}_{\alpha}(G) = \sum_{k=0}^{\infty} \frac{\text{tr}(A_{\alpha}^k(G))}{k!},$$

$$\text{EE}_{\alpha}(G) \geq n + \text{tr}(A_{\alpha}^2(G)) + \frac{\text{tr}(A_{\alpha}^3(G))}{2!} + \frac{\text{tr}(A_{\alpha}^4(G))}{3!}$$

$$+ \frac{\text{tr}(A_{\alpha}^5(G))}{4!}.$$ 

(10)

According to the H"{o}lder inequality, we have $2m = \sum_{i \in V(G)} d_i \leq n^{(r-1)/r} \left( \sum_{i \in V(G)} d_i^r \right)^{1/r}$ for any positive integer $t$. Hence

$$\sum_{i \in V(G)} d_i^t \geq \frac{(2m)^t}{n^{t-1}}.$$ 

(11)
By (3)–(11) and Proposition 2, we have

\[
\begin{align*}
\EE_a(G) & \geq n + \frac{1}{2} \left( 2(1 - \alpha)^2 m + \alpha^2 \sum_{i \in V(G)} d_i^2 \right) \\
& \quad + \frac{1}{6} \left( \alpha^3 \sum_{i \in V(G)} d_i^2 + 3 \alpha(1 - \alpha)^2 \sum_{i \in V(G)} d_i^2 + 6(1 - \alpha)^3 t \right) \\
& \quad + \frac{1}{24} \left( \alpha^4 \sum_{i \in V(G)} d_i^4 + 4 \alpha^2(1 - \alpha)^2 \sum_{i \in V(G)} d_i^2 \\
& \quad + 8 \alpha(1 - \alpha)^3 \sum_{(i,j) \in E(G)} (d_i + d_j + d_k) + 4 \alpha^2(1 - \alpha)^2 \gamma \\
& \quad + (1 - \alpha)^4(2m + 4\beta + 8\xi) \right) + 2am \geq n + 2am \\
& \quad + \frac{1}{2} \left( 2(1 - \alpha)^2 m + \alpha^2 \frac{4m^2}{n} \right) \\
& \quad + \frac{1}{6} \left( \alpha^3 \frac{8m^3}{n^2} + 3 \alpha(1 - \alpha)^2 \frac{4m^2}{n} + 6(1 - \alpha)^3 t \right) \\
& \quad + \frac{1}{24} \left( \alpha^4 \frac{16m^4}{n^3} + \alpha^2(1 - \alpha)^2 \frac{32m^3}{n^2} + 8 \alpha(1 - \alpha)^3 \zeta \\
& \quad + 4 \alpha^2(1 - \alpha)^2 \gamma + (1 - \alpha)^4(2m + 4\beta + 8\xi) \right) \\
& = n + \left( 2 \alpha + (1 - \alpha)^2 + \frac{1}{12} (1 - \alpha)^4 \right) m \\
& \quad + (2 \alpha^2 + 2 \alpha(1 - \alpha)^2) \frac{m^2}{n} + \frac{4}{3} (\alpha^3 + \alpha^2(1 - \alpha)^2) \frac{m^3}{n^2} \\
& \quad + \frac{2}{3} \alpha^4 \frac{m^4}{n^3} + (1 - \alpha)^3 t + \frac{1}{3} \alpha(1 - \alpha)^3 \zeta \\
& \quad + \frac{1}{6} \alpha^2(1 - \alpha)^2 \gamma + \frac{1}{6} (1 - \alpha)^4(\beta + 2\xi),
\end{align*}
\]

(12)

where \( \gamma = \sum_{(i,j) \in E(G)} d_i d_j, \ \zeta = \sum_{(i,j,k) \in E(G)} (d_i + d_j + d_k). \)

**Corollary 4.** Let \( G \) be an \( r \)-regular graph with \( n \) vertices and \( t \) triangles. Then

\[
\begin{align*}
\EE_a(G) & > n + \left( \alpha + \frac{1}{2} (1 - \alpha)^2 + \frac{1}{24} (1 - \alpha)^4 \right) nr \\
& \quad + \frac{1}{2} \left( \alpha^2 + \alpha(1 - \alpha)^2 \right) nr^2 + \left( \frac{1}{6} \alpha^3 + \frac{1}{4} \alpha^2(1 - \alpha)^2 \right) \\
& \quad \cdot nr^3 + \frac{1}{24} \alpha^4 nr^4 + (1 - \alpha)^3 t + \alpha(1 - \alpha)^3 rt \\
& \quad + \frac{1}{6} (1 - \alpha)^4(\beta + 2\xi).
\end{align*}
\]

(13)

**Proof.** Since \( G \) is an \( r \)-regular graph, then \( m = (1/2)nr, \ \gamma = \sum_{i \in V(G)} d_i = (1/2)n r^2, \ \zeta = \sum_{(i,j,k) \in E(G)} (d_i + d_j + d_k) = 3rt. \) By Theorem 3, we have

\[
\EE_a(G) > n + \left( \alpha + \frac{1}{2} (1 - \alpha)^2 + \frac{1}{24} (1 - \alpha)^4 \right) nr \\
& \quad + \frac{1}{2} \left( \alpha^2 + \alpha(1 - \alpha)^2 \right) nr^2 + \frac{1}{6} (\alpha^3 + \alpha^2(1 - \alpha)^2) nr^3 \\
& \quad + \frac{1}{24} \alpha^4 nr^4 + (1 - \alpha)^3 t + \alpha(1 - \alpha)^3 rt \\
& \quad + \frac{1}{6} (1 - \alpha)^4(\beta + 2\xi).
\]

(14)

Also, we give another lower bound for the \( \alpha \)-Estrada index of a graph including the parameter \( \alpha \), the vertex number, the edge number, and the numbers of triangles of \( G \).

**Theorem 5.** Let \( G \) be a graph with \( n \) vertices, \( m \) edges, and \( t \) triangles. Then

\[
\begin{align*}
\EE_a(G) & \geq \sqrt{n^2 + (8 \alpha^2 + 8 \alpha(1 - \alpha)^2) m^2 + (2(1 - \alpha)^2 + 4 \alpha^2) mn + \alpha^2 \frac{12m^2}{3n} + 2(1 - \alpha)^4 nt.}
\end{align*}
\]

(15)

**Proof.** Let \( \lambda_1, \cdots, \lambda_n \) be eigenvalues of \( \tilde{A}_a(G) \). By the Taylor expansion theorem, then

\[
e^{\xi} \geq 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!},
\]

(16)

with equality if and only if \( x = 0. \)

\[
\begin{align*}
\EE_a(G)^2 & = \sum_{\beta=1}^n \sum_{\alpha=1}^n \alpha^{k_1} \beta^{k_2} \\
& \geq \sum_{\beta=1}^n \sum_{\alpha=1}^n \left( 1 + \lambda_\beta + \lambda_\alpha + \frac{\lambda_\beta + \lambda_\alpha}{2!} + \frac{(\lambda_\beta + \lambda_\alpha)^3}{3!} \right) \\
& = \sum_{\beta=1}^n \sum_{\alpha=1}^n \left( 1 + \lambda_\beta + \lambda_\alpha \lambda_\beta + \lambda_\beta^2 + \lambda_\alpha^2 + \lambda_\beta^3 + \lambda_\alpha^3 \right) \\
& \quad + \frac{\lambda_\beta \lambda_\alpha^2}{2} + \frac{\lambda_\beta^3}{6} + \frac{\lambda_\alpha^3}{6}.
\end{align*}
\]

(17)

By (3), we have

\[
\sum_{i=1}^n \lambda_i = 2am.
\]

(18)
\[
\sum_{i=1}^{n} \sum_{j=1}^{n} (\lambda_i + \lambda_j) = n \sum_{i=1}^{n} \lambda_i + n \sum_{j=1}^{n} \lambda_j = 4amn,
\]
\[
\sum_{i=1}^{n} \sum_{j=1}^{n} (\lambda_i \lambda_j) = \left( \sum_{i=1}^{n} \lambda_i \right)^2 = 4a^2m^2.
\]

By (4) and (11), we have
\[
\sum_{i=1}^{n} \lambda_i^2 \geq 2(1 - \alpha)^3m + \alpha^2 \frac{4m^2}{n}.
\]

So
\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \left( \frac{\lambda_i^2}{2} + \frac{\lambda_j^2}{2} \right) = \frac{n}{2} \left( \sum_{i=1}^{n} \lambda_i^2 + \sum_{j=1}^{n} \lambda_j^2 \right) \\
\geq 2(1 - \alpha)^3mn + 4a^2m^2, \quad \sum_{i=1}^{n} \sum_{j=1}^{n} \left( \frac{\lambda_i^2 \lambda_j + \lambda_j^2 \lambda_i}{2} \right) \\
= \frac{1}{2} \left( \sum_{i=1}^{n} \lambda_i^2 + \sum_{j=1}^{n} \lambda_j^2 \right) + \frac{1}{2} \left( \sum_{i=1}^{n} \lambda_i \sum_{j=1}^{n} \lambda_j \right) \\
\geq 4\alpha(1 - \alpha)^2m^3 + \frac{8a^3m^3}{n}.
\]

By (5) and (11), we have
\[
\sum_{i=1}^{n} \lambda_i^3 \geq \alpha^3 \frac{8m^3}{n^2} + 3\alpha(1 - \alpha)^2 \frac{4m^2}{n} + 6(1 - \alpha)^3t.
\]

So
\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \left( \frac{\lambda_i^3}{6} + \frac{\lambda_j^3}{6} \right) = \frac{n}{3} \sum_{i=1}^{n} \lambda_i^3 \geq 2(1 - \alpha)^3nt + 4\alpha(1 - \alpha)^2m^2 \\
+ \frac{8a^3m^3}{3n}.
\]

Summarize the above conclusions, we have
\[
\text{EE}_\alpha(G)^2 \geq n^2 + 4amn + 4\alpha^2m^2 + 2(1 - \alpha)^2mn + 4a^2m^2 \\
+ 4\alpha(1 - \alpha)^2m^2 + \frac{8a^3m^3}{n} + 2(1 - \alpha)^3nt \\
+ 4\alpha(1 - \alpha)^2m^2 + \frac{8a^3m^3}{n} \\
= n^2 + \left( 8\alpha^2 + 8\alpha(1 - \alpha)^2 \right)m^2 + \left( 2(1 - \alpha)^2 + 4a^2 \right)mn \\
+ \alpha^3 \frac{32m^3}{3n} + 2(1 - \alpha)^3nt.
\]

In order to prove Theorem 8, we give two lemmas as follows:

**Lemma 6** (see [27]). Let \(x_1, x_2, \ldots, x_n\) be nonnegative real numbers, and \(k > 2\), then
\[
\sum_{i=1}^{n} x_i^k \leq \left( \sum_{i=1}^{n} x_i^2 \right)^{k/2}.
\]

**Lemma 7** (see [30]). Let \(G\) be a graph with \(n\) vertices and \(m\) edges. Then
\[
\sum_{i \in V(G)} d_i^2 \leq m \left( \frac{2m}{n-1} + n - 2 \right).
\]

Inspired by literatures [14, 18], we obtained some bounds on the \(\alpha\)-Estrada index by arithmetic-geometric inequality.

**Theorem 8.** Let \(G\) be a graph with \(n\) vertices and \(m\) edges. Then
\[
\sqrt{n + 4am + n(n - 1)e^{\alpha mn}} \leq \text{EE}_\alpha(G) \leq n + 2am - 1 - \omega + e^\omega,
\]
where \(\omega = \sqrt{2(1 - \alpha)^2m(n - 1) + 2a^2m^2 - a^2(n - 1)(n - 2)m}/(n - 1)\).

**Proof.** Let \(\lambda_1, \ldots, \lambda_n\) be eigenvalues of \(\tilde{A}_\alpha(G)\). Then
\[
\text{EE}_\alpha(G)^2 = \sum_{i=1}^{n} e^{2\lambda_i} + 2 \sum_{i<j} e^{\lambda_i} e^{\lambda_j}.
\]

By the arithmetic-geometric inequality, we have
\[
2 \sum_{i<j} e^{\lambda_i} e^{\lambda_j} \geq n(n - 1) \left( \prod_{i<j} e^{\lambda_i} e^{\lambda_j} \right)^{2/(n(n - 1))} = n(n - 1) \left( \prod_{i=1}^{n} e^{\lambda_i} \right)^{2/(n(n - 1))} = n(n - 1)e^{2amn/n}.
\]

By the Taylor expansion theorem, we have
\[
\sum_{i=1}^{n} e^{2\lambda_i} = \sum_{i=1}^{n} \sum_{k=0}^{n} \frac{(2\lambda_i)^k}{k!} = n + 4am + \sum_{i=1}^{n} \sum_{k=2}^{n} \frac{(2\lambda_i)^k}{k!}.
\]
Let $i \in [0, 4]$, we have
\[
\sum_{i=1}^{n} \lambda^i_i \geq n + 4am + i \sum_{k=2}^{n} \frac{\lambda^k_k}{k!}
\]
\[
= n + 4am - m - 2am + i \sum_{k=2}^{n} \frac{\lambda^k_k}{k!}
\]
\[
= (1 - i)n + (4a - 2a)m + iEE_a(G).
\]

By substituting the above formula and solving for $EE_a(G)$, we obtain
\[
EE_a(G)^2 \geq (1 - i)n + (4a - 2a)m + iEE_a(G) + n(n - 1)e^{2am/n},
\]
\[
EE_a(G) \geq \frac{i}{2} + \sqrt{(1 - i)n + (4a - 2a)m + \frac{i^2}{4} + n(n - 1)e^{2am/n}}.
\]
\[
\text{(32)}
\]

It is elementary to show for $n \geq 2$; let the function
\[
f(x) = \frac{x}{2} + \sqrt{(1 - x)n + (4a - 2a)m + \frac{x^2}{4} + n(n - 1)e^{2am/n}},
\]
\[
\text{(33)}
\]

where $0 \leq \alpha \leq 1$; then $f(x)$ monotonically decrease in the interval $[0, 4]$. Let $x = 0$; $f(x)$ is max; that is to say, $i = 0$, $EE_a(G)$ is a better lower bound.

By Lemmas 6 and 7, we have
\[
EE_a(G) = n + 2am + \sum_{i=1}^{n} \frac{\lambda^i_i}{i!}
\]
\[
\leq n + 2am + \sum_{k=2}^{n} \sum_{i=2}^{n} \frac{|\lambda^k_k|^{i-k}}{k!}
\]
\[
= n + 2am + \sum_{k=2}^{n} \frac{1}{k!} \sum_{i=2}^{n} |\lambda^k_k|^{i-k}
\]
\[
\leq n + 2am + \frac{1}{k!} \left( \sum_{i=1}^{n} \lambda^i_i \right)^{k/2}
\]
\[
= n + 2am + \frac{1}{k!} \left( \sum_{i=1}^{n} \lambda^i_i \right)^{k/2}
\]
\[
= n + 2am + \frac{1}{k!} \left( 2(1 - a)^2m + a^2 \sum_{i=1}^{n} d^2_i \right)^{k/2}
\]
\[
\leq n + 2am + \frac{1}{k!} \left( 2(1 - a)^2m + a^2m \left( \frac{2m}{n - 1} + n - 2 \right) \right)^{k/2}
\]
\[
= n + 2am - 1 - \omega + \frac{1}{k!} \omega^k
\]
\[
= n + 2am - 1 - \omega + e^\omega,
\]
\[
\text{(34)}
\]

where $\omega = \sqrt{2(1 - a)^2m(n - 1) + 2a^2m^2 - a^2(n - 1)(n - 2)m}/(n - 1)$.

In what follows, let $\lambda_1$ and $\lambda_n$ be the largest and the smallest of $A_a(G)$, respectively.

**Lemma 9** (see [1]). Let $G$ be a graph on $n$ vertices with $m$ edges. Then
\[
\lambda_1 \geq \frac{2m}{n}.
\]
\[
\text{(35)}
\]

The equality holds if and only if $G$ is a regular graph.

**Theorem 10.** Let $G$ be a graph on $n$ vertices with $m$ edges. Then
\[
EE_a(G) \geq e^{2mn/n} + (n - 1) + 2am - \frac{2m}{n}.
\]
\[
\text{(36)}
\]

**Proof.** Consider the function
\[
f(x) = (x - 1) - \ln x, \quad x > 0.
\]
\[
\text{(37)}
\]

Obviously, the function $f(x)$ is decreasing in $x \in (0, 1]$ and increasing in $x \in [1, +\infty)$; then $f(x) \geq f(1) = 0$, implying that
\[
x \geq 1 + \ln x, \quad x > 0.
\]
\[
\text{(38)}
\]

The equality holds if and only if $x = 1$. By Lemma 1, we have
\[
EE_a(G) \geq e^{h_1} + (n - 1) + \sum_{k=2}^{n} \ln e^{h_k}
\]
\[
= e^{h_1} + (n - 1) + \sum_{k=2}^{n} \lambda_k
\]
\[
= e^{h_1} + (n - 1) + 2am - \lambda_1.
\]
\[
\text{(39)}
\]

Define another function
\[
\Phi(x) = e^x + (n - 1) + 2am - x, \quad x > 0.
\]
\[
\text{(40)}
\]

Clearly, this is an increasing function on $x \in (0, +\infty)$. On the other hand, by Lemma 9,
\[
\lambda_1 \geq \frac{2m}{n} \geq 0.
\]
\[
\text{(41)}
\]

Then,
\[
\Phi(\lambda_1) \geq \Phi \left( \frac{2m}{n} \right).
\]
\[
\text{(42)}
\]

Finally, we get
\[
EE_a(G) \geq e^{2mn/n} + (n - 1) + 2am - \frac{2m}{n}.
\]
\[
\text{(43)}
\]

From Theorem 10, we have the following result.

**Corollary 11.** Let $G$ be a $r$-regular graph with $n$ vertices. Then
\[
EE_a(G) \geq e^r + (n - 1) + anr - r.
\]
\[
\text{(44)}
\]
In the following, we also obtained some other bounds for the $\alpha$-Estrada index through Sarasija’s [31], Ozeki’s [32], Polya’s [33], and Guo’s [34] inequalities, respectively.

**Lemma 12** (see [31]). Let $x_1, x_2, \cdots, x_n$ be nonnegative real numbers. Then

$$\left(\frac{1}{n} \sum_{i=1}^{n} x_i - \left(\prod_{i=1}^{n} x_i\right)^{1/n}\right)^2 \leq n \left(\frac{1}{n} \sum_{i=1}^{n} x_i - \left(\prod_{i=1}^{n} x_i\right)^{1/n}\right)^2$$

$$\leq n(n-1) \left(\frac{1}{n} \sum_{i=1}^{n} x_i - \left(\prod_{i=1}^{n} x_i\right)^{1/n}\right).$$

(45)

**Theorem 13.** Let $G$ be a graph on $n$ vertices with $m$ edges. Then

$$\frac{(\sum_{i=1}^{n} e^{\lambda_i}/2)^2 - n e^{2\lambda_m/n}}{n-1} \leq EE_{a}(G) \leq \frac{(\sum_{i=1}^{n} e^{\lambda_i}/2)^2}{n-1} - n(n-1) e^{2\lambda_m/n}.$$  

(46)

**Proof.** By Lemma 1 and Lemma 12, let $x_i = e^{\lambda_i}$ ($i = 1, 2, \cdots, n$); we have

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

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

(47)

Then

$$\sum_{i=1}^{n} e^{\lambda_i} - n e^{2\lambda_m/n} \leq n \sum_{i=1}^{n} e^{\lambda_i} - \left(\sum_{i=1}^{n} e^{\lambda_i}/2\right)^2$$

$$\leq n(n-1) \sum_{i=1}^{n} e^{\lambda_i} - n(n-1) e^{2\lambda_m/n}.$$  

(48)

Consider the left and right sides of inequality, respectively, we have

$$\sum_{i=1}^{n} e^{\lambda_i} - n e^{2\lambda_m/n} \leq n \sum_{i=1}^{n} e^{\lambda_i} - \left(\sum_{i=1}^{n} e^{\lambda_i}/2\right)^2,$$

$$EE_{a}(G) \geq \frac{(\sum_{i=1}^{n} e^{\lambda_i}/2)^2 - n e^{2\lambda_m/n}}{n-1}.$$  

(49)

Similarly,

$$EE_{a}(G) \leq \frac{(\sum_{i=1}^{n} e^{\lambda_i}/2)^2}{n-1} - n(n-1) e^{2\lambda_m/n}.$$  

(50)

**Lemma 14** (see [32]). If $a_i$ and $b_i$ are positive real numbers for $1 \leq i \leq n$, then

$$\left(\sum_{i=1}^{n} a_i^2\right) \left(\sum_{i=1}^{n} b_i^2\right) - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \frac{n^2}{4} \left(M_1M_2 - m_1m_2\right)^2,$$

(51)

where $M_1 = \max_{i \leq n} a_i$, $M_2 = \max_{i \leq n} b_i$, $m_1 = \min_{i \leq n} a_i$, and $m_2 = \min_{i \leq n} b_i$.

**Theorem 15.** Let $G$ be a graph on $n$ vertices with $m$ edges. Then

$$EE_{a}(G) \geq \sqrt{n \left(\sum_{i=1}^{n} e^{\lambda_i}\right) - \frac{n^2}{4} \left(e^{\lambda_1} - e^{\lambda_n}\right)^2}.$$  

(52)

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

**Proof.** Let $a_i = e^{\lambda_i}$ and $b_i = 1$; then $m_1 = e^{\lambda_n}$, $M_1 = e^{\lambda_1}$, and $m_2 = M_2 = 1$, respectively. According to Lemma 14, we have

$$\left(\sum_{i=1}^{n} e^{\lambda_i}\right) \left(\sum_{i=1}^{n} 1\right) - \left(\sum_{i=1}^{n} e^{\lambda_i}\right)^2 \leq \frac{n^2}{4} \left(e^{\lambda_1} - e^{\lambda_n}\right)^2.$$  

(53)

Then

$$EE_{a}(G) \geq \sqrt{n \left(\sum_{i=1}^{n} e^{\lambda_i}\right) - \frac{n^2}{4} \left(e^{\lambda_1} - e^{\lambda_n}\right)^2}.$$  

(54)

**Lemma 16** (see [33]). Suppose $a_i$ and $b_i$ are positive real numbers for $1 \leq i \leq n$; then

$$\left(\sum_{i=1}^{n} a_i^2\right) \left(\sum_{i=1}^{n} b_i^2\right) \leq \frac{1}{4} \left(M_1 M_2 + m_1 m_2\right) \left(M_1 M_2 - m_1 m_2\right)^2 \left(\sum_{i=1}^{n} a_i b_i\right)^2,$$

(55)

where $M_1 = \max_{i \leq n} a_i$, $M_2 = \max_{i \leq n} b_i$, $m_1 = \min_{i \leq n} a_i$, and $m_2 = \min_{i \leq n} b_i$. 


Theorem 17. Let $G$ be a graph on $n$ vertices with $m$ edges. Then

$$EE_a(G) \geq \frac{2\sqrt{n}}{\lambda_1 + \lambda_n} \left( \sum_{i=1}^{n} e^{\lambda_i} \right) \left( \sum_{i=1}^{n} e^{-\lambda_i} \right) .$$

(56)

Proof. Let $a_i = e^{\lambda_i}$ and $b_i = 1$; then $m_1 = e^{\lambda_1}$, $M_1 = e^{\lambda_1}$, and $m_2 = M_2 = 1$, respectively. By Lemma 16, we have

$$\left( \sum_{i=1}^{n} e^{\lambda_i} \right) \left( \sum_{i=1}^{n} e^{-\lambda_i} \right) \leq \frac{1}{4} \left( \sum_{i=1}^{n} e^{\lambda_i} \right) \left( \sum_{i=1}^{n} e^{-\lambda_i} \right) .$$

(57)

Then

$$EE_a(G) \geq \frac{2\sqrt{n}}{\lambda_1 + \lambda_n} \left( \sum_{i=1}^{n} e^{\lambda_i} \right) \left( \sum_{i=1}^{n} e^{-\lambda_i} \right) .$$

(58)

Lemma 18 (see [34]). For $a_1, a_2, \ldots, a_n \geq 0$ and $p_1, p_2, \ldots, p_n \geq 0$ such that $\sum_{i=1}^{n} p_i = 1$, then

$$\sum_{i=1}^{n} a_i \geq \left( \sum_{i=1}^{n} a_i^{1/n} \right) .$$

(59)

where $T = \min \{ p_1, p_2, \ldots, p_n \}$. Equality holds if and only if $a_1 = a_2 = \cdots = a_n$.

Theorem 19. Let $G$ be a graph with $n$ vertices with $m$ edges. Then

$$EE_a(G) \geq e^{\lambda_1} + 2(n - 1)\Delta - (n - 1)e^{2am/n},$$

(60)

where $\Delta = e^{(2am/(2n-1))}/(2n(n-1))$. Equality holds if and only if $G \cong K_n$.

Proof. Let $p_i = 1/2n$, $p_i = (2n - 1)/((2n(n-1)))$ for $i = 2, \cdots, n$, $a_i = e^{\lambda_i}$ and for $i = 2, \cdots, n$. Obviously, $T = \min \{ 1/2n, (2n - 1)/(2n(n-1)) \} = 1/2n$, according to Lemma 18; we have

$$\frac{e^{\lambda_1}}{2n} + \frac{2n - 1}{2n(n-1)} \sum_{i=2}^{n} e^{\lambda_i} - \Delta \geq \frac{1}{2} \left( \sum_{i=1}^{n} e^{\lambda_i} - \Pi_{i=1}^{n} e^{\lambda_i/n} \right) .$$

(61)

where $\Delta = e^{(2am/2n(n-1))}/(2n(n-1))$. We consider $\Delta$ is

$$\Delta = e^{(2am/(2n-1))}/(2n(n-1)) \cdot e^{\left( \frac{n}{2} \right) \sum_{i=1}^{n} \lambda_i / (2n(n-1))} \cdot e^{(2n - 1)/((2n(n-1)))} .$$

(62)

Since

$$\frac{e^{\lambda_1}}{2n} + \frac{2n - 1}{2n(n-1)} \left( \sum_{i=1}^{n} e^{\lambda_i} \right) - \Delta \geq \frac{1}{2} \sum_{i=1}^{n} e^{\lambda_i} - \frac{1}{2} e^{2am/n},$$

(63)

then

$$EE_a(G) \geq e^{\lambda_1} + 2(n - 1)\Delta - (n - 1)e^{2am/n},$$

(64)

equality holds if and only if $G \cong K_n$.

In the Hückel molecular orbital theory, graph energy is defined as the sum of the absolute values of the eigenvalues of the adjacency matrix of the molecular graph [35, 36]. In [28], the $\alpha$-energy of $G$ is defined as $\kappa_\alpha(G) = \sum_{i=1}^{n} |\lambda_i - (2am/n)|$, where $\lambda_1, \cdots, \lambda_n$ are the eigenvalues of $A(G)$. New bounds for the $\alpha$-Estrada index in terms of the $\alpha$-energy of the graph $G$ are established.

In [37], the Estrada index-like quantity is defined by

$$EE_\alpha(G) = \sum_{i=1}^{n} e^{x_{i}},$$

(65)

where $x_1, x_2, \cdots, x_n$ are arbitrary real numbers and $\bar{x}$ is their arithmetic mean. Let $x_1, x_2, \cdots, x_n$ and $\bar{x}$ be $\lambda_1, \cdots, \lambda_n$ and $2 am/n$, respectively. Evidently, $EE_a(G) = e^{2am/n}EE_\alpha(G)$, and therefore, results obtained for $EE_a(G)$ can be immediately restated for $EE_\alpha(G)$ and vice versa.

Theorem 20. Let $G$ be a graph on $n$ vertices with $m$ edges. Then

$$EE_a(G) \leq e^{2am/n} \left( \sum_{i=1}^{n} (\lambda_i - (2am/n)) = 0 \right).$$

(66)

Proof. Note that $\sum_{i=1}^{n} (\lambda_i - (2am/n)) = 0$. By Lemma 9, we have
$e^{-(2am/n)}$EE$_n(G) = E\tilde{E}_n(G)$

$$= n + \sum_{i=1}^{n} \sum_{k \geq 2} \left( \lambda_i - (2am/n) \right)^k \frac{k!}{k!}$$

$$\leq n + \sum_{i=1}^{n} \sum_{k \geq 2} \lambda_i \frac{\lambda_i}{k!}$$

$$\leq n + \frac{1}{k!} \zeta_a(G)$$

$$= n - 1 - \zeta_a(G) + e^{\zeta_a(G)}.$$ (67)

In order to prove Theorems 21 and 22, let $\lambda_i - (2am/n) = \delta_i$ (i = 1, ..., n), and let $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_k \geq 0 \geq \cdots \geq \delta_m$. By Lemma 1, we obtained $\sum_{i=1}^{n} \delta_i = 0$. The $\alpha$-energy of the graph $G$ is $\zeta_a(G) = \sum_{i=1}^{n} \delta_i$; then $(\zeta_a(G))/2 = \sum_{i=1}^{n} \delta_i = -\sum_{i<n} \delta_i$.

In the following, some relations between the $\alpha$-Estrada index and $\alpha$-energy are established.

**Theorem 21.** Let $G$ be a graph on $n$ vertices with $m$ edges. Then

$$EE_n(G) \geq e^{2am/n} \left( \frac{\zeta_a(G)}{2} - \delta_1 + (k-1) + e^{\delta_1} \right).$$ (68)

**Proof.** Let $x \geq 0$, considering the following function:

$$f(x) = -1 - x + e^x,$$ (69)

in which equality holds if and only if $x = 0$. The function $f(x)$ is increasing in $[0, +\infty)$. The $f(x) \geq f(0)$, implying that

$$x \leq e^x - 1, x \geq 0.$$ (70)

By (70), we have

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

$$= \delta_1 + \sum_{i=2, \delta_i \geq 0}^{k} \delta_i$$

$$\leq \delta_1 + \sum_{i=2, \delta_i \geq 0}^{k} (\delta_i - 1)$$

$$= \delta_1 - (k-1) + \sum_{i=1, \delta_i \geq 0}^{k} \delta_i$$

$$\leq \delta_1 - (k-1) + \sum_{i=1, \delta_i \geq 0}^{k} \delta_i$$

$$= \delta_1 - (k-1) + \sum_{i=1}^{n} \delta_i - \delta_1$$

$$= \delta_1 - (k-1) + EE_n(G) - \delta_1.$$ (71)

**Theorem 22.** Let $G$ be a graph on $n$ vertices with $m$ edges. Then

$$EE_n(G) \geq e^{2am/n} \left( k e^{\zeta(G)/2k} + (n-k) e^{-\zeta(G)/(2(n-k))} \right),$$ (72)

in which equality holds if and only if $\delta_1 = \cdots = \delta_k$ and $\delta_{k+1} = \cdots = \delta_m$.

**Proof.** By the Mean Quadratic inequality, we have

$$\sum_{i=1, \delta_i \geq 0}^{k} e^{\delta_i} \geq k e^{(\delta_1+\delta_2+\cdots+\delta_k)/k} = k e^{\zeta(G)/2k}.$$ (73)

Similarly,

$$\sum_{i=k+1, \delta_i < 0}^{n} e^{\delta_i} \geq (n-k) e^{-\zeta(G)/(2(n-k))}.$$ (74)

Then

$$EE_n(G) = e^{2am/n} \tilde{E}_n(G)$$

$$\geq e^{2am/n} \left( k e^{\zeta(G)/2k} + (n-k) e^{-\zeta(G)/(2(n-k))} \right).$$ (75)

The equality holds in (75) if and only if equalities hold in both (73) and (74). By the equality case in the Mean Quadratic inequality, equality occurs in (73) and (74) if and only if $\delta_1 = \cdots = \delta_k$ and $\delta_{k+1} = \cdots = \delta_m$; that is to say, the equality holds in (75) if and only if $\delta_1 = \cdots = \delta_k$ and $\delta_{k+1} = \cdots = \delta_m$. This means all negative eigenvalues and all nonnegative eigenvalues which completes the proof.

**3. Numerical Examples**

In this section, we list some computational experiments to compare our new bounds to previous results for certain connected graphs, benchmark graphs, and random graphs, where the results of the benchmark graphs and random graphs are the average of 20 independent experiments. We listed the lower bound of Theorem 1 (Th. 1) [23], the lower bound of Theorem 10 (Th. 10), the lower bound of Theorem 13 (Th. 13'), the upper bound of Theorem 2.1 (Th. 2.1) [38], the upper bound of Theorem 13 (Th. 13'), and the numerical value of $EE_n(G)$ (see Table 1).

The $C_{20}$, $C_{40}$, and $C_{46}$ are fullerenes (letter C is followed by the number of carbon atoms). ER(1) is the Erdös-Rényi random graph with $n = 100$ and $p = 0.05$. ER(2) is the Erdös-Rényi random graph with $n = 100$ and $p = 0.5$. BA is the Barabási-Albert random graph with $n = 100$, $m = 5$, and $n_0 = 50$. WS(1) is the Watts-Strogatz random graph with $n = 100$, $K = 6$, and $p = 0.1$. WS(2) is the Watts-Strogatz random graph with $n = 100$ and $K = 6$, and $p = 0.5$. GN is the GN (Girvan-Newman) Benchmark graph with $n = 128$, $k = 16$, $\max k = 16$, $\max k = 40$, $\min c = 32$, and $\max c = 32$. LFR is the LFR (Lancichinetti-Fortunato-Radicchi) Benchmark graph with $n = 1000$, $k = 10$, $\max k = 40$, $\min c = 0.2$, and $\max c = 60$ (for related parameters, see...
In this paper, we give some bounds on the α-Estrada index of $G$, some relations between the α-Estrada index and α-energy are established. At the same time, we also analyze the advantages and disadvantages of different bounds for certain connected graphs, benchmark graphs, and random graphs by numerical experiments. Our future work will focus on exploring the practical applications of the α-Estrada index in physical, chemical, and network sciences.

### Data Availability

The Estrada index is a spectral measure to character efficiently the strongness of complex networks. These prior studies (and datasets) are cited at relevant places within the text as references [7–11, 29]. Since the paper is a theoretical study, so no data were used to support this study.

### Conflicts of Interest

The authors declare that they have no conflicts of interest.

### Acknowledgments

This work was supported by the National Natural Science Foundation of China (No. 11801115 and No. 11601102), [39, 40]). We use $f^3$ instead of $10^3$ in Table 1. The results are kept to four decimal places.

According to the information in Table 1, we know that the lower bounds in Th. 2.10 and Th. 2.13 are better than the lower bound of Th. 1; the upper bound of Th. 2.13 is better than the upper bound of Th. 2.1. We also get some other results in Table 1 as follows: The lower bound of Th. 2.10 is better than the lower bounds of Th. 2.13 in the cycle graph, bipartite graph, Petersen graph, ER(2), WS(2), and LFR; Th. 2.13 is good in other cases. For sparse graphs, Th. 2.13 is good in most cases. For dense graph, Th. 2.10 is good in most cases.

### 4. Conclusion

In this paper, we give some bounds on the α-Estrada index of $G$, some relations between the α-Estrada index and α-energy are established. At the same time, we also analyze the advantages and disadvantages of different bounds for certain connected graphs, benchmark graphs, and random graphs by numerical experiments. Our future work will focus on exploring the practical applications of the α-Estrada index in physical, chemical, and network sciences.

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