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Research Article

A New Like Quantity Based on "Estrada Index"

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We first define a new Laplacian spectrum based on Estrada index, namely, *Laplacian Estrada-like invariant*, *LEEL*, and two new *Estrada index-like quantities*, denoted by S and EE_X, respectively, that are generalized versions of the Estrada index. After that, we obtain some lower and upper bounds for *LEEL*, S, and EE_X.

1. Introduction and Preliminaries

It is known that, for an (n, m)-graph G (i.e., an undirected graph with no loops and multiple edges), the numbers of vertices and edges of G are denoted by n and m, respectively. Throughout this paper, all graphs will be concerned as an (n, m)-graph.

Let $\mathbf{A} = \mathbf{A}(G)$ be the adjacency matrix of G, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues. By [1], it is known that these eigenvalues form the spectrum of the graph G. Let G be connected graph on the vertex set $V = \{v_1, v_2, \ldots, v_n\}$. Then the distance matrix $\mathbf{D} = \mathbf{D}(G)$ of G is defined as its (i, j)-entry is equal to $d_G(v_i, v_j)$, denoted by d_{ij}, the distance (in other words, the length of the shortest path) between the vertices v_i and v_j of G. Let the eigenvalues of $\mathbf{D}(G)$ be $\rho_1, \rho_2, \ldots, \rho_n$. Moreover let $\mathbf{L} = \mathbf{L}(G)$ be the Laplacian matrix of G (formally it is denoted by $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$), and let $\mu_1, \mu_2, \ldots, \mu_n$ be its eigenvalues. These eigenvalues form the Laplacian spectrum of the graph G (see [2–4]). Since $\mathbf{A}(G)$, $\mathbf{L}(G)$, and $\mathbf{D}(G)$ are real symmetric matrices, their eigenvalues are real numbers and so we can order them as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$, and $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. These eigenvalues are shortly called $\mathbf{A}$-eigenvalues, $\mathbf{L}$-eigenvalues, and $\mathbf{D}$-eigenvalues, respectively. The fundamental properties of graph eigenvalues can be found in the study in [1].

Now we recall that the Estrada index of a simple connected graph G is defined by

$$EE = EE(G) = \sum_{i=1}^{n} e^{\lambda_i}, \tag{1.1}$$

where, as depicted above, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the $\mathbf{A}$-eigenvalues (see [5–8]). Denoting by $M_k = M_k(G)$ the kth moment of the graph G, we get $M_k = M_k(G) = \sum_{i=1}^{n}(\lambda_i)^k$, and recalling the power-series expansion of e^x, we have

$$EE = \sum_{k=0}^{\infty}\frac{M_k}{k!}. \tag{1.2}$$

The Estrada index EE has an important role in Chemistry, since it is a proposed molecular structure descriptor, used in the modeling of certain features of the 3D structure of organic molecules, in particular of the degree of folding of proteins and other long-chain biopolymers. There exists a vast literature that studies Estrada index. For example, in [9] it has been examined Estrada index in the case of benzenoid hydrocarbons with a fixed number of carbon atoms and a fixed number of carbon-carbon bonds. Also, in [10], Gutman et al. determined its relation with the spectral radius (i.e., the greatest graph eigenvalue). In addition to Estrada's and Gutman's papers depicted above, we may also refer the reader [11–17] for more detail investigation about this special index and its lower and upper bounds, and some inequalities between EE and the energy of some graph G. Recently, there have been found two new papers [18, 19] that are concerned with the bounds of distance Estrada index and Harary Estrada index of the graph G, respectively.

As an additional preliminary material for this paper, we should recall that a graph-spectrum-based invariant, namely, the graph energy,is defined by

$$E = E(G) = \sum_{i=1}^{n}|\lambda_i|, \tag{1.3}$$

where each of λ_i is as above (see [20, 21]). Depending on this, a Laplacian-spectral of the graph energy, namely, Laplacian energy, is defined (see [22, 23]) by

$$LE = LE(G) = \sum_{i=1}^{n}\left|\mu_i - \frac{2m}{n}\right|. \tag{1.4}$$

It is known that LE and E have a number of common properties. As depicted in [24], Laplacian energy is currently much investigated and so many chemical applications can be found for it. Furthermore, in [25], it has been proposed another Laplacian spectrum based on "energy", and it has been called Laplacian-energy-like invariant, LEL, which is defined as

$$LEL = LEL(G) = \sum_{i=1}^{n}\sqrt{\mu_i}, \tag{1.5}$$

where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ are the $\mathbf{L}$-eigenvalues. (We should note that, since one of the $\mathbf{L}$-eigenvalues is necessarily equal to zero, μ_n is chosen as zero).

In the light of the above material, in this paper, we did propose another Laplacian spectrum based on "Estrada index", and called it *Laplacian Estrada-like invariant*, denoted by *LEEL*. In fact it is defined as

$$LEEL = LEEL(G) = \sum_{i=1}^{n} e^{\sqrt{\mu_i}}, \tag{1.6}$$

where each of μ_i is defined as in *LEL*.

For a well understanding of the definition and properties of *LEEL*, and of the dependence of it with the graph structure, in this paper, we mainly establish lower and upper bounds for *LEEL* in terms of n, m, and *LEL*. Moreover we also present Nordhaus-Gaddum-type bounds for *LEEL*. Finally, by considering an arbitrary quantity defined from the graph G, we also generalize some of the known results on lower and upper bounds that are obtained previously (see [12, 17, 18]) and our results that will be given in the second section.

2. Bounds for Laplacian Estrada-Like Invariant in terms of Laplacian Energy-Like Invariant

As a new derivation for obtaining bounds in indexes, we will at first determine some lower and upper bounds for Laplacian Estrada-like invariant, *LEEL*. So the following theorem is the first main result of this section.

Theorem 2.1. *For an* (n, m)*-graph* G*, one has*

$$\sqrt{n\left[(n-1)e^{2LEL/n} + 1\right] + 2LEL + 4m} \leq LEEL \leq n - 1 + e^{\sqrt{2m}}. \tag{2.1}$$

Moreover equality holds in (2.1) *if and only if* $G \cong \overline{K_n}$.

Proof.

The Lower Bound

By a direct calculation from (1.6), we have

$$LEEL^2 = \sum_{i=1}^{n} e^{2\sqrt{\mu_i}} + 2\sum_{i<j} e^{\sqrt{\mu_i}} e^{\sqrt{\mu_j}}. \tag{2.2}$$

By the arithmetic-geometric mean inequality, we get

$$\begin{aligned}
2\sum_{i<j} e^{\sqrt{\mu_i}} e^{\sqrt{\mu_j}} &\geq n(n-1)\left[\prod_{i<j} e^{\sqrt{\mu_i}} e^{\sqrt{\mu_j}}\right]^{2/n(n-1)} \\
&= n(n-1)\left[\left(\prod_{i=1}^{n} e^{\sqrt{\mu_i}}\right)^{n-1}\right]^{2/n(n-1)} \\
&= n(n-1)e^{2LEL/n}.
\end{aligned} \tag{2.3}$$

By means of a power-series expansion and $M_0 = n$, $M_1 = 2LEL$, and $M_2 = 4m$, and using a multiplier $\gamma \in [0,8]$ (since we require a lower bound as good as possible, it looks reasonable to use such a multiplier), we obtain

$$\begin{aligned}
\sum_{i=1}^{n} e^{2\sqrt{\mu_i}} &= \sum_{i=1}^{n}\sum_{k\geq 0} \frac{\left(2\sqrt{\mu_i}\right)^k}{k!} = n + 2LEL + 4m + \sum_{i=1}^{n}\sum_{k\geq 3} + \frac{\left(2\sqrt{\mu_i}\right)^k}{k!} \\
&\geq n + 2LEL + 4m + \gamma\sum_{i=1}^{n}\sum_{k\geq 3} \frac{\left(\sqrt{\mu_i}\right)^k}{k!} \\
&= n + 2LEL + 4m - \gamma n - \gamma LEL - \gamma m + \gamma\sum_{i=1}^{n}\sum_{k\geq 0} \frac{\left(\sqrt{\mu_i}\right)^k}{k!} \\
&= (1-\gamma)n + (2-\gamma)LEL + (4-\gamma)m + \gamma LEEL.
\end{aligned} \tag{2.4}$$

By substituting (2.3) and (2.4) back into (2.2), and then solving it for $LEEL$, we get

$$LEEL \geq \frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{4} + n\left[(n-1)e^{2LEL/n} + 1 - \gamma\right] + (2-\gamma)LEL + (4-\gamma)m}\cdot \tag{2.5}$$

Meanwhile, for $n \geq 2$ and $m \geq 1$, it is easy to check that the function

$$f(x) := \frac{x}{2} + \sqrt{\frac{x^2}{4} + n\left[(n-1)e^{2LEL/n} + 1 - x\right] + (2-x)LEL + (4-x)m} \tag{2.6}$$

monotonically decreases in the interval $[0,8]$. As a result, the best lower bound for $LEEL$ is attained for $\gamma = 0$. This gives us the validity of the left-hand side of the inequality in (2.1).

The Upper Bound

By (1.6), we clearly have

$$LEEL = \sum_{k\geq 0} \frac{M_k}{k!}, \quad \text{where } M_k = \sum_{i=1}^{n} \left(\sqrt{\mu_i}\right)^k. \tag{2.7}$$

After this, we also have

$$\begin{aligned} LEEL &= n + \sum_{i=1}^{n} \sum_{k\geq 1} \frac{\left(\sqrt{\mu_i}\right)^k}{k!} \\ &= n + \sum_{k\geq 1} \frac{1}{k!} \sum_{i=1}^{n} \left[\left(\sqrt{\mu_i}\right)^2\right]^{k/2} \\ &\leq n + \sum_{k\geq 1} \frac{1}{k!} \left[\sum_{i=1}^{n} \left(\sqrt{\mu_i}\right)^2\right]^{k/2} \\ &= n + \sum_{k\geq 1} \frac{1}{k!} (2m)^{k/2} = n - 1 + \sum_{k\geq 0} \frac{\left(\sqrt{2m}\right)^k}{k!} \\ &= n - 1 + e^{\sqrt{2m}}, \end{aligned} \tag{2.8}$$

as required by the right-hand side of the inequality in (2.1).

Let us consider again inequality given in (2.1). For this, it is easy to check that equality will be held if and only if the graph G has no nonzero eigenvalues. Actually this situation can happen only in the case of the edgeless graph $\overline{K_n}$, that is, in the case of $G \cong \overline{K_n}$.

Hence the result is mentioned. □

In the following, we will determine two upper bounds for Laplacian Estrada like invariant, $LEEL$, in terms of Laplacian energy-like invariant , LEL.

Theorem 2.2. *Let G be a connected (n, m)-graph, and let LEL and $LEEL$ be as defined in* (1.5) *and* (1.6)*, respectively. Then*

$$LEEL - LEL \leq n - 1 - \sqrt{2m} + e^{\sqrt{2m}}, \tag{2.9}$$

or

$$LEEL \leq n - 1 + e^{LEL}. \tag{2.10}$$

Equality holds for both (2.9) *and* (2.10) *if and only if $G \cong \overline{K_n}$.*

Proof. In (2.8) in the proof of Theorem 2.1

$$LEEL = n + \sum_{i=1}^{n}\sum_{k\geq 1}\frac{\left(\sqrt{\mu_i}\right)^k}{k!}. \tag{2.11}$$

Taking into account the definition of LEL given in (1.5), we may also have the inequality

$$LEEL \leq n + LEL + \sum_{i=1}^{n}\sum_{k\geq 2}\frac{\left(\sqrt{\mu_i}\right)^k}{k!} \tag{2.12}$$

which leads to

$$LEEL - LEL \leq n + \sum_{i=1}^{n}\sum_{k\geq 2}\frac{\left(\sqrt{\mu_i}\right)^k}{k!} = n - 1 - \sqrt{2m} + e^{2m}, \tag{2.13}$$

as required in (2.9). In fact this inequality holds for all (n, m)-graphs. Additionally, a similar thought as in the proof of Theorem 2.1 gives that equality is attained in (2.9) if and only if $G \cong \overline{K_n}$.

Furthermore, again by considering (2.8) as in the above, there exists another route to connect $LEEL$ and LEL as in the following:

$$\begin{aligned}LEEL &= n + \sum_{i=1}^{n}\sum_{k\geq 1}\frac{\left(\sqrt{\mu_i}\right)^k}{k!} \leq n + \sum_{k\geq 1}\frac{1}{k!}\left[\sum_{i=1}^{n}\left(\sqrt{\mu_i}\right)\right]^k \\ &= n + \sum_{k\geq 1}\frac{(LEL)^k}{k!} = n - 1 + \sum_{k\geq 0}\frac{(LEL)^k}{k!},\end{aligned} \tag{2.14}$$

and then, by considering the definition of LEL in (1.5), this implies that

$$LEEL \leq n - 1 + e^{LEL}, \tag{2.15}$$

as claimed in (2.10).

As in the other upper bound case defined in (2.9), equality also occurs in (2.10) if and only if $G \cong \overline{K_n}$. □

In [26], it has been given bounds for the sum of the chromatic numbers of a graph G and its complement $\overline{G}$. After that, in general meanings, so many people investigated a number of graph invariants in terms of G and $\overline{G}$, and collected these studies in the literature under the name of “Nordhaus-Gaddum-type results”. For example, in a recent paper [24], Gutman et al. have studied the Nordhaus-Gaddum-type results and then they transferred the Nordhaus-Gaddum-type results for graph energy E (which was obtained in [27]) into Nordhaus-Gaddum-type results for Laplacian energy-like invariant , LEL.

In the following we will give a theorem that considers Nordhaus-Gaddum-type results for Laplacian Estrada energy like , $LEEL$.

Theorem 2.3. *Let G be a connected graph on $n \geq 2$ vertices and m edges with a connected component $\overline{G}$. Then*

$$n\sqrt{2e^{\sqrt{n}}} \leq LEEL(G) + LEEL\left(\overline{G}\right) \leq 2(n-1) + e^{\sqrt{2m}} + e^{\sqrt{n(n-1)-2m}}. \tag{2.16}$$

Proof.

The Lower Bound

Let $\overline{\mu_1}, \overline{\mu_2}, \ldots, \overline{\mu_n}$ be the Laplacian eigenvalues of $\overline{G}$ arranged in a nonincreasing order. Then, for $i = 1, 2, \ldots, n-1$, $\overline{\mu_i} = n - \mu_{n-i}$. By considering (1.6), a direct calculation gives that

$$LEEL(G) + LEEL\left(\overline{G}\right) = \sum_{i=1}^{n}\left(e^{\sqrt{\mu_i}} + e^{\sqrt{n-\mu_i}}\right) \geq \sum_{i=1}^{n}\sqrt{2e^{\sqrt{n}}} = n\sqrt{2e^{\sqrt{n}}}. \tag{2.17}$$

The Upper Bound

By (2.1) in Theorem 2.1, we did obtain an upper bound $n - 1 + e^{\sqrt{2m}}$ for $LEEL(G)$. Now recalling that $\overline{m} = (n(n-1) - 2m)/2$, again a direct calculation shows that

$$LEEL(G) + LEEL\left(\overline{G}\right) \leq 2(n-1) + e^{\sqrt{2m}} + e^{\sqrt{n(n-1)-2m}}. \tag{2.18}$$

Hence the result is attained. □

2.1. Laplacian Estrada-Like Invariant is Estrada Like

As depicted in [24], starting with the work of McClelland (in [28]), the basic results over bounds for graph energy could be deduced by relying to a limited number of simple properties of the graph eigenvalues (see, for instance, [29]).

Let us suppose that G is a molecular (n, m)-graph. Also let N and M be two positive integers. Consider an auxiliary quantity S, defined as

$$S = S(G) = \sum_{i=1}^{N} e^{s_i}, \tag{2.19}$$

where s_i's are some numbers (for $i = 1, 2, \ldots, N$) which somehow can be computed from the graph G, for which we only need to know that they satisfy the conditions

$$\sum_{i=1}^{N} s_i = F, \tag{2.20}$$

$$\sum_{i=1}^{N} (s_i)^2 = 2M. \tag{2.21}$$

Actually, from (2.20) and (2.21), it is possible to deduce both lower and upper bounds for S as in the following.

What now needs to be observed is that if we choose $N = n$, $M = m$, and $s_i = \lambda_i$ (for $i = 1, 2, \ldots, n$), then the auxiliary quantity S will be turned out to the Estrada index, as defined in (1.1). Now, all of the two conditions (2.20) and (2.21) are obeyed for the choice $N = n$, $M = m$, and $s_i = \sqrt{\mu_i}$ (where $i = 1, 2, \ldots, n$), in which case the quantity S will be thought as $LEEL$, as defined in (1.6).

Keeping the above in mind, in other words, if all of the two conditions (2.20) and (2.21) are taken into account, then, as a generalization, we have the following three results for S similar to results for $LEEL$ (given in the previous section) and results for Estrada index deduced previously by some other authors (see [12, 17, 18]):

(1) $N - 1 + e^{\sqrt{2M}} \leq S \leq \sqrt{N + 2F + N(N-1)e^{2F/N}}$,

(2) $S - F \leq N - 1 - \sqrt{2M} + e^{\sqrt{2M}}$,

(3) $S \leq N - 1 + e^{F}$.

In detail, the following are considered.

(i) If we take $N = n$, $M = m$, and $s_i = \lambda_i$ (where $i = 1, 2, \ldots, n$), then results presented in (1), (2), and (3) correspond to the bounds (6), (14), and (15) in [12], respectively.

(ii) If we take $N = n$, $M = m$, and $s_i = \rho_i$ (where $i = 1, 2, \ldots, n$), then results presented in (1), (2), and (3) correspond to the bounds (11), (15), and (16) in [18], respectively.

(iii) If we take $N = n$, $M = m$, and $s_i = \mu_i - 2m/n$ (where $i = 1, 2, \ldots, n$), then results presented in (1), (2), and (3) correspond to the bounds (11), (17), and (18) in [17], respectively.

(iv) If we take $N = n$, $M = m$, and $s_i = \sqrt{\mu_i}$ (where $i = 1, 2, \ldots, n$), then results presented in (1), (2), and (3) correspond to the bounds obtained in this paper in Theorems 2.1 and 2.2.

3. On the Estrada Index-Like Quantity

It is a well known fact that there are so many papers in the literature that study indexes and energies. In [28], McClelland obtained lower and upper bounds for the total π-electron energy. In [30, Theorems 1 and 2], Gutman et al. formulated the generalized version of these bounds, applicable to the energy-like expression E_X and defined this by

$$E_X = \sum_{i=1}^{n} |x_i - \overline{x}|, \tag{3.1}$$

where $x_1, x_2, \ldots, x_n$ are any real numbers, and $\overline{x}$ is their arithmetic mean. As depicted in the same paper, if $x_1, x_2, \ldots, x_n$ are the eigenvalues of the adjacency, Laplacian, or distance matrix of some graph G, then *graph energy, Laplacian energy,* and *distance energy* are the special cases of E_X. (We note that, in [19, Theorem 2.3], as another special case of E_X, it has been recently shown a lower bound and an upper bound for the Harary energy).

By considering the Estrada index defined in (1.1), the other *Estrada index-like quantity* can be defined as

$$EE_X = \sum_{i=1}^{n} e^{x_i - \overline{x}}, \tag{3.2}$$

where $x_1, x_2, \dots, x_n$ are arbitrary real numbers, and $\overline{x}$ is their arithmetic mean. In particular, as similarly in E_X, if $x_1, x_2, \dots, x_n$ are the eigenvalues of the adjacency, Laplacian, or distance matrix of some of G, then EE_X is the Estrada index (see [5, 8, 14, 15]), Laplacian Estrada index (see [17]), or distance Estrada index (see [18]), respectively, of some graph G.

Let

$$N_k' = \sum_{i=1}^{n} (x_i - \overline{x})^k. \tag{3.3}$$

Then

$$EE_X = \sum_{k=0}^{\infty} \frac{N_k'}{k!}. \tag{3.4}$$

We remind two basic facts in the statistics that, for arbitrary real numbers $x_1, x_2, \dots, x_n$, the arithmetic mean and variance are defined by

$$\overline{x} = \frac{1}{n} \sum_{i=1}^{n} x_i, \tag{3.5}$$

$$\operatorname{Var}(x) = \frac{1}{n} \sum_{i=1}^{n} (x_i - \overline{x})^2. \tag{3.6}$$

By considering (3.2), (3.3), and (3.6), one can show the following results as proved in Theorems 2.1 and 2.2.

Theorem 3.1. *Let EE_X be the Estrada index-like expression as defined in* (1.6)*. Then*

$$\sqrt{n^2 + 2n \operatorname{Var}(x)} \le EE_X \le n - 1 + e^{\sqrt{n \operatorname{Var}(x)}}. \tag{3.7}$$

Equality holds if and only if $x_1 = x_2 = \cdots = x_n$.

Theorem 3.2. *Let E_X and EE_X be as defined in* (1.5) *and* (1.6)*, respectively. Then*

$$EE_X - E_X \le n - 1 - \sqrt{n \operatorname{Var}(x)} + e^{\sqrt{n \operatorname{Var}(x)}}, \tag{3.8}$$

or

$$EE_X \le n - 1 + e^{E_X}. \tag{3.9}$$

In Theorem 3.2, equality holds in both inequalities if and only if $x_1 = x_2 = \cdots = x_n$ (or, equivalently, $\mathrm{Var}(x) = 0$), as given in the proof of Theorem 3.1.

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