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The Normalized Laplacian Estrada Index of a Graph

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Abstract. In this paper, we define and investigate the normalized Laplacian Estrada index of a graph. Some bounds for the normalized Laplacian Estrada index of a graph in term of its vertex number, maximum (or minimum) degree are obtained, some inequalities between the normalized Laplacian Estrada and the normalized Laplacian energy are also obtained.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Its *order* is $|V(G)|$, denoted by n, and its *size* is $|E(G)|$, denoted by m. For $v \in V(G)$, let $d(v)$ be the degree of v. The maximum and minimum degrees of G are denoted by Δ and δ, respectively.

Let $A(G)$ and $D(G)$ be the adjacency matrix and the diagonal matrix of vertex degrees of G, respectively. The Laplacian and normalized Laplacian matrices of G are defined as $L(G) = D(G) - A(G)$ and $\mathcal{L}(G) = D(G)^{-1/2}L(G)D(G)^{-1/2}$, respectively. The eigenvalues of $A(G)$, $L(G)$ and $\mathcal{L}(G)$ are called the eigenvalues, the Laplacian eigenvalues and the normalized Laplacian eigenvalues of G, denoted by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$, $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$ and $\gamma_1(G) \geq \gamma_2(G) \geq \cdots \geq \gamma_n(G)$, respectively.

When only one graph G is under consideration, we sometimes use λ_i, μ_i and γ_i instead of $\lambda_i(G)$, $\mu_i(G)$ and $\gamma_i(G)$ for $i = 1, 2, \ldots, n$, respectively. The basic properties on the eigenvalues, the Laplacian eigenvalues and the normalized Laplacian eigenvalues of G can be founded in [5], [2]and [4], respectively.

The Estrada index of the graph G was defined in [11] as

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

motivated by its chemical applications, proposed earlier by Ernesto Estrada [7, 8]. The mathematical properties of the Estrada index have been studied in a number of recent works [6, 10, 11, 14].

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The Laplacian Estrada index of the graph G was defined in [12] as

$$LEE = LEE(G) = \sum_{i=1}^{n} e^{(\mu_i - 2m/n)}. \tag{2}$$

Remark 1.1. Independently of [12], another variant of the Laplacian Estrada index was put forward in [9], defined as

$$LEE_{[9]} = LEE_{[9]}(G) = \sum_{i=1}^{n} e^{\mu_i}.$$

Evidently, $LEE_{[9]}(G) = e^{2m/n} LEE(G)$, and therefore results obtained for LEE can be immediately re-stated for $LEE_{[9]}$ and vice versa. Some basic properties of the Laplacian Estrada index were determined in [9, 12, 13, 15–17]. In particular, the appropriate relations between the Laplacian Estrada index and the Laplacian energy, the first Zagreb index, the Estrada index of the graph and the Estrada index of its line graph were established in [9, 12, 15, 16].

In full analogy with (1) and (2), we now define the normalized Laplacian Estrada index of a graph as follows.

Definition. Let G be a connected graph of order n. The normalized Laplacian Estrada index of G, denoted by $NEE(G)$, is equal to

$$NEE = NEE(G) = \sum_{i=1}^{n} e^{(\gamma_i - 1)}. \tag{3}$$

Remark 1.2. Note that if G is a k-regular graph, then $\gamma_i = \frac{\mu_i}{k}$ for $i = 1, 2, \ldots, n$ (see [4]). Hence we have $e^k NEE = LEE$ for any k-regular graph. Therefore, in the case of G is regular, results obtained for LEE can be immediately re-stated for NEE.

In this paper, we investigate the normalized Laplacian Estrada index of G, and get some lower (or upper) bounds for the normalized Laplacian Estrada index of G in term of its vertex number, maximum (or minimum) degree, and also obtained some inequalities between the normalized Laplacian Estrada index and the normalized Laplacian energy.

At the outset we note that

$$NEE = NEE(G) = \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{i=1}^{n} (\gamma_i - 1)^k,$$

where the standard notational convention that $0^0 = 1$ is used.

2. Preliminaries

Firstly, we select some basic properties on the normalized Laplacian eigenvalues of G which will be used in this paper.

Lemma 2.1 ([4]). *Let G be a connected graph of order $n \geq 2$.*

(1) $\sum_{i=1}^{n} \gamma_i = n$ *and* $\sum_{i=1}^{n} \gamma_i^2 = n + 2 \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}$.
(2) $\gamma_1(G) \geq \frac{n}{n-1}$ *with equality holding if and only if G is a complete graph.*
(3) $\gamma_1(G) = 2$ *with equality holding if and only if G is a bipartite graph.*
(4) *For each* $1 \leq i \leq n$, *we have* $\gamma_i \in [0, 2]$ *and* $\gamma_n = 0$.

Lemma 2.2 ([3]). *Let G be a connected graph of order $n \geq 3$. Then the following statements hold.*

(1) *G has exactly two distinct normalized Laplacian eigenvalues if and only if G is the complete graph.*
(2) *G has an normalized Laplacian eigenvalue with multiplicity exactly $n-2$ if and only if G is a complete bipartite graph.*

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

$$R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha,$$

where the summation is over all edges uv in G, and $\alpha \neq 0$ is a fixed real number.

The general Randić index when $\alpha = 1$ is

$$R_{-1} = R_{-1}(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}.$$

Combing the form of $R_{-1}(G)$ and Lemma 2.1, we have $\sum_{i=1}^{n} \gamma_i^2 = n + 2R_{-1}$ holds for any graph G of order n. Some properties on $R_{-1}(G)$ can be founded in [3]. In particular, the following upper and lower bounds on $R_{-1}(G)$ in terms of maximum and minimum degrees are obtained.

Lemma 2.3 ([3]). *Let G be a connected graph of order n with maximum degree Δ and minimum degree δ. Then*

$$\frac{n}{2\Delta} \leq R_{-1}(G) \leq \frac{n}{2\delta}.$$

Equality occurs in both bounds if and only if G is a regular graph.

3. The main results

In this section, we deduce some bounds for the normalized Laplacian Estrada index of a (bipartite) graph in term of its vertex number, maximum (or minimum) degree, respectively. Some inequalities between NEE and NE are also obtained.

Theorem 3.1. *Let G be a connected graph of order n. Then*

$$NEE \geq (n-1)e^{1/(n-1)} + e^{-1}. \tag{4}$$

Moreover, the equality holds if and only if $G \cong K_n$.

Proof. Recall that $\gamma_n = 0$. Directly from (3), we have

$$\begin{aligned} NEE &= e^{(\gamma_1 - 1)} + e^{(\gamma_2 - 1)} + \cdots + e^{(\gamma_{n-1} - 1)} + e^{-1} \\ &\geq e^{(\gamma_1 - 1)} + (n-2)\left(\prod_{i=2}^{n-1} e^{(\gamma_i - 1)}\right)^{1/(n-2)} + e^{-1} \\ &= e^{(\gamma_1 - 1)} + (n-2)e^{(2-\gamma_1)/(n-2)} + e^{-1} \quad \text{as} \quad \sum_{i=1}^{n} (\gamma_i - 1) = 0. \end{aligned}$$

Let $f(x) := e^x + (n-2)e^{(1-x)/(n-2)} + e^{-1}$. Then we have $f'(x) = e^x - e^{(1-x)/(n-2)} \geq 0$ for $x \geq \frac{1}{n-1}$. Hence, $f(x)$ is an increasing function for $x \geq \frac{1}{n-1}$. On the other hand, by Lemma 2.1, we have $\gamma_1 - 1 \geq \frac{1}{n-1}$. Therefore, we get

$$NEE \geq f(\gamma_1 - 1) \geq f(\frac{n}{n-1} - 1) = (n-1)e^{1/(n-1)} + e^{-1}.$$

Suppose that the equality in (4) holds. Then all inequalities in the above argument must be equalities, i.e., $\gamma_1 = \frac{n}{n-1}$ and $\gamma_2 = \cdots = \gamma_{n-1}$. Hence by Lemmas 2.1 and 2.2, we have $G \cong K_n$.

Conversely, it is easy to check that the equality in (4) holds for K_n, which completes the proof. □

Moreover, if G is a bipartite graph, then $\gamma_1 = 2$ by Lemma 2.1. Using the same way as in Theorem 3.1, we then have the following bound.

Theorem 3.2. *Let G be a bipartite graph of order n. Then*

$$NEE \geq e + (n-2) + e^{-1}.$$

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

Remark 3.3. In fact, Theorem 3.1 concludes that among all graphs of order n, the complete graph K_n with minimum normalized Laplacian Estrada index; and Theorem 3.2 concludes that among all bipartite graphs of order n, the complete bipartite graphs with minimum normalized Laplacian Estrada index.

Theorem 3.4. *Let G be a bipartite graph of order n with maximum degree Δ and minimum degree δ. Then the normalized Laplacian Estrada index of G is bounded as*

$$e^{-1} + e + \sqrt{(n-2)^2 + \frac{2(n-2\Delta)}{\Delta}} \leq NEE \leq e^{-1} + e + (n-3) - \sqrt{\frac{n-2\delta}{\delta}} + e^{\sqrt{\frac{n-2\delta}{\delta}}}. \tag{5}$$

Equality occurs in both bounds if and only if G is a complete bipartite regular graph.

Proof. Note that by Lemma 2.1, $\gamma_n(G) = 0$ and $\gamma_1(G) = 2$ for any bipartite graph G. Directly from (3), we get

$$(NEE - e^{-1} - e)^2 = \sum_{i=2}^{n-1} e^{2(\gamma_i - 1)} + 2 \sum_{2 \leq i < j \leq n-1} e^{(\gamma_i - 1)} e^{(\gamma_j - 1)}. \tag{6}$$

In view of the inequality between the arithmetic and geometric means,

$$\begin{aligned} 2 \sum_{2 \leq i < j \leq n-1} e^{(\gamma_i - 1)} e^{(\gamma_j - 1)} &\geq (n-2)(n-3) \left(\prod_{2 \leq i < j \leq n-1} e^{(\gamma_i - 1)} e^{(\gamma_j - 1)} \right)^{2/[(n-2)(n-3)]} \\ &= (n-2)(n-3) \left[\left(\prod_{i=2}^{n-1} e^{(\gamma_i - 1)} \right)^{n-3} \right]^{2/[(n-2)(n-3)]} \\ &= (n-2)(n-3), \quad \text{since } \sum_{i=2}^{n-1} (\gamma_i - 1) = 0. \end{aligned} \tag{7}$$

Note that $\sum_{i=2}^{n-1} (\gamma_i - 1)^0 = n - 2$, $\sum_{i=2}^{n-1} (\gamma_i - 1) = 0$ and $\sum_{i=2}^{n-1} (\gamma_i - 1)^2 = 2R_{-1} - 2$. By means of a power-series expansion and Lemma 2.3, we get

$$\begin{aligned} \sum_{i=2}^{n-1} e^{2(\gamma_i - 1)} &= \sum_{k \geq 0}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} [2(\gamma_i - 1)]^k \\ &= n - 2 + 4(R_{-1} - 1) + \sum_{k \geq 3}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} [2(\gamma_i - 1)]^k \\ &\geq n - 2 + 4(R_{-1} - 1) + t \sum_{k \geq 3}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} (\gamma_i - 1)^k \quad \text{for } t \in [0, 4] \\ &= (1-t)(n-2) + (4-t)(R_{-1} - 1) + t(NEE - e^{-1} - e) \\ &\geq (1-t)(n-2) + (4-t)\left(\frac{n}{2\Delta} - 1\right) + t(NEE - e^{-1} - e). \end{aligned} \tag{8}$$

By substituting (7) and (8) back into (6), and solving for $NEE - e^{-1} - e$, we have

$$NEE - e^{-1} - e \geq \frac{t}{2} + \frac{\sqrt{[t-2(n-2)]^2 + \frac{2(n-2\Delta)}{\Delta}(4-t)}}{2}.$$

It is elementary to show that for $n \geq 2$ and $\Delta \leq \lceil \frac{n}{2} \rceil$ the function

$$f(x) := \frac{x}{2} + \frac{\sqrt{[x-2(n-2)]^2 + \frac{2(n-2\Delta)}{\Delta}(4-x)}}{2}$$

monotonically decreases in the interval $[0,4]$. Consequently, the best lower bound for $NEE - e^{-1} - e$ is attained for $t = 0$. Then we arrive at the first half of Theorem 3.4.

Starting from the following inequality, we get

$$\begin{aligned}
NEE - e^{-1} - e &= n - 2 + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} (\gamma_i - 1)^k \\
&\leq n - 2 + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} |\gamma_i - 1|^k \\
&= n - 2 + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} [(\gamma_i - 1)^2]^{k/2} \\
&\leq n - 2 + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \left[\sum_{i=2}^{n-1} (\gamma_i - 1)^2\right]^{k/2} \\
&= n - 2 + \sum_{k\geq 2}^{\infty} \frac{(2R_{-1} - 2)^{k/2}}{k!} \\
&= (n-3) - \sqrt{2R_{-1} - 2} + \sum_{k\geq 0}^{\infty} \frac{\left(\sqrt{2R_{-1} - 2}\right)^k}{k!} \\
&= (n-3) - \sqrt{2R_{-1} - 2} + e^{\sqrt{2R_{-1}-2}}.
\end{aligned}$$

It is elementary to show that the function $g(x) := e^x - x$ monotonically increases in the interval $[0, +\infty]$. Consequently, by Lemma 2.3, the best lower bound for $NEE - e^{-1} - e$ is attained for $R_{-1} = \frac{n}{2\delta}$. This directly leads to the right-hand side inequality in (5).

From the derivation of (5) and Lemmas 2.1 and 2.3 it is evident that equality will be attained if and only if $\gamma_2(G) = \cdots = \gamma_{n-1}(G) = 1$ and G is regular. By Lemma 2.2, this happens only in the case of G is complete bipartite and regular . The proof now is completed. □

Recall that for a general graph G, we have $\gamma_1(G) \leq 2$ and $\gamma_n(G) = 0$ by Lemma 2.1. If we consider $NEE - e^{-1} = \sum_{i=1}^{n-1} e^{(\gamma_i - 1)}$ in the same way as in Theorem 3.4, we then have the following bounds for the general graphs.

Theorem 3.5. *Let G be a graph of order n with maximum degree Δ and minimum degree δ. Then the normalized Laplacian Estrada index of G is bounded as*

$$e^{-1} + \sqrt{(n-1)[1 + (n-2)e^{2/(n-1)}] + \frac{2n}{\Delta}} < NEE \leq e^{-1} + n - 1 - \sqrt{\frac{n-\delta}{\delta}} + e^{\sqrt{\frac{n-\delta}{\delta}}}.$$

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

Recall that the normalized Laplacian energy of a graph G is defined in [3] as

$$NE = NE(G) = \sum_{i=1}^{n} |\gamma_i - 1|. \tag{9}$$

Some properties on $NE(G)$ can be founded in [3]. In what follows, we give some inequalities between NEE and NE.

Theorem 3.6. *Let G be a bipartite graph of order n with minimum degree δ. Then*

$$NEE - NE \leq (n-5) + e^{-1} + e - \sqrt{\frac{n-2\delta}{\delta}} + e^{\sqrt{\frac{n-2\delta}{\delta}}} \tag{10}$$

or

$$NEE + NE \leq (n-1) + e^{-1} + e + e^{(NE-2)}. \tag{11}$$

Equality (10) or (11) is attained if and only if G is a complete bipartite regular graph.

Proof. Note that $\gamma_n = 0$ and $\gamma_1 = 2$. Then we get

$$NEE - e^{-1} - e = (n-2) + \sum_{k\geq 1}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} (\gamma_i - 1)^k \leq (n-2) + \sum_{k\geq 1}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} |\gamma_i - 1|^k.$$

Taking into account the definition of graph normalized Laplacian energy (9), we have

$$NEE - e^{-1} - e \leq (n-2) + (NE-2) + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} |\gamma_i - 1|^k,$$

which, as in Theorem 3.4, leads to

$$\begin{aligned} NEE - NE &\leq (n-4) + e^{-1} + e + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} |\gamma_i - 1|^k \\ &\leq (n-5) + e^{-1} + e - \sqrt{2R_{-1} - 2} + e^{\sqrt{2R_{-1}-2}} \\ &\leq (n-5) + e^{-1} + e - \sqrt{\frac{n-2\delta}{\delta}} + e^{\sqrt{\frac{n-2\delta}{\delta}}}. \end{aligned}$$

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

Another route to connect NEE and NE, is the following:

$$\begin{aligned} NEE - e^{-1} - e &= (n-2) + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} (\gamma_i - 1)^k \\ &\leq (n-2) + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} |\gamma_i - 1|^k \\ &\leq (n-2) + \sum_{k\geq 2}^{\infty} \frac{\left[\sum_{i=2}^{n-1} |\gamma_i - 1|\right]^k}{k!} \\ &= (n-2) - 1 - (NE-2) + \sum_{k\geq 0}^{\infty} \frac{(NE-2)^k}{k!} \\ &= (n-1) - NE + e^{(NE-2)} \end{aligned}$$

implying

$$NEE + NE \leq n - 1 + e^{-1} + e + e^{(NE-2)}.$$

Also on this formula equality occurs if and only if G is a complete bipartite regular graph. This completes the proof. □

Similarly, if we consider $NEE - e^{-1} = \sum_{i=1}^{n-1} e^{(\gamma_i - 1)}$ in the same way as in Theorem 3.6, we then have the following inequalities for the general graphs.

Theorem 3.7. *Let G be a graph of order n with minimum degree δ. Then*

$$NEE - NE \leq (n-3) + e^{-1} - \sqrt{\frac{n-\delta}{\delta}} + e^{\sqrt{\frac{n-\delta}{\delta}}} \tag{12}$$

or

$$NEE + NE \leq n + e^{-1} + e^{(NE-1)}. \tag{13}$$

Equality (12) or (13) is attained if and only if G is a complete bipartite regular graph.

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