On the Laplacian Estrada index of graphs with given chromatic number *

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Abstract

Assume that $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of the Laplacian matrix of a graph G. The Laplacian Estrada index of G, is defined as $LEE(G) = \sum_{i=1}^{n} e^{\mu_i}$. In this note, we give an upper bound on $LEE(G)$ in terms of chromatic number and characterize the corresponding extremal graph.

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1 Introduction

Throughout this paper all graphs are finite and simple. Let $G = (V(G), E(G))$ be a graph with n vertices. The *join*, $G_1 \bigvee G_2$, of the graphs G_1 and G_2 is the graph obtained from disjoint union $G_1 \bigcup G_2$ by adding new edges from each vertex in G_1 to every vertex in G_2. By $G - U$ we mean the induced subgraph $G[V - U]$, if $U \subset V(G)$. The *adjacency matrix* of G is

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$A(G) = (a_{ij})_{n\times n}$, where $a_{ij} = 1$ if two vertices u_i and u_j are adjacent in G and $a_{ij} = 0$ otherwise. Let $D(G) = \text{diag}(d_1, d_2, \ldots, d_n)$ be the the diagonal matrix of vertex degrees of G. We call the matrix $L(G) = D(G) - A(G)$ *Laplacian matrix* of G. Clearly, $L(G)$ is a real symmetric matrix. From this fact and Geršgorin's theorem, it follows that its eigenvalues are nonnegative real numbers. Moreover, since its rows sum to 0, 0 is the smallest eigenvalue of $L(G)$. Thus, all eigenvalues of $L(G)$ can be arranged in order as $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) = 0$. Denote the spectrum of $L(G)$ by $S(G) = (\mu_1, \mu_2, \ldots, \mu_n)$. It is well known that $\mu_i(G) = n - \mu_{n-i}(\overline{G})$ for $1 \leq i \leq n-1$, since $L(G)+L(\overline{G}) = nI - J$, where I and J denote the identity matrix and the matrix all of whose entries being equal to 1, respectively. In particular, for any graph G of order n, we have $\mu_1(G) \leq n$ with the equality if and only if $\overline{G}$ is disconnected. We refer reader to [12, 16] for further information on the Laplacian matrix. Recall that the Estrada index of a simple connected graph G, put forward by Estrada [5], is defined by

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

The Estrada index has already found extensive applications, e. g., in chemistry [5, 6], in complex networks [7], in statistical thermodynamics [8, 9]. Quite recently, in full analogy with the Estrada index, the Laplacian Estrada index of the graph G, LEE for short, was introduced in [10] as

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i} . \tag{1.1}$$

Given a graph G of order n with m edges, independently, in [15] the Laplacian Estrada index was defined as

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

It is easy to see that two "Laplacian Estrada indices" are essentially equivalent in view of $LEE(G) = LEE_{LSC}(G) \times e^{2m/n}$. In the following we use the definition (1.1). Some properties of LEE have been reported in [1, 3, 4, 10, 15, 18, 13, 19, 20].

A *coloring* of a graph is an assignment of colors to its vertices such that any two adjacent vertices have different colors. The *chromatic number* $\chi(G)$ of the graph G is the minimum number of colors in any coloring of G. The set of vertices with any one color in a coloring of G is said to be a color class. Evidently, any color class is independent. Let $K_{n_1,n_2,n_3,\ldots,n_k}$ denote the complete k-partite graph. For the other graph theoretical terms used but not defined, we follow [2]. In this note, we characterize the extremal graphs with given chromatic number $\chi(G)$ maximizing the Laplacian Estrada index. The main result of this note is as follows.

Theorem 1. *Let G be a connected graph with n vertices and chromatic number χ.*

(i) *If $\chi > \lfloor n/2 \rfloor$, then $LEE(G) \leq 1+(\chi-1)\,e^n+(n-\chi)\,e^{n-2}$ with equality if and only if $G \cong K_{\underbrace{1,\ldots,1}_{2\chi-n},\underbrace{2,\ldots,2}_{n-\chi}}$.*

(ii) *If $1 \leq \chi \leq \lfloor n/2 \rfloor$, then $LEE(G) \leq 1+(\chi-1)\,e^n+(\chi-1)\,e^{n-2}+(n-2\chi+1)\,e^{2\chi-2}$ with equality if and only if $G \cong K_{\underbrace{2,\ldots,2}_{\chi-1},n-2(\chi-1)}$.*

2 The proof of Theorem 1

In to show Theorem 1, we need the following two lemmas.

Lemma 1. [11, p. 291] *Let G be a simple non-complete graph with n vertices. If $G+e$ is obtained from G by adding an edge e to G, then $0 = \mu_n(G) \leq \mu_n(G+e) \leq \cdots \leq \mu_2(G) \leq \mu_2(G+e) \leq \mu_1(G) \leq \mu_1(G+e)$.*

Since $\sum_{i=1}^{n} \mu_i(G+e) - \sum_{i=1}^{n} \mu_i(G) = 2$, the next result follows immediately from Lemma 1.

Lemma 2. *Let G be a simple non-complete graph with n vertices. Then $LEE(G) < LEE(G+e)$.*

In what follows, we prove the main theorem.

Proof. Let G be a graph with the maximum LEE of all connected graphs with vertices and chromatic number χ. Thus, we can divide $V(G)$ into χ color classes, say $V_1, V_2, \ldots, V_\chi$. By virtue of Lemma 2, we know that each vertex in V_i is adjacent to all vertices in V_j for any $1 \leq i < j \leq \chi$. Consequently, G can be written as $K_{n_1,n_2,\ldots,n_\chi}$, where $n_i = |V_i|$ for $1 \leq i \leq \chi$. Without loss of generality, we can assume that $1 \leq n_1 \leq n_2 \leq \ldots \leq n_\chi$. It is obvious that

$$\begin{aligned} S(\overline{G}) &= S\left(K_{n_1} \bigcup K_{n_2} \bigcup \cdots \bigcup K_{n_\chi}\right) \\ &= (\underbrace{n_\chi, \ldots, n_\chi}_{n_\chi - 1}, \ldots, \underbrace{n_1, \ldots, n_1}_{n_1 - 1}, \underbrace{0, \ldots, 0}_{\chi}). \end{aligned}$$

So we have

$$S(G) = (\underbrace{n, \ldots, n}_{\chi-1}, \underbrace{n - n_1, \ldots, n - n_1}_{n_1 - 1}, \ldots, \underbrace{n - n_\chi, \ldots, n - n_\chi}_{n_\chi - 1}, 0).$$

As a result, we obtain that

$$LEE(G) = 1 + (\chi - 1)\, e^n + \sum_{i=1}^{\chi} (n_i - 1)\, e^{n - n_i}$$

with $\sum_{i=1}^{\chi} n_i = n$. Assume that

$$f(x) = (x-1)\, e^{n-x} + (m - x - 1)\, e^{n-m+x}.$$

It is easy to show that

$$\begin{aligned} f'(x) &= (2-x)\, e^{n-x} + (m-x-2)\, e^{n-m+x} \\ &= e^{n-2}\left[(m-x-2)\, e^{-(m-x-2)} - (x-2)\, e^{-(x-2)}\right] \\ &= (m-2x)(1-\xi)\, e^{n-2-\xi} \\ &\le 0 \end{aligned}$$

for $3 \le x \le m/2$ and $x-2 < \xi < m-x-2$, where equality holds if and only if $x = m/2$. This implies that

$$(n_i - 1)\, e^{n-n_i} + (n_j - 1)\, e^{n-n_j} > n_i\, e^{n-n_i+1} + (n_j - 2)\, e^{n-n_j-1}$$

for $4 \le n_i \le n_j$. Thus, by replacing any pair (n_i, n_j) with $4 \le n_i \le n_j$ by $(n_i - 1, n_j + 1)$ in the sum $\sum_{i=1}^{\chi}(n_i - 1)\, e^{n-n_i}$, we increase the sum. By repeating this process, we attain the maximum of $1+(\chi-1)\, e^{n}+\sum_{i=1}^{\chi}(n_i-1)\, e^{n-n_i}$ only when $n_{\chi-1} \le 3$. In what follows, we divide the proof into two cases.

Case 1. If $n_\chi > 3$, then it is not hard to obtain

$$e^{n-2} + n_\chi\, e^{n-n_\chi-1} > 2\, e^{n-3} + (n_\chi - 1)\, e^{n-n_\chi}.$$

Consequently, by replacing any pair $(3, n_\chi)$ by $(2, n_\chi + 1)$ in the sum $\sum_{i=1}^{\chi-1}(n_i - 1)e^{n-n_i} + (n_\chi - 1)e^{n-n_\chi}$ for $1 \le n_1 \le \dots \le n_{\chi-1} \le 3$, we increase the sum. By a repeated using, we attain the maximum of $1+(\chi-1)\, e^{n}+\sum_{i=1}^{\chi-1}(n_i-1)\, e^{n-n_i}+(n_\chi-1)\, e^{n-n_\chi}$ only when $n_{\chi-1} \le 2$ and $n_\chi > 3$. Note that

$$e^{n-2} + (n_\chi - 1)\, e^{n-n_\chi} > n_\chi\, e^{n-n_\chi-1}$$

for $n_\chi > 3$ implies $n_1 \ge 2$. We have $G \cong K_{\underbrace{2,\dots,2}_{\chi-1},n-2(\chi-1)}$ and

$$\begin{aligned} LEE(G) &= 1 + (\chi-1)\, e^{n} + \sum_{i=1}^{\chi}(n_i - 1)\, e^{n-n_i} \\ &= 1 + (\chi-1)\, e^{n} + (\chi-1)\, e^{n-2} + (n - 2\chi + 1)\, e^{2\chi-2} \end{aligned}$$

for $\chi \le \lfloor n/2 \rfloor - 1$. Case 2. If $n_\chi \le 3$, then $e^{n-2} + e^{n-2} > 2\, e^{n-3}$ implies that at most one of $n_1 = 1$ and $n_\chi = 3$ holds. Thus, we can suppose that $n_1 = n_2 = \cdots = n_a = 1$ and $n_{a+1} = \cdots =$

$n_\chi = 2$ or $n_1 = n_2 = \cdots = n_a = 2$ and $n_{a+1} = \cdots = n_\chi = 3$. Consequently, we have $G \cong K_{\underbrace{1,\ldots,1}_{2\chi-n},\underbrace{2,\ldots,2}_{n-\chi}}$ for $\chi \geq n/2$ with

$$\begin{aligned} LEE(G) &= 1 + (\chi - 1)\, e^n + \sum_{i=1}^{\chi} (n_i - 1)\, e^{n-n_i} \\ &= 1 + (\chi - 1)\, e^n + (n - \chi)\, e^{n-2} \end{aligned}$$

or $G \cong K_{\underbrace{2,\ldots,2}_{3\chi-n},\underbrace{3,\ldots,3}_{n-2\chi}}$ for $n/3 \leq \chi \leq n/2$ with

$$\begin{aligned} LEE(G) &= 1 + (\chi - 1)\, e^n + \sum_{i=1}^{\chi} (n_i - 1)\, e^{n-n_i} \\ &= 1 + (\chi - 1)\, e^n + (3\chi - n)\, e^{n-2} + 2(n - 2\chi)\, e^{n-3}. \end{aligned}$$

Comparing the results in above two cases, we complete the proof. □

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