

On the Laplacian Estrada Index of Graphs

Bao-Xuan Zhu*

School of Mathematical Sciences, Dalian University of Technology,
Dalian 116024, P. R. China

e-mail: zhubaoxuan@yahoo.com.cn

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Abstract

Assume that $\mu_1, \mu_2, \dots, \mu_n$ 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 upper bounds for $LEE(G)$ in terms of connectivity or matching number and characterize the corresponding extremal graphs.

1 Introduction

In this paper all graphs are finite and simple. The *join*, $G_1 \vee G_2$, of the graphs G_1 and G_2 is the graph obtained from the disjoint union $G_1 \cup G_2$ by adding new edges from each vertex in G_1 to every vertex in G_2 . Let $G = (V(G), E(G))$ be a graph with n vertices. By $G - U$ we mean the induced subgraph $G[V - U]$, if $U \subset V(G)$. The *adjacency matrix* of G is $A(G) = ||a_{ij}||_{n \times n}$, where $a_{ij} = 1$ if two vertices u_i and u_j are adjacent in G and $a_{ij} = 0$ otherwise. Since $A(G)$ is a real symmetric, it has only real eigenvalues, which can be ordered as $\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$.

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Let $D(G) = \text{diag}(d_1, d_2, \dots, d_n)$ be the the diagonal matrix of vertex degrees of G . We call the matrix $L(G) = D(G) - A(G)$ *Laplacian matrix* of G . It is well known that $L(G)$ is a real positive semidefinite matrix and its eigenvalues can be ordered as $\mu_1(G) \geq \mu_2(G) \geq \dots \geq \mu_n(G) = 0$. Denote the spectrum of $L(G)$ by $S(G) = (\mu_1, \mu_2, \dots, \mu_n)$. It is well known that $\mu_i(G) = n - \mu_{n-i}(\overline{G})$ for $1 \leq i \leq n - 1$. We refer the reader to [13, 18] for further information on the Laplacian matrix.

Recall that the Estrada index of a simple connected graph G , recently put forward by Estrada [6], is defined by

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

The Estrada index has already found extensive applications, e. g., in chemistry [6, 7], in complex networks [8], in statistical thermodynamics [9, 10]. For recent research on EE see [3, 4, 15, 19, 20].

Quite recently, in full analogy with the Estrada index, the Laplacian Estrada index of the graph G , LEE for short, was introduced in [11] as

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

Given a graph G of order n with m edges, independently, in [16] 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). Some properties of LEE have been reported in [1, 5, 11, 14, 16, 21, 22].

Let $k \geq 1$. We say that a graph G is k -connected if either G is the complete graph K_{k+1} , or G has at least $k + 2$ vertices and contains no $(k - 1)$ -vertex cut. Similarly, G is k -edge-connected if it has at least two vertices and does not contain $(k - 1)$ -edge cut. The maximum value of k for which a connected graph G is k -connected is the connectivity of G , denoted by $\kappa(G)$. If G is disconnected, we define $\kappa(G) = 0$. The edge-connectivity $\kappa'(G)$ is defined analogously. If G is a graph of order n , then (1) $\kappa(G) \leq \kappa'(G) \leq n - 1$, and (2) the three statements $\kappa(G) = n - 1$, $\kappa'(G) = n - 1$ and $G \cong K_n$ are equivalent.

Two distinct edges in a graph G are *independent* if they are not incident with a common vertex in G . A set of pairwise independent edges in G is called a *matching* in G . A matching of maximum cardinality is a *maximum matching* in G . The *matching number* $\beta(G)$ of G is the cardinality of a maximum matching of G . It is well known that $\beta(G) \leq n/2$ with equality if and only if G has a perfect matching. For the other graph theoretical terms used but not defined, we follow the book [2].

In this note, we determine the extremal graphs with given connectivity k maximizing the Laplacian Estrada index. Moreover, we also characterize the n -vertex graphs with given matching number having the maximal Laplacian Estrada index.

2 The Laplacian Estrada index and connectivity

Lemma 1. [12, 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 $0 = \mu_n(G) \leq \mu_n(G + e) \leq \dots \leq \mu_2(G) \leq \mu_2(G + e) \leq \mu_1(G) \leq \mu_1(G + e)$.*

Noting that $\sum_{i=1}^n \mu_i(G+e) - \sum_{i=1}^n \mu_i(G) = 2$, we immediately obtain the following result by Lemma 1.

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

In the following, we will present one main result of this paper.

Theorem 1. *Let G be a graph of order n with vertex connectivity k . Then $LEE(G) \leq k e^n + (n - k - 2) e^{n-1} + e^k + 1$ with equality if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.*

Proof. Let G be a graph of order n with given vertex connectivity k . It is clear for $k = n - 1$. Thus, we can suppose that $1 \leq k \leq n - 2$ in the following. Assume that G has the maximal Laplacian Estrada index among all all connected graphs with n vertices and vertex connectivity k . By hypothesis there exists a vertex cut set U of order k such that $G - U$ is disconnected. Let G_1, G_2, \dots, G_r be connected components of $G - U$. If $r > 2$, then adding an edge between G_1 and G_2 will preserve the connectivity of G but increase the Laplacian Estrada index by Lemma 2, a contradiction. Thus, $r = 2$. Similarly, we also have all of $G[U]$, G_1 and G_2 are cliques

and every vertex in U is adjacent to all vertices in G_1 and G_2 in view of Lemma 2. Consequently, G can be written as $K_k \vee (K_i \cup K_{n-k-i})$ for $1 \leq i \leq (n-k)/2$.

It is well known that $S(K_p) = (\underbrace{p, p, \dots, p}_{p-1}, 0)$. Noting that

$$\begin{aligned} S(\overline{G}) &= S(K_{i, n-k-i} \cup \overline{K_k}) \\ &= \left(\underbrace{n-k, n-k-i, \dots, n-k-i}_{i-1}, \underbrace{i, \dots, i}_{n-k-i-1}, \underbrace{0, \dots, 0}_{k+1} \right) \end{aligned}$$

we have

$$S(G) = (\underbrace{n, \dots, n}_k, \underbrace{n-i, \dots, n-i}_{n-k-i-1}, \underbrace{i+k, \dots, i+k}_{i-1}, k, 0).$$

Consequently, we obtain that

$$LEE(G) = k e^n + e^k + (i-1)e^{i+k} + (n-k-i-1)e^{n-i} + 1.$$

Assume that $g(x) = (x-1)e^{x+k} + (n-k-x-1)e^{n-x}$. It is clear that

$$g'(x) = x e^{x+k} - (n-k-x)e^{n-x} \leq 0$$

for $1 \leq x \leq (n-k)/2$ with equality if and only if $x = (n-k)/2$. Hence, we have

$$LEE(G) \leq k e^n + e^k + (n-k-2)e^{n-1} + 1$$

where equality holds if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$, as required. □

As well known, $\kappa(G) \leq \kappa'(G) \leq \delta(G)$. Note that $K_k \vee (K_1 \cup K_{n-k-1})$ has minimum degree k and edge connectivity k and the function $k e^n + e^k + (n-k-2)e^{n-1} + 1$ is increasing with respect to k . Thus the following corollaries immediately follows from Theorem 1.

Corollary 1. *Let G be a graph of order n with given edge connectivity k . Then $LEE(G) \leq k e^n + e^k + (n-k-2)e^{n-1} + 1$, where equality holds if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.*

Corollary 2. *Let G be a graph with n vertices and minimum degree k . Then $LEE(G) \leq k e^n + e^k + (n-k-2)e^{n-1} + 1$, where equality holds if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.*

3 The Laplacian Estrada index and chromatic number

Obviously, $\beta(G) = 0$ if and only if G is an empty graph. A component of a graph is said to be *even* (respectively *odd*) if it has an even (respectively odd) number of vertices. The following Tutte–Berge formula is very important.

Lemma 3. [17] *Let G be a graph of order n with matching number β . Let $o(G)$ be the number of odd components of G . Then*

$$n - 2\beta = \max\{o(G - S) - |S| : S \subset V(G)\}.$$

In what follows we present a result for Laplacian Estrada index related to matching number.

Theorem 2. *Let G be a connected graph with n vertices and matching number β .*

- (i) *If $\beta = \lfloor n/2 \rfloor$, then $LEE(G) \leq (n-1)e^n + 1$ with equality if and only if $G \cong K_n$.*
- (ii) *If $1 \leq \beta < \lfloor n/2 \rfloor$, then $LEE(G) \leq 1 + \beta e^n + (n - \beta - 1)e^\beta$ with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$.*

Proof. Let G be a graph with the maximum LEE among all connected graphs with n vertices and matching number β . Then by Lemma 3 there exists a subset S of $V(G)$ on s vertices such that $G - S$ has $n + s - 2\beta$ odd components.

Assume that $s = 0$. It follows that $G - S = G$ and $n - 2\beta \leq 1$. If $n - 2\beta = 0$, then $\beta = n/2$, and if $n - 2\beta = 1$, then $\beta = (n - 1)/2$. In either case, by Lemma 2 we have $G = K_n$ and $LEE(G) = (n - 1)e^n + 1$.

In what follows, we suppose that $s \geq 1$. So $n - 2\beta + s \geq 1$. Let $G_1, G_2, \dots, G_{n-2\beta+s}$ be the odd components of $G - S$. If $G - S$ has an even component, then by adding an edge to G joining a vertex of an even component and a vertex of an odd component of $G - S$, we obtain a graph G^* , for which $n - 2\beta(G^*) \geq o(G^* - S) - s = o(G - S) - s$. This implies that $\beta(G^*) = \beta$. However $LEE(G^*) > LEE(G)$ by Lemma 2, a contradiction. Hence $G - S$ does not have an even component. Similarly, $G_1, G_2, \dots, G_{n-2\beta+s}$ and $G[S]$ are all cliques, and every vertex in S is adjacent to all vertices in $G_1, G_2, \dots, G_{n-2\beta+s}$. Consequently, we can write G as

$K_s \vee (K_{n_1} \cup K_{n_2} \cup \dots \cup K_{n_{n-2\beta+s}})$, where $n_i = |V(G_i)|$ for $1 \leq i \leq n-2\beta+s$. Without loss of generality, we can suppose that $n_1 \leq n_2 \leq \dots \leq n_{n-2\beta+s}$. Note that

$S(K_p) = (\underbrace{p, p, \dots, p}_{p-1}, 0)$. It is easy to obtain that

$$\begin{aligned} S\left(K_{n_1} \cup K_{n_2} \cup \dots \cup K_{n_{n-2\beta+s}}\right) &= (\underbrace{n_{n-2\beta+s}, \dots, n_{n-2\beta+s}}_{n_{n-2\beta+s}-1}, \dots \\ &\quad \dots, \underbrace{n_1, \dots, n_1}_{n_1-1}, \underbrace{0, \dots, 0}_{n-2\beta+s}) \\ S\left(\overline{K_{n_1} \cup K_{n_2} \cup \dots \cup K_{n_{n-2\beta+s}}}\right) &= (\underbrace{n-s, \dots, n-s}_{n-2\beta+s-1}, \dots \\ &\quad \dots, \underbrace{n-s-n_1, \dots, n-s-n_1}_{n_1-1}, \dots, \underbrace{n-s-n_{n-2\beta+s}, \dots, n-s-n_{n-2\beta+s}}_{n_{n-2\beta+s}-1}, 0) \\ S(\overline{G}) &= S\left(\overline{K_s \cup K_{n_1} \cup K_{n_2} \cup \dots \cup K_{n_{n-2\beta+s}}}\right) \\ &= (\underbrace{n-s, \dots, n-s}_{n-2\beta+s-1}, \underbrace{n-s-n_1, \dots, n-s-n_1}_{n_1-1}, \dots, \\ &\quad \dots, \underbrace{n-s-n_{n-2\beta+s}, \dots, n-s-n_{n-2\beta+s}}_{n_{n-2\beta+s}-1}, \underbrace{0, \dots, 0}_{s+1}). \end{aligned}$$

Thus, we have

$$\begin{aligned} S(G) &= (\underbrace{n, \dots, n}_s, \underbrace{s+n_{n-2\beta+s}, \dots, s+n_{n-2\beta+s}}_{n_{n-2\beta+s}-1}, \dots, \\ &\quad \dots, \underbrace{s+n_1, \dots, s+n_1}_{n_1-1}, \underbrace{s, \dots, s}_{n-2\beta+s-1}, 0). \end{aligned}$$

Therefore, we obtain that

$$LEE(G) = 1 + s e^n + (n - 2\beta + s - 1) e^s + \sum_{i=1}^{n-2\beta+s} (n_i - 1) e^{s+n_i}.$$

Assume that $g(x) = (x - 1) e^{s+x} + (m - x - 1) e^{s+m-x}$. It is easy to show that

$$g'(x) = x e^{s+x} - (m - x) e^{s+m-x} \leq 0$$

for $1 \leq x \leq m/2$, where equality holds if and only if $x = m/2$. This implies that

$$(n_i - 1) e^{n-n_i} + (n_j - 1) e^{n-n_j} < (n_i - 2) e^{n-n_i+1} + n_j e^{n-n_j-1}$$

for $n_i \leq n_j$. Thus, by replacing any pair (n_i, n_j) with $n_i \leq n_j$ by $(n_i - 1, n_j + 1)$ in the sum $\sum_{i=1}^{n-2\beta+s} (n_i - 1) e^{s+n_i}$, we increase the sum. By repeating this process, we attain the maximum of $1 + s e^n + (n - 2\beta + s - 1) e^s + \sum_{i=1}^{n-2\beta+s} (n_i - 1) e^{s+n_i}$ if and only if $n_1 = n_2 = \dots = n_{n-2\beta+s-1} = 1$ and $n_{n-2\beta+s} = 2\beta - 2s + 1$. It follows that G can be written as

$$K_s \sqrt{\overline{K_{n-2\beta+s-1}}} \cup K_{2\beta-2s+1}$$

and

$$LEE(G) = 1 + s e^n + (n - 2\beta + s - 1) e^s + (2\beta - 2s) e^{2\beta-s+1}.$$

Since $n - s \geq n - 2\beta + s$, we we have $s \leq \beta$. Suppose that $h(s) = 1 + s e^n + (n - 2\beta + s - 1) e^s + (2\beta - 2s) e^{2\beta-s+1}$. By taking derivatives, we have

$$h''(s) = (n - 2\beta + s + 1) e^s + 2(\beta - s + 2) e^{2\beta-s+1} > 0.$$

It follows that $h(s)$ is a strictly convex function for $1 \leq s \leq \beta$, and the maximum is achieved for $s = 1$ or $s = \beta$. It is easy to show that

$$\begin{aligned} h(\beta) - h(1) &= (\beta - 1) e^n - 2(\beta - 1) e^{2\beta} + (n - \beta - 1) e^\beta - (n - 2\beta) e \\ &\geq (\beta - 1) e^{2\beta+1} - 2(\beta - 1) e^{2\beta} + (n - \beta - 1) e^\beta - (n - 2\beta) e \\ &\geq 0 \end{aligned}$$

where equalities hold if and only if $\beta = 1$. Thus, $LEE(G) \leq 1 + \beta e^n + (n - \beta - 1) e^\beta$ with equality if and only if $G \cong K_\beta \sqrt{\overline{K_{n-\beta}}}$. This completes the proof. □

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