

MORE ON THE NORMALIZED LAPLACIAN ESTRADA INDEX

Yilun Shang

Let G be a simple graph of order N . The normalized Laplacian Estrada index of G is defined as $NEE(G) = \sum_{i=1}^N e^{\lambda_i^{-1}}$, where $\lambda_1, \lambda_2, \dots, \lambda_N$ are the normalized Laplacian eigenvalues of G . In this paper, we give a tight lower bound for NEE of general graphs. We also calculate NEE for a class of treelike fractals, which contains T fractal and Peano basin fractal as its limiting cases. It is shown that NEE scales linearly with the order of the fractal, in line with a best possible lower bound for connected bipartite graphs.

1. INTRODUCTION

Let G be a simple undirected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_N\}$. Denote by $A = A(G) \in \mathbb{R}^{N \times N}$ the adjacency matrix of G , and $\lambda_1(A) \geq \lambda_2(A) \geq \dots \geq \lambda_N(A)$ the eigenvalues of A in non-increasing order. The Laplacian and normalized Laplacian matrices of G are defined as $L = L(G) = D - A$ and $\mathcal{L} = \mathcal{L}(G) = D^{-1/2}LD^{-1/2}$, respectively, where $D = D(G)$ is a diagonal matrix with d_i on the main diagonal being the degree of vertex v_i , $i = 1, \dots, N$. Here, by convention $d_i^{-1} = 0$ if $d_i = 0$. The eigenvalues of L and \mathcal{L} are referred to as the Laplacian and normalized Laplacian eigenvalues of graph G , denoted by $\lambda_1(L) \geq \lambda_2(L) \geq \dots \geq \lambda_N(L)$ and $\lambda_1(\mathcal{L}) \geq \lambda_2(\mathcal{L}) \geq \dots \geq \lambda_N(\mathcal{L})$, respectively. Details of the theory of graph eigenvalues can be found in [4, 5].

The Estrada index of a graph G is defined in [6] as

$$EE = EE(G) = \sum_{i=1}^N e^{\lambda_i(A)},$$

2010 Mathematics Subject Classification. 05C50, 15A18, 05C05.

Keywords and Phrases. Normalized Laplacian Estrada index, bound, eigenvalue, fractal.

which was first introduced in 2000 as a molecular structure-descriptor by ERNESTO ESTRADA [7]. The Laplacian Estrada index of a graph G is defined in [21, 22] as

$$LEE = LEE(G) = \sum_{i=1}^N e^{(\lambda_i(L) - 2E/N)},$$

where E is the number of edges in G . Another essentially equivalent definition for the Laplacian Estrada index is given by $LEE = \sum_{i=1}^N e^{\lambda_i(L)}$ in [14] independently.

Albeit young, the Estrada index has already found a variety of chemical applications in the degree of folding of long-chain polymeric molecules [7, 8], extended atomic branching [13], and the Shannon entropy descriptor [9]. On top of that, the Estrada index based on the adjacency matrix emerges naturally in many physical-mathematical contexts, such as the analysis of vibrations in networks [11, 12, 24, 26, 27]. We refer to the recent survey [10] for more results and applications concerning (Laplacian) Estrada index in terms of network communicability.

Mathematical properties of EE and LEE , especially the upper and lower bounds, are investigated in, e.g., [1, 3, 15, 16, 17, 20, 25, 29, 32]. From a numerical analysis perspective, more accurate bounds for EE are obtained by BENZI and BOITO [2] using quadrature rule techniques. Such techniques turn out to be very useful for deriving sharp bounds of indices involving adjacency matrices. Moreover, a framework for calculating EE of general weighted graphs is formulated in [28].

Very recently, in full analogy with the (Laplacian) Estrada index, the normalized Laplacian Estrada index of a graph G is introduced in [19] as

$$(1) \quad NEE = NEE(G) = \sum_{i=1}^N e^{\lambda_i(\mathcal{L}) - 1}.$$

Among other things, the following tight bounds for NEE are obtained.

Theorem 1. [19] *If G is a connected graph of order N , then*

$$(2) \quad NEE \geq (N - 1)e^{1/(N-1)} + e^{-1}.$$

The equality holds if and only if $G = K_N$, i.e., a complete graph.

Theorem 2. [19] *Let G be a connected bipartite graph of order N with maximum degree Δ and minimum degree δ . Then*

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

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

In this paper, we find a tight lower bound for NEE of a general graph (not necessarily connected) by extending Theorem 1. We also calculate NEE for a class of treelike fractals, which subsume some chemical trees as special cases, through an explicit recursive relation. We unveil that NEE scales linearly with the order of the fractal, i.e., $NEE \propto N$ for large N , in line with the lower bound in Theorem 2.

2. A NEW LOWER BOUND FOR GENERAL GRAPHS

We begin with some basic properties of the normalized Laplacian eigenvalues of a connected graph G . In the rest of the paper, to ease notation, we use λ_i , $i = 1, \dots, N$ to represent the normalized Laplacian eigenvalues of a graph of order N .

Lemma 1. [4] *Let G be a connected graph of order $N \geq 2$. Then*

$$(i) \sum_{i=1}^N \lambda_i = N.$$

$$(ii) \lambda_N = 0 \text{ and } \lambda_i \in (0, 2] \text{ for every } 1 \leq i \leq N - 1.$$

$$(iii) \text{ If } G \text{ is a bipartite graph, then } \lambda_1 = 2 \text{ and } \lambda_2 < 2.$$

Theorem 3. *Let G be a graph of order N . If G possesses c connected components, r of which are isolated vertices, then*

$$(4) \quad NEE \geq (N - c)e^{\frac{c-r}{N-c}} + ce^{-1}.$$

The equality holds if and only if G is a union of copies of K_s , for some fixed $s \geq 2$, and r isolated vertices.

Clearly, we reproduce Theorem 1 when $c = 1$ (and $r = 0$).

Proof. From Lemma 1 and the fact that the normalized Laplacian eigenvalue for an isolated vertex is zero, we obtain $\lambda_N = \dots = \lambda_{N-c+1} = 0$ and $\lambda_1 + \dots + \lambda_{N-c} = N - r$. Hence,

$$NEE = e^{-1} \left(c + \sum_{i=1}^{N-c} e^{\lambda_i} \right) \geq e^{-1} \left(c + (N - c)e^{\frac{\lambda_1 + \dots + \lambda_{N-c}}{N-c}} \right) = ce^{-1} + (N - c)e^{\frac{c-r}{N-c}},$$

where the arithmetic-geometric mean inequality is utilized.

Now suppose $G = (c-r)K_s \cup rK_1$ for some integers $0 \leq r \leq c$ and $s \geq 2$. Then $N = (c-r)s + r = cs - r(s-1)$, and the normalized Laplacian eigenvalues of G can be computed as 0 with multiplicity c and $s/(s-1)$ with multiplicity $(c-r)(s-1)$. Therefore,

$$NEE(G) = ce^{-1} + (c-r)(s-1)e^{\frac{s}{s-1}-1} = ce^{-1} + (N-c)e^{\frac{c-r}{N-c}}.$$

Conversely, suppose that the equality holds in (4). Then from the above application of the arithmetic-geometric mean inequality we know that all the non-zero normalized Laplacian eigenvalues of G must be mutually equal. Suppose that a connected graph H with order s has normalized Laplacian eigenvalues $\lambda > 0$ with multiplicity $s - 1$ and a single zero eigenvalues. It now suffices to show $H = K_s$.

The case of $s = 1$ holds trivially. In what follows, we assume $s \geq 2$. We first claim that

$$(5) \quad \mathcal{L}(H)(\mathcal{L}(H) - \lambda I_s) = \mathbf{0},$$

where $I_s \in \mathbb{R}^{s \times s}$ is the identity matrix and $\mathbf{0}$ is the zero matrix. Indeed, for any vector $x \in \mathbb{R}^s$, we can decompose it as $x = a_1 D^{1/2} \mathbf{1} + \sum_{i=2}^s a_i x_i$, where $a_i \in \mathbb{R}$, $\mathbf{1}$ is a column vector with all elements being 1, and $x_i, i = 2, \dots, s$ are eigenvectors associated with λ . Thus, the equation (5) follows by the fact that $\mathcal{L}(H)(\mathcal{L}(H) - \lambda I_s)x = 0$ for all x .

In the light of (5), all columns of $\mathcal{L}(H) - \lambda I_s$ belong to the null space of $\mathcal{L}(H)$. It follows from Lemma 1 that the null space of $\mathcal{L}(H)$ is of dimension one and is spanned by $D^{1/2} \mathbf{1}$. Therefore, each column of $\mathcal{L}(H) - \lambda I_s$ is of the form $\alpha D^{1/2} \mathbf{1}$ for some $\alpha \in \mathbb{R}$. Since H is connected, $\alpha \neq 0$ and $d_i > 0$ for all i . It follows that any pair of vertices in H must be adjacent in view of the definition of $\mathcal{L}(H)$. This means $H = K_s$.

REMARK 1. Theorem 3 extends the result in Theorem 1 to the case when the graphs are not connected. From a practical perspective, nevertheless, bounds obtained on the basis of the number of vertices are not so useful because these indices change with the structure of the graphs.

For instance, let us consider Erdős-Rényi random graphs with 100 vertices and m edges. Some values of the index NEE are as follows. These tiny variations in the index

	$m = 400$	$m = 600$	$m = 800$	$m = 1000$
NEE	288.89	283.02	280.07	278.32

are the ones which are important. Thus, the lower bound of 100.37 (by Theorem 1) is reached only for very dense graphs of no interest whatsoever in practice. We refer to [3, 26, 30] for more results in the random graph setting.

3. THE NORMALIZED LAPLACIAN ESTRADA INDEX OF TREELIKE FRACTALS

In this section, we analytically calculate NEE for a class of treelike fractals through a recursive relation deduced from the self-similar structure of the fractals. It is of great interest to seek NEE (also LEE and EE) for specific graphs due to the following two reasons: Firstly, a universal approach for evaluating these

structure descriptors of general graphs, especially large-scale graphs, is out of reach so far; and secondly, the known upper and lower bounds (such as (3)) are too far away apart to offer any meaningful guide for a given graph.

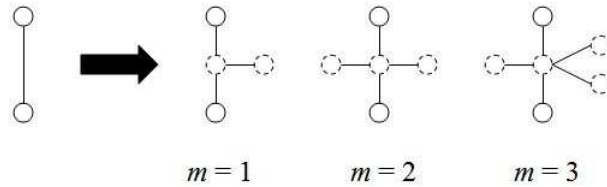


Figure 1. Building blocks of the fractals. The next generation is obtained from current generation through replacing each edge by the stars on the right-hand side of the arrow.

The fractal graphs in question are constructed in an iterative manner [23]. For integers $n \geq 0$ and $m \geq 1$, let $G_n(m)$ represent the graph after n iterations (generations). When $n = 0$, $G_0(m)$ is an edge linking two vertices. In each following iteration $n \geq 1$, $G_n(m)$ is built from $G_{n-1}(m)$ by conducting such operations on each existing edges as shown in Fig. 1: subdivide the edge into two edges, connecting to a new vertex; then, generate m new vertices and attach each of them to the middle vertex of the length-2 path. The first several steps of the iterative construction process corresponding to $m = 1$ are illustrated in Fig. 2. Clearly, it reduces to two classes of well-known fractals: the T fractal (when $m = 1$) and the Peano basin fractal (when $m = 2$).

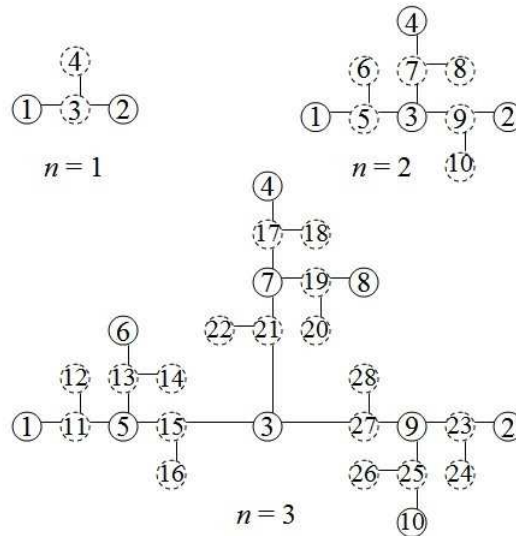


Figure 2. Growth process for a fractal corresponding to $m = 1$. The vertex with index 3 is called the *inmost* vertex since it is in the center of the graph, and those vertices farthest from the inmost vertex are called the *outmost* vertices (e.g. vertices with indices 1, 2, and 4).

Another intuitive generation approach of the fractal $G_n(m)$, which will be used later, highlights the self-similarity. Taking $G_n(m)$ with $n = 3$ and $m = 1$ as an example (see Fig. 2), $G_n(m)$ can be obtained by coalescing $m + 2$ replicas of $G_{n-1}(m)$ (denoted by $G_{n-1}^{(i)}(m)$, $i = 1, \dots, m + 2$) with the $m + 2$ outmost vertices in separate duplicates being merged into one single new vertex – the inmost vertex of $G_n(m)$ (e.g. the vertex with index 3 in Fig. 2).

Since our results will be stated for any fixed m , we often suppress the index m in notations. Some basic properties of $G_n = G_n(m)$ are easy to derive. For example, the number of vertices and edges are given by $N_n = (m + 2)^n + 1$ and $E_n = (m + 2)^n$, respectively. We write $\mathcal{L}_n = \mathcal{L}(G_n)$ as the normalized Laplacian matrix of G_n . Its eigenvalues are denoted by $\lambda_1(n) \geq \lambda_2(n) \geq \dots \geq \lambda_{N_n}(n)$. Therefore, the normalized Laplacian Estrada index

$$(6) \quad NEE(G_n) = \sum_{i=1}^{N_n} e^{\lambda_i(n)-1}$$

can be easily derived provided we have all the eigenvalues.

Theorem 4. *All the eigenvalues $\{\lambda_i(n)\}_{i=1}^{N_n}$, $n \geq 1$ can be obtained by the following recursive relations:*

- (i) 0 and 2 are both single eigenvalues for every $n \geq 1$.
- (ii) 1 is an eigenvalue with multiplicity $m(m + 2)^{n-1} + 1$ for $n \geq 1$.
- (iii) For $n \geq 1$, all eigenvalues $\lambda(n + 1)$ (except 0, 1, and 2) at generation $n + 1$ are exactly those produced via

$$(7) \quad \lambda(n + 1) = 1 \pm \sqrt{1 - \frac{\lambda(n)}{m + 2}}$$

by using eigenvalues $\lambda(n)$ (except 0 and 2) at generation n .

Proof. We start with checking the completeness of the eigenvalues provided by the rules (i), (ii), and (iii). It is direct to check that the eigenvalues for $G_1(m)$ (0, 2, and 1 with multiplicity $m + 1$) given by (i) and (ii) are complete. Therefore, all eigenvalues (except 0, 1, and 2) for $G_n(m)$, $n \geq 2$ are descendants of eigenvalue 1 following (7). Each father eigenvalue produces 2 child eigenvalues in the next generation. Thus, the total number of eigenvalues of $G_n(m)$ is found to be

$$2 + \sum_{i=0}^{n-1} (m(m + 2)^{n-1-i} + 1) 2^i = (m + 2)^n + 1 = N_n,$$

which implies that all eigenvalues are obtained.

Since G_n is connected and bipartite, (i) follows by Lemma 1. It suffices to show (ii) and that each eigenvalue $\lambda_i(n + 1)$ (except 0, 1, and 2) can be derived

through (7) by some eigenvalue $\lambda_i(n)$. Since \mathcal{L}_n is similar to $I_{N_n} - D^{-1}(G_n)A(G_n)$ thus having the same eigenvalues, we will focus on $I_{N_n} - D^{-1}(G_n)A(G_n)$ in the sequel and write it as \mathcal{L}_n for simplicity.

To derive the recursive relation (7), we resort to the so-called decimation method [18]. Let α denote the set of vertices belonging to G_n and β the set of vertices created at iteration $n + 1$. Assume that $\lambda_i(n + 1)$ is an eigenvalue of \mathcal{L}_{n+1} and $\lambda_i(n + 1) \neq 0, 1, 2$. Then the eigenvalue equation for \mathcal{L}_{n+1} can be recast in the following block form

$$(8) \quad \mathcal{L}_{n+1} \begin{bmatrix} u_\alpha \\ u_\beta \end{bmatrix} = \begin{bmatrix} I_{N_n} & \mathcal{L}_{\alpha,\beta} \\ \mathcal{L}_{\beta,\alpha} & \mathcal{L}_{\beta,\beta} \end{bmatrix} \begin{bmatrix} u_\alpha \\ u_\beta \end{bmatrix} = \lambda_i(n + 1) \begin{bmatrix} u_\alpha \\ u_\beta \end{bmatrix},$$

where $\mathcal{L}_{\beta,\beta} = I_{E_n} \otimes B$ with

$$B = \begin{bmatrix} 1 & -\frac{1}{m+2} & -\frac{1}{m+2} & \cdots & -\frac{1}{m+2} \\ -1 & 1 & 0 & \cdots & 0 \\ -1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & \cdots & 1 \end{bmatrix} \in \mathbb{R}^{(m+1) \times (m+1)}.$$

By eliminating u_β from (8) we arrive at

$$(9) \quad (I_{N_n} + \mathcal{L}_{\alpha,\beta}(\lambda_i(n + 1)I_{(m+1)E_n} - \mathcal{L}_{\beta,\beta})^{-1}\mathcal{L}_{\beta,\alpha}) u_\alpha = \lambda_i(n + 1)u_\alpha,$$

provided the concerned matrix is invertible. Let $\mathcal{P}_n = I_{N_n} + \mathcal{L}_{\alpha,\beta}(\lambda_i(n + 1)I_{(m+1)E_n} - \mathcal{L}_{\beta,\beta})^{-1}\mathcal{L}_{\beta,\alpha}$ and $\mathcal{Q}_n = (x + y)I_{N_n} - y\mathcal{L}_n$, with

$$(10) \quad x = \frac{\lambda_i(n + 1) - 1}{(m + 2)(\lambda_i(n + 1) - 2)\lambda_i(n + 1) + 2} + 1 = y + 1.$$

It is not difficult to see that $\mathcal{P}_n = \mathcal{Q}_n$.

Indeed,

$$\begin{aligned} (\lambda_i(n + 1)I_{(m+1)E_n} - \mathcal{L}_{\beta,\beta})^{-1} &= I_{E_n} \otimes (\lambda_i(n + 1)I_{m+1} - B)^{-1} \\ &= I_{E_n} \otimes \frac{\text{adj}((\lambda_i(n + 1)I_{m+1} - B))}{\det((\lambda_i(n + 1)I_{m+1} - B))}, \end{aligned}$$

where $\text{adj}(\cdot)$ means the adjugate matrix. Let z be the element on the first row and the first column of $(\lambda_i(n + 1)I_{m+1} - B)^{-1}$. We have

$$z = \frac{(\lambda_i(n + 1) - 1)^m}{\det((\lambda_i(n + 1)I_{m+1} - B))} = \frac{(m + 2)(\lambda_i(n + 1) - 1)}{2 + (m + 2)\lambda_i(n + 1)(\lambda_i(n + 1) - 2)},$$

which is well-defined since $\lambda_i(n + 1) \neq 0, 2$. With these preparations, it is easy to make an entry-wise comparison between \mathcal{P}_n and \mathcal{Q}_n . Clearly, $(\mathcal{Q}_n)_{i,i} = x = 1 + d_i(-1/d_i)z(-1/(m + 2)) = (\mathcal{P}_n)_{i,i}$; for $i \neq j$, if i and j are not adjacent,

$(\mathcal{Q}_n)_{i,j} = (\mathcal{P}_n)_{i,j} = 0$, while if i and j are adjacent, $(\mathcal{Q}_n)_{i,j} = -y(-1/d_i) = (-1/d_i)z(-1/(m+2)) = (\mathcal{P}_n)_{i,j}$. Hence, we conclude $\mathcal{P}_n = \mathcal{Q}_n$.

Inserting the equality $\mathcal{P}_n = \mathcal{Q}_n$ into (9) we get

$$\mathcal{L}_n u_\alpha = \left(\frac{x + y - \lambda_i(n+1)}{y} \right) u_\alpha,$$

where $y \neq 0$ since $\lambda_i(n+1) \neq 1$. This indicates that $\lambda_i(n) = (x + y - \lambda_i(n+1))/y$, where $\lambda_i(n)$ is an eigenvalue of \mathcal{L}_n associated with the eigenvector u_α . Combining this with (10) yields a quadratic equation, whose solution gives the formula (7) as desired.

It remains to show (ii). Let $M_n(\lambda)$ represent the multiplicity of eigenvalue λ of \mathcal{L}_n . We have

$$M_n(\lambda = 1) = N_n - \text{rank}(\mathcal{L}_n - I_{N_n}).$$

The problem of determining multiplicity is reduced to evaluating $\text{rank}(\mathcal{L}_n - I_{N_n})$.

(ii) follows by showing that

$$(11) \quad \text{rank}(\mathcal{L}_n - I_{N_n}) = 2(m+2)^{n-1}$$

for each $n \geq 1$.

To show (11) we use the method of induction. For $n = 1$, we have

$$\mathcal{L}_1 - I_{N_1} = \begin{bmatrix} 0 & -\frac{1}{m+2} & \cdots & -\frac{1}{m+2} \\ -1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{(m+3) \times (m+3)}.$$

Thus, $\text{rank}(\mathcal{L}_1 - I_{N_1}) = 2$. For $n = 2$, we have

$$\mathcal{L}_2 - I_{N_2} = \begin{bmatrix} 0 & -\frac{1}{m+2} & \cdots & -\frac{1}{m+2} \\ 0 & \cdots & \cdots & \cdots \\ \vdots & & I_{m+2} \otimes F & \\ 0 & & & \end{bmatrix},$$

where $F \in \mathbb{R}^{(m+2) \times (m+2)}$ is the matrix $\mathcal{L}_1 - I_{N_1}$ deleting the last column and the last row. Accordingly, $\text{rank}(\mathcal{L}_2 - I_{N_2}) = 2(m+2)$. For $n \geq 2$, we have

$$\mathcal{L}_{n+1} - I_{N_{n+1}} = \begin{bmatrix} 0 & -\frac{1}{m+2} & \cdots & -\frac{1}{m+2} \\ 0 & \cdots & \cdots & \cdots \\ \vdots & & I_{m+2} \otimes F_n & \\ 0 & & & \end{bmatrix},$$

where $F_n + I_{(m+2)^n} = \mathcal{L}(G_n \setminus \{\text{an outmost vertex}\})$. Moreover, F_n can be iteratively expressed as

$$F_n = \begin{bmatrix} F_{n-1} & 0 & \cdots & 0 & w_1 \\ 0 & F_{n-1} & \cdots & 0 & w_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & F_{n-1} & w_{m+1} \\ w_1^T & w_2^T & \cdots & w_{m+1}^T & F_{n-1} \end{bmatrix},$$

where each $w_i \in \mathbb{R}^{(m+2)^{n-1} \times (m+2)^{n-1}}$ is a matrix containing only one non-zero element $-1/(m+2)$ describing the edge linking the inmost vertex in G_n to one vertex in the replica $G_{n-1}^{(i)}$. For any vertex u in G_n that is adjacent to the inmost vertex of G_n , it has a neighbor v with degree one. Hence, there is only one non-zero element for row v and for column v , respectively, that is, $(F_n)_{v,u} = -1$ and $(F_n)_{u,v} = -1/(m+2)$. By using some basic operations for the matrix, we can eliminate all non-zero elements at the last row and the last column of F_n . Thus, $\text{rank}(\mathcal{L}_{n+1} - I_{N_{n+1}}) = (m+2) \cdot \text{rank}(F_n) = (m+2) \cdot \text{rank}(\mathcal{L}_n - I_{N_n})$. This yields (11), and finally concludes the proof.

REMARK 2. We mention that although the eigenvalues of a related matrix of $G_n(m)$ have been computed in [31] by a semi-analytical method, the normalized Laplacian eigenvalues cannot be derived directly from results therein.

REMARK 3. Note that the graph G_n is studied in a diffusion-like problem in [31]. Moreover, $NEE(G_n)$ is also related to network of quantum harmonic oscillators. Assume that each vertex of G_n is a ball of mass m , and each edge is a spring with the spring constant $m\omega^2$ connecting two balls. Let us consider the Hamiltonian of the oscillator network in the form

$$(12) \quad \mathcal{H} = \sum_i \frac{p_i^2}{2m} + \frac{m\omega^2}{2} \sum_{i < j} A(G_n)_{i,j} (x_i - x_j)^2,$$

where p_i and x_i are the momentum and coordinate of the ball i , respectively. In (12), the first term of the right-hand side is the kinetic energy of the ball i , whereas the second term is the potential energy of the springs connecting the balls. This network can move as a whole since it is not tied to the ground. It is shown in [10] (see Eqs. (25)-(30) therein)

$$\mathcal{H} = \sum_i \frac{p_i^2}{2m} + \frac{m\omega^2}{2} \sum_{i,j} (x_i \sqrt{d_i}) \mathcal{L}(G_n)_{i,j} (x_j \sqrt{d_j}),$$

and the thermal Green's function of the network of quantum oscillators with Hamiltonian \mathcal{H} corresponds to a network communicability function related to $NEE(G_n)$. We refer to [10, Section 3] for details.

With Theorem 4 at hand, the normalized Laplacian Estrada index can be easily evaluated through (6). Note that $G_n(m)$ is a connected bipartite graph with maximum degree $\Delta = m+2$ and minimum degree $\delta = 1$. In Fig. 3, we display $NEE(G_n(m))$ for $n = 1, \dots, 7$, $m = 1, \dots, 5$ together with the obtained bounds in Theorem 2. The results gathered in Fig. 3 allow us to draw several interesting comments. First, as expected from Theorem 2, all values of $NEE(G_n(m))$ lie

between the upper and lower bounds. Second, the lower bounds for different values of Δ are collapsed together and they scale with the order of the graph as $NEE \propto N$, which can be derived from (3). Similarly, the upper bound scales with N as $NEE \propto e^{\sqrt{N}}$. Third, $NEE(G_n(m))$ also scales linearly with the order of the fractal, i.e., $NEE(G_n(m)) \propto N_n$, in parallel with the lower bound.

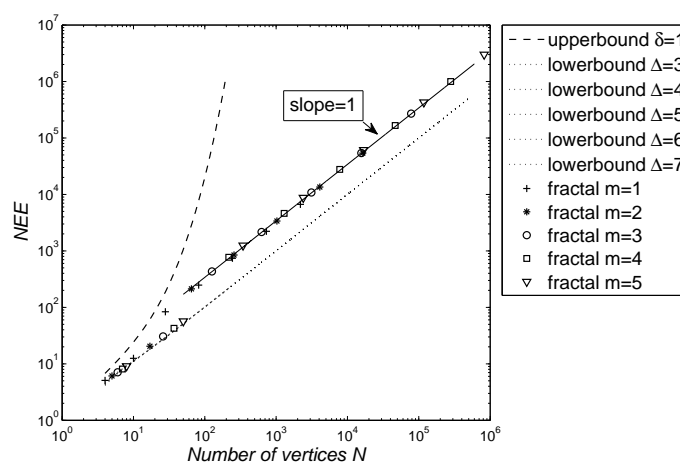


Figure 3. The normalized Laplacian Estrada index NEE versus the number of vertices N in log-log scale. Markers represent $NEE(G_n(m))$ for $n = 1, \dots, 7$, $m = 1, \dots, 5$; dashed and dotted lines represent the bounds given by (3).

Acknowledgements. The author acknowledges SUTD-MIT International Design Center, where most of this research was carried through. The author also thanks the referees for their careful reading and interesting suggestions.

REFERENCES

1. H. BAMDAD, F. ASHRAF, I. GUTMAN: *Lower bounds for Estrada index and Laplacian Estrada index*. Appl. Math. Lett., **23** (2010), 739–742.
2. M. BENZI, P. BOITO: *Quadrature rule-based bounds for functions of adjacency matrices*. Linear Algebra Appl., **433** (2010), 637–652.
3. Z. CHEN, Y. Z. FAN, W. X. DU: *Estrada index of random graphs*. MATCH Commun. Math. Comput. Chem., **68** (2012), 825–834.
4. F. CHUNG: *Spectral Graph Theory*. Amer. Math. Soc., Providence, 1997.
5. D. M. CVETKOVIĆ, M. DOOB, H. SACHS: *Spectra of Graphs: Theory and Application*. Johann Ambrosius Bart Verlag, Heidelberg, 1995.
6. J. A. DE LA PEÑA, I. GUTMAN, J. RADA: *Estimating the Estrada index*. Linear Algebra Appl., **427** (2007), 70–76.
7. E. ESTRADA: *Characterization of 3D molecular structure*. Chem. Phys. Lett., **319** (2000), 713–718.

8. E. ESTRADA: *Characterization of the folding degree of proteins*. *Bioinformatics*, **18** (2002), 697–704.
9. E. ESTRADA, N. HATANO: *Statistical-mechanical approach to subgraph centrality in complex networks*. *Chem. Phys. Lett.*, **439** (2007), 247–251.
10. E. ESTRADA, N. HATANO, M. BENZI: *The physics of communicability in complex networks*. *Phys. Rep.*, **514** (2012), 89–120.
11. E. ESTRADA, J. A. RODRÍGUEZ-VELÁZQUEZ: *Subgraph centrality in complex networks*. *Phys. Rev. E*, **71** (2005), 056103.
12. E. ESTRADA, J. A. RODRÍGUEZ-VELÁZQUEZ: *Spectral measures of bipartivity in complex networks*. *Phys. Rev. E*, **72** (2005), 046105.
13. E. ESTRADA, J. A. RODRÍGUEZ-VELÁZQUEZ, M. RANDIĆ: *Atomic branching in molecules*. *Int. J. Quantum Chem.*, **106** (2006), 823–832.
14. G. H. FATH-TABAR, A. R. ASHRAFI, I. GUTMAN: *Note on Estrada and L-Estrada indices of graphs*. *Bull. Acad. Serbe Sci. Arts Cl. Sci. Math.*, **139** (2009), 1–16.
15. B. FURTULA, I. GUTMAN, T. MANSOUR, S. RADENKOVIĆ, M. SCHORK: *Relating Estrada index with spectral radius*. *J. Serbian Chem. Soc.*, **72** (2007), 1371–1376.
16. Y. GINOSAR, I. GUTMAN, T. MANSOUR, M. SCHORK: *Estrada index and Chbeyshev polynomials*. *Chem. Phys. Lett.*, **454** (2008), 145–147.
17. I. GUTMAN: *Lower bounds for Estrada index*. *Publ. Inst. Math. Beograd*, **83** (2008), 1–7.
18. N. LAL, M. L. LAPIDUS: *The decimation method for Laplacians on fractals: spectra and complex dynamics*. *Fractal Geometry and Dynamical Systems in Pure and Applied Mathematics II: Fractals in Applied Mathematics* (D. Carfi, M. L. Lapidus, E. P. J. Pearse, and M. van Frankenhuijsen, eds.), Amer. Math. Soc., Providence, 2013.
19. J. LI, J.-M. GUO, W. C. SHIU: *The normalized Laplacian Estrada index of a graph*. *Filomat*, **28** (2014), 365–371.
20. J. LI, W. C. SHIU, W. H. CHAN: *Note on the Laplacian Estrada index of a graph*. *MATCH Commun. Math. Comput. Chem.*, **66** (2011), 777–784.
21. J. LI, W. C. SHIU, A. CHANG: *On the Laplacian Estrada index of a graph*. *Appl. Anal. Discrete Math.*, **3** (2009), 147–156.
22. J. LI, J. ZHANG: *On the Laplacian Estrada index of unicyclic graphs*. *MATCH Commun. Math. Comput. Chem.*, **68** (2012), 835–842.
23. Y. LIN, B. WU, Z. ZHANG: *Determining mean first-passage time on a class of treelike regular fractals*. *Phys. Rev. E*, **82** (2010), 031140.
24. Y. SHANG: *Perturbation results for the Estrada index in weighted networks*. *J. Phys. A: Math. Theor.*, **44** (2011), 075003.
25. Y. SHANG: *Lower bounds for the Estrada index of graphs*. *Electron. J. Linear Algebra*, **23** (2012), 664–668.
26. Y. SHANG: *Random lifts of graphs: network robustness based on the Estrada index*. *Appl. Math. E-Notes*, **12** (2012), 53–61.
27. Y. SHANG: *Biased edge failure in scale-free networks based on natural connectivity*. *Indian J. Phys.*, **86** (2012), 485–488.

28. Y. SHANG: *Estrada index of general weighted graphs*. Bull. Aust. Math. Soc., **88** (2013), 106–112.
29. Y. SHANG: *Lower bounds for the Estrada index using mixing time and Laplacian spectrum*. Rocky Mountain J. Math., **43** (2013), 2009–2016.
30. Y. SHANG: *Distance Estrada index of random graphs*. Linear Multilinear Algebra, <http://dx.doi.org/10.1080/03081087.2013.872640>.
31. Z. ZHANG, B. WU, G. CHEN: *Complete spectrum of the stochastic master equation for random walks on treelike fractals*. EPL, **96** (2011), 40009.
32. B. ZHOU: *On Estrada index*. MATCH Commun. Math. Comput. Chem., **60** (2008), 485–492.

Einstein Institute of Mathematics,
Hebrew University of Jerusalem,
91904 Jerusalem
Israel
E-mail: shylymath@hotmail.com

(Received January 15, 2014)
(Revised July 7, 2014)