MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **77** (2017) 673-690

ISSN 0340 - 6253

Novel Bounds for the Normalized Laplacian Estrada Index and Normalized Laplacian Energy*

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(Received July 6, 2016)

Abstract

For a simple and connected graph, several lower and upper bounds of graph invariants expressed in terms of the eigenvalues of the normalized Laplacian matrix have been proposed in literature. In this paper, through a unified approach based on majorization techniques, we provide some novel inequalities depending on additional information on the localization of the eigenvalues of the normalized Laplacian matrix. Some numerical examples show how sharper results can be obtained with respect to those existing in literature.

1 Introduction

In literature, several topological indices, related to the structural properties of graphs, have been widely explored. We focus here on the normalized Laplacian Estrada index (see [22] and [23]) and the normalized Laplacian energy (see [11]), that are based on a particular matrix associated with a graph, called the normalized Laplacian matrix. Properties about the spectrum of this matrix and its relationship to the Randić index have been investigated in several works (see [10], [11], [12] and [17]). In this paper we use a powerful methodology that relies on majorization techniques (see [1], [3], [4] and [6]) in order to localize the graph topological indices we consider. In particular, through this technique, we derive new

*We thank Monica Bianchi and Anna Torriero for their valuable comments and suggestions.

bounds for these indices taking advantage of additional information on the localization of the eigenvalues of normalized Laplacian matrix. Furthermore, this additional information can be quantified by using numerical approaches developed in [13] and [15] and extended for normalized Laplacian matrix in [14]. Finally, some existing bounds (see [22] and [23]), depending on well-known inequalities on Randić index, have been also improved by using some novel results proposed in [5].

The paper is organized as follows: in Section 2 some preliminaries are given. In Section 3 we provide, through majorization techniques, new bounds for topological indices expressed in terms of the eigenvalues of the normalized Laplacian matrix and we also recover in a straightforward way some results proposed in [23]. The relation between normalized Laplacian Estrada index and Randić index has been used in Section 4 to obtain new inequalities on normalized Laplacian Estrada index. Finally, in Section 5 several numerical results are reported, showing how the proposed bounds are tighter than those given in literature.

2 Notations and Preliminaries

2.1 Basic graph concepts

We consider a simple, connected and undirected graph $G = (V, E)$ where $V = \{1, 2, \ldots, n\}$ is the set of vertices and $E \subseteq V \times V$ the set of edges, $|E| = m$.

The degree sequence of G is denoted by $\pi = (d_1, d_2, .., d_n)$ and it is arranged in non-increasing order $d_1 \geq d_2 \geq \cdots \geq d_n$, where d_i is the degree of vertex i.

It is well known that $\sum_{i=1}^{n} d_i = 2m$ and that if G is a tree, i.e. a connected graph without cycles, $m = n - 1$.

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

We now recall some properties of normalized Laplacian eigenvalues useful for our purpose. For more details we refer the reader to [10], [12] and [17].

Lemma 1. *(see [12]) Given a connected graph G of order $n \geq 2$, the following properties of the spectrum of $\mathcal{L}(G)$ hold:*

1. $\sum_{i=1}^{n} \gamma_i = \mathrm{tr}(\mathcal{L}(G)) = n$;
2. $\sum_{i=1}^{n} \gamma_i^2 = \mathrm{tr}(\mathcal{L}^2(G)) = n + 2\sum_{(i,j)\in E} \frac{1}{d_i d_j}$;
3. $\frac{n}{n-1} \leq \gamma_1 \leq 2$. *The left inequality is attained if and only if G is a complete graph, while the right inequality holds when G is a bipartite graph;*
4. $\gamma_n = 0$, $\gamma_{n-1} \neq 0$ *if G is connected.*

2.2 Normalized Laplacian indices

The normalized Laplacian Estrada index has been proposed in [23] and it is defined as:

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

In [22], an alternative definition of normalized Laplacian Estrada index has been provided:

$$\ell EE(G) = \sum_{i=1}^{n} e^{\gamma_i}. \tag{2}$$

Notice that $NEE(G) = \frac{1}{e}\ell EE(G)$, any results derived for $NEE(G)$ can be trivially re-stated for $\ell EE(G)$ and viceversa.

Another graph invariant, introduced in [11], is the normalized Laplacian energy of a graph denoted by:

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

In literature, (3) is also known as Randić energy (see [18] and [21]).

2.3 Randić index and Majorization techniques

The Randić index is defined as:

$$R_{-1}(G) = \sum_{(i,j)\in E} \left(\frac{1}{d_i d_j}\right),$$

and it can be equivalently expressed as:

$$R_{-1}(G) = \frac{1}{2}\left(\sum_{(i,j)\in E}\left(\frac{1}{d_i} + \frac{1}{d_j}\right)^2 - \sum_{i=1}^{n}\frac{1}{d_i}\right).$$

Given a fixed degree sequence π, let $\mathbf{x} \in \mathbb{R}^m$ be the vector whose components are $\dfrac{1}{d_i} + \dfrac{1}{d_j}$, with $(i,j) \in E$.

Since $\sum_{i=1}^m x_i = \sum_{(i,j)\in E}\left(\frac{1}{d_i}+\frac{1}{d_j}\right) = n$, let $\Sigma_n = \{\mathbf{x} \in \mathbb{R}_+^m : \sum_{i=1}^m x_i = n, x_1 \geq x_2 \geq \cdots \geq x_m\}$. By considering a closed subset S of Σ_n whose maximal and minimal elements with respect to the majorization order are $\mathbf{x}^*(S)$ and $\mathbf{x}_*(S)$, the Randić index can be bounded as follows (see (5) in [5]):

$$L_1 = \frac{\|\mathbf{x}_*(S)\|_2^2 - \sum_{i=1}^n \frac{1}{d_i}}{2} \leq R_{-1}(G) \leq \frac{\|\mathbf{x}^*(S)\|_2^2 - \sum_{i=1}^n \frac{1}{d_i}}{2} = U_1. \tag{4}$$

Inequalities (4) will be used in Section 4 in order to derive new bounds for $NEE(G)$.

Using the information available on the degree sequence of G and characterizing the set S, the minimal and maximal elements $\mathbf{x}^*(S)$ and $\mathbf{x}_*(S)$ can be easily computed.

In this paper, we focus on a specific case of a graph G with h pendent vertices, whose degree sequence is of the type

$$\pi = (d_1, \cdots, d_{n-h}, \underbrace{1, \cdots, 1}_{h}), \tag{5}$$

where $h > 0$ and $n - h \geq 2$ (we do not consider the star graph S_n since it is well-known that $R_{-1}(S_n) = 1$).

It is noteworthy that this method could be applied to other suitable degree sequences.

Pointing out that $\frac{1}{d_{n-h}} + \frac{1}{d_{n-h-1}} < 1 + \frac{1}{d_1}$ holds, we face the set

$$\begin{aligned} S_1 = \Bigg\{ &\mathbf{x} \in \mathbb{R}_+^m : \sum_{i=1}^m x_i = n,\ \ 1 + \frac{1}{d_1} \leq x_h \leq \cdots \leq x_1 \leq \frac{1}{d_{n-h}} + 1\,, \\ &\frac{1}{d_1} + \frac{1}{d_2} \leq x_m \leq \cdots \leq x_{h+1} \leq \frac{1}{d_{n-h}} + \frac{1}{d_{n-h-1}} \Bigg\}. \end{aligned} \tag{6}$$

For convenience of the reader, we report the expressions of the maximal and minimal elements of S_1.

The maximal element is derived by means of Corollary 3 in [5] as follows:

$$\mathbf{x}^*(S_1) = \begin{cases} \Big[\underbrace{M_1, \ldots\ldots, M_1}_{k}, \theta, \underbrace{m_1, \ldots\ldots, m_1}_{h-k-1}, \underbrace{m_2, \ldots\ldots, m_2}_{m-h}\Big] & \text{if} \quad n < a^* \\ \Big[\underbrace{M_1, \ldots\ldots, M_1}_{h}, \underbrace{M_2, \ldots\ldots, M_2}_{k-h}, \theta, \underbrace{m_2, \ldots\ldots m_2}_{m-k-1}\Big] & \text{if} \quad n \geq a^* \end{cases}, \tag{7}$$

where

$$k = \begin{cases} \left\lfloor \dfrac{n - h(m_1 - m_2) - mm_2}{M_1 - m_1} \right\rfloor & \text{if} \quad n < a^* \\ \\ \left\lfloor \dfrac{n - h(M_1 - M_2) - mm_2}{M_2 - m_2} \right\rfloor & \text{if} \quad n \geq a^* \end{cases},$$

$a^* = hM_1 + (m-h)m_2$, $m_1 = 1 + \dfrac{1}{d_1}$, $m_2 = \dfrac{1}{d_1} + \dfrac{1}{d_2}$, $M_1 = 1 + \dfrac{1}{d_{n-h}}$, $M_2 = \dfrac{1}{d_{n-h}} + \dfrac{1}{d_{n-h-1}}$ and θ is obtained as the difference between n and the sum of the other components of the vector $\mathbf{x}^*(S_1)$.

The minimal element is instead obtained by Corollary 10 in [5] as follows:

$$\mathbf{x}_*(S_1) = \begin{cases} \left[\underbrace{m_1, ..., m_1}_{h}, \underbrace{\dfrac{n - hm_1}{m-h}, ..., \dfrac{n - hm_1}{m-h}}_{m-h} \right] & \text{if} \quad n < \widetilde{a} \\ \left[\underbrace{\dfrac{n - M_2(m-h)}{h}, ..., \dfrac{n - M_2(m-h)}{h}}_{h}, \underbrace{M_2, ..., M_2}_{m-h} \right] & \text{if} \quad n \geq \widetilde{a}, \end{cases} \tag{8}$$

where $\widetilde{a} = hm_1 + (m-h)M_2$ and m_1, M_2 have the same meaning of before.

3 Bounds for normalized Laplacian indices via majorization techniques

In this section we provide bounds for normalized Laplacian Estrada index and normalized Laplacian energy. These descriptors can be expressed in terms of Schur-convex or Schur-concave functions of suitable variables. We briefly recall that Schur-convex (Schur-concave) functions preserve (reverse) the majorization order (see [24] for details).

3.1 Normalized Laplacian Estrada index

Firstly, we focus on $NEE(G)$. Let us consider the set

$$S_0 = \{\gamma \in \mathbb{R}^{n-1} : \sum_{i=1}^{n-1} \gamma_i = n, \ \gamma_1 \geq \gamma_2 \geq ... \geq \gamma_{n-2} \geq \gamma_{n-1} \geq 0 \ \}.$$

We can now consider a subset S_0^1 of S_0:

$$S_0^1 = \{\gamma \in S_0 : \gamma_1 \geq \alpha\},$$

with $\alpha \geq \frac{n}{n-1}$.

In order to compute the minimal element of S_0^1, we apply Corollary 14 in [6] and we obtain:

$$x_*(S_0^1) = \left(\alpha, \underbrace{\frac{n-\alpha}{n-2}, ..., \frac{n-\alpha}{n-2}}_{n-2} \right).$$

By the Schur-convexity of the function $NEE(G)$, we get the following bound:

$$NEE(G) \geq \frac{1}{e} + e^{\alpha-1} + (n-2)e^{\frac{2-\alpha}{n-2}}. \tag{9}$$

Setting $\alpha = \dfrac{n}{n-1}$, we can easily derive the same result proved in [23], Theorem 3.1:

$$NEE(G) \geq (n-1)\, e^{\dfrac{1}{n-1}} + \frac{1}{e}. \tag{10}$$

Furthermore, by applying a theoretical and numerical methodology (see [7] and [14]), it is possible to compute a different lower bound α for the first eigenvalue of γ_1 in a fairly straightforward way, that is $\gamma_1 \geq Q$, where

$$Q = \frac{\left(n + \sqrt{\frac{b(h^*+1)-n^2}{h^*}} \right)}{(1+h^*)},$$

with $b = n + 2\sum_{(i,j)\in E} \frac{1}{d_i dj}$ and $h^* = \left\lfloor \frac{n^2}{b} \right\rfloor$.
It is well-known that, for every connected graph of order n:

$$\left(\frac{2}{n}\right) \sum_{(i,j)\in E} \frac{1}{d_i d_j} \geq \frac{1}{n-1}, \tag{11}$$

with inequality attained when $G \cong K_n$ (see [2]). It has been shown in [14] that $Q \geq \frac{n}{n-1}$ and thus we assure that bound (9), by placing $\alpha = Q$, is sharper than (10) (see [5] and [6] for more theoretical details).

We can further improve bound (9) by identifying additional information on γ_2. In this case we face the set:

$$S_0^2 = \{\gamma \in S_0 : \gamma_1 \geq \alpha \ , \gamma_2 \geq \beta\}.$$

Under the assumptions $\alpha \geq \beta$ and $\alpha + \beta(n-2) > n$, by Corollary 14 in [6], the minimal element of S_0^2 with respect to the majorization order is given by

$$x_*(S_0^2) = \left(\alpha, \beta, \underbrace{\frac{n-\alpha-\beta}{n-3}, ..., \frac{n-\alpha-\beta}{n-3}}_{n-3} \right)$$

and we can provide the following bound:

$$NEE(G) \geq \frac{1}{e} + e^{\alpha-1} + e^{\beta-1} + (n-3)e^{\frac{3-\alpha-\beta}{n-3}}. \qquad (12)$$

In [14] the authors found a lower bound β for γ_2, that is $\gamma_2 \geq R$, where: $R = \frac{n-\sqrt{\frac{b(n-1)-n^2}{n-2}}}{n-1}$. They proved that $R \leq Q$ and numerically showed, for some classes of graphs, that $Q + R(n-2) > n$, satisfying the conditions underlying Corollary 14 in [6]. In virtue of these relations it is possible to compute bound (12) that is tighter than (9) with $\alpha = Q$ and (10) (see [5] and [6] for more theoretical details).

Finally, for bipartite graphs, it is well-known that $\gamma_1 = 2$. Hence

$$S_0^b = \{\gamma \in \mathbb{R}^{n-2} : \sum_{i=2}^{n-1} \gamma_i = n-2,\ 2 \geq \gamma_2 \geq ... \geq \gamma_{n-2} \geq \gamma_{n-1} \geq 0\}.$$

By applying Corollary 14 in [6], we recover the following bound provided in [23], Theorem 3.2:

$$NEE(G) \geq \frac{1}{e} + e + (n-2). \qquad (13)$$

Also in this case, we can improve this bound by identifying additional information on γ_2. We face the set:

$$S_0^{2b} = \{\gamma \in S_0^b : \gamma_2 \geq \beta\},$$

under the assumption $1 < \beta \leq 2$. By Corollary 14 in [6], the minimal element of S_0^2 with respect of majorization order is given by

$$x_*(S_0^{2b}) = \left(\beta, \underbrace{\frac{n-2-\beta}{n-3}, ..., \frac{n-2-\beta}{n-3}}_{n-3}\right)$$

and we can provide the following bound:

$$NEE(G) \geq \frac{1}{e} + e + e^{\beta-1} + (n-3)e^{\frac{1-\beta}{n-3}}, \qquad (14)$$

where the lower bound $\beta = R$ of γ_2 derived in [14] can be also used to compute (14).

In analogy with the results (9) and (12) on $NEE(G)$, we can easily derive the following bounds for $\ell EE(G)$ for connected non bipartite graphs:

$$\ell EE(G) \geq 1 + e^{\alpha} + (n-2)e^{\frac{n-\alpha}{n-2}} \qquad (15)$$

and

$$\ell EE(G) \geq e^{\alpha} + e^{\beta} + (n-3)e^{\frac{n-\alpha-\beta}{n-3}}, \qquad (16)$$

with $\gamma_1 \geq \alpha$, $\gamma_2 \geq \beta$ and $\alpha + \beta(n-2) > n$.

In Section 5 we will compare these bounds with those proposed in [22] and [23].

3.2 Normalized Laplacian energy

The normalized Laplacian energy $NE(G)$ can be rewritten as a Schur-concave function of the variables $(\gamma_i - 1)^2, i = 1, \cdots, n$:

$$NE(G) = 1 + \sum_{i=1}^{n-1} \sqrt{(\gamma_i - 1)^2}. \tag{17}$$

If a lower bound for γ_1 is available, i.e. $\gamma_1 \geq \alpha \left(\geq \frac{n}{n-1} \right)$, introducing the new variables $x_i = (\gamma_i - 1)^2$ as a function of the eigenvalue γ_i arranged in nonincreasing order, we get:

$$x_1 \geq k_1 = (\alpha - 1)^2.$$

Let us consider the set

$$S_{NE} = \{\mathbf{x} \in \mathbb{R}^{n-1} : \sum_{i=1}^{n-1} x_i = 2 \sum_{(i,j)\in E} \frac{1}{d_i d_j} - 1, x_1 \geq k_1\},$$

where the relation $\sum_{i=1}^{n-1} x_i = 2 \sum_{(i,j)\in E} \frac{1}{d_i d_j} - 1$ has been obtained by using properties recalled in Lemma 1.

With the same methodology described for $NEE(G)$, we can derive the minimal element of S_{NE} and then the following upper bound:

$$NE(G) \leq 1 + \sqrt{k_1} + \sqrt{(n-2)(a - k_1)}, \tag{18}$$

with $a = 2 \sum_{(i,j)\in E} \frac{1}{d_i d_j} - 1$. This bound could be computed by placing $k_1 = (Q-1)^2$.

Considering also an additional information on γ_2 (i.e. $\gamma_2 \geq \beta$), we may face the set:

$$S_{NE}^2 = \{\mathbf{x} \in S_{NE} : x_2 \geq k_2\}$$

under the assumptions $\alpha \geq \beta$ and $\alpha + \beta(n-2) > a$.

In this case, by means of the minimal element of S_{NE}^2, we can provide the bound:

$$NE(G) \leq 1 + \sqrt{k_1} + \sqrt{k_2} + \sqrt{(n-3)(a - k_1 - k_2)}, \tag{19}$$

where we can place $k_1 = (Q-1)^2$ and $k_2 = (R-1)^2$.

Finally, for bipartite graphs, taking into account that $\gamma_1 = 2$, we set:

$$S_{NE}^b = \{\mathbf{x} \in \mathbb{R}^{n-2} : \sum_{i=2}^{n-1} x_i = 2 \sum_{(i,j)\in E} \frac{1}{d_i d_j} - 2\},$$

and we derive the bound:

$$NE(G) \leq 2 + \sqrt{a(n-2)}, \tag{20}$$

where $a = 2\sum_{(i,j)\in E} \frac{1}{d_i d_j} - 2$.

Also in this case, we can improve this result by identifying additional information on γ_2. We face the set:

$$S_{NE}^{2b} = \{\mathbf{x} \in S_{NE}^{b} : x_2 \geq k_2\}$$

under the assumption $\dfrac{a-2}{n-2} < \beta \leq 2$ and we can provide the bound:

$$NE(G) \leq 2 + \sqrt{k_2} + \sqrt{(n-3)\,(a-k_2)}, \tag{21}$$

where the information $k_2 = (R-1)^2$ can be used to compute (21).

4 Bounds through Randić Index

In Theorem 3.4 and Theorem 3.5 in [23], the authors provided lower and upper bounds for $NEE(G)$ of a (bipartite) graph in terms of n and maximum (or minimum) degree. This result has been obtained through well-known inequalities on Randić index (see [25]), i.e. $\dfrac{n}{2d_1} \leq R_{-1}(G) \leq \dfrac{n}{2d_n}$.

Following this idea, we now deduce some bounds for $NEE(G)$ and its variant $\ell EE(G)$ by using the methodology based on majorization recalled in Section 2.3. In Section 5.2 we will numerically show that the bounds obtained are tighter than those provided in [22] and [23].

In virtue of (4) and by means of Theorem 3.4 in [23], we easily get the following result for bipartite graph:

Proposition 1. *Let G be a simple, connected and bipartite graph of order n. Then the normalized Laplacian Estrada index of G is bounded as:*

$$\frac{1}{e}+e+\sqrt{(n-2)^2+4(L_1-1)} \leq NEE(G) \leq \frac{1}{e}+e+(n-3)-\sqrt{2(U_1-1)}+e^{2(U_1-1)}. \tag{22}$$

In the same way as before, by Theorem 3.5 in [23] we have the following bounds for non-bipartite graphs:

Proposition 2. *Let G be a simple and connected graph of order n. Then the normalized Laplacian Estrada index of G is bounded as follows:*

$$\sqrt{(n-1)(1+(n-2)e^{\frac{2}{n-1}})+4L_1} \leq NEE(G) \leq \frac{1}{e} + (n-1) - \sqrt{2U_1 - 1} + e^{2U_1 - 1}. \quad (23)$$

Notice that, replacing $L_1 = \dfrac{n}{2d_1}$ and $U_1 = \dfrac{n}{2d_n}$, we recover the same bounds provided in [23], Theorem 3.4 and 3.5.

Bounds (22) and (23) can be trivially derived for $\ell EE(G)$ by using the proportionality relationship with $NEE(G)$. For the comparisons provided in Section 5.2, we only report the bound obtained for non-bipartite graph:

$$\sqrt{(n-1)(e+(n-2)e^{\frac{n+1}{n-1}})+4eL_1} \leq \ell EE(G) \leq 1+e\left[(n-1) - \sqrt{2U_1 - 1}\right] + e^{2U_1}. \quad (24)$$

5 Numerical Results

5.1 Comparing Bounds derived via majorization techniques

5.1.1 Normalized Laplacian Estrada index

Firstly, we focus on $NEE(G)$ by comparing for non-bipartite graphs bounds (9) and (12) with (10) proposed in [23]. It has been already analytically proved in Section 3.1 that, when the additional information $\gamma_1 \geq Q$ is considered, bound (9) with $\alpha = Q$ is tighter than (10). We now show how these bounds behave according to different graphs. In particular we analyze two alternative classes of graphs generated by using either the Erdös-Rényi (ER) model $G_{ER}(n, q)$ (see [9], [12], [19] and [20]) or the Watts and Strogatz (WS) model (see [26]). Both models have been generated by using a well-known package of R (see [16]) and by assuring that the graph obtained is connected. The ER is constructed by connecting nodes randomly such that edges are included with probability q independent from every other edge. The WS networks have been derived beginning by a simulated n-node lattice and rewiring each edge at random to a new target node with probability p. As described by [26], we choose a vertex and the edge that connects it to its nearest neighbor in a clockwise sense. With probability p, we reconnect this edge to a vertex chosen uniformly at random over the entire ring, with duplicate edges forbidden; otherwise we leave the edge in place. We repeat this process by moving clockwise around the ring, considering each vertex in turn until one lap is completed. Next, we consider the edges that connect vertices to their second-nearest neighbors clockwise. As before, we randomly rewire each of these edges with probability p and continue this process, circulating around the ring and proceeding outward to more distant neighbors after each lap, until each edge in the original lattice has been considered once. This construction allows to analyze the behavior of networks between regularity ($p = 0$) and disorder ($p = 1$).

In Table 1 we report the $NEE(G)$ index and the values of the three mentioned bounds evaluated on non-bipartite graphs generated by using ER model with different number of vertices and with q equal to 0.5. Relative errors r measures the absolute value of the difference between the lower bounds and $NEE(G)$ divided by the value of $NEE(G)$.

n	$NEE(G)$	bound (10)	bound (9)	bound (12)	r(10)	r(9)	r(12)
4	5.0862	4.5547	4.6783	4.7112	10.4488%	8.0184%	7.3717%
5	6.6073	5.5040	5.6407	5.6935	16.6991%	14.6301%	13.8304%
6	6.9783	6.4749	6.5088	6.5265	7.2140%	6.7287%	6.4748%
7	8.4965	7.4560	7.5345	7.5559	12.2457%	11.3223%	11.0700%
8	9.3463	8.4428	8.4778	8.4933	9.6663%	9.2921%	9.1266%
9	10.0295	9.4331	9.4456	9.4541	5.9466%	5.8219%	5.7365%
10	10.9027	10.4256	10.4334	10.4391	4.3768%	4.3048%	4.2528%
20	20.9252	20.3947	20.3963	20.3977	2.5353%	2.5274%	2.5206%
30	30.9411	30.3853	30.3860	30.3867	1.7963%	1.7940%	1.7919%
50	50.9236	50.3782	50.3784	50.3786	1.0710%	1.0705%	1.0701%
100	100.9001	100.3729	100.3730	100.3731	0.5225%	0.5224%	0.5223%

Table 1. Lower bounds for $NEE(G)$ and relative errors for graphs generated by $ER(n, 0.5)$ model.

As expected, using bound (12) we observe an improvement with respect to existing bound according to all the analyzed graphs. The improvement is very significant for graphs with a small number of vertices, while it reduces for very large graphs. However, for large graphs formula (10) provided in [23] already gives a very low relative error.

The comparison has been extended in order to test the behaviour of the bounds on alternative graphs generated by using always the ER model with a different probability q. For sake of simplicity we report only the relative errors derived for graphs generated by using respectively $q = 0.1$ and $q = 0.9$ (see Table 2). In all cases bound (12) assures the best approximation to $NEE(G)$. We observe a best behaviour of all bounds when $q = 0.9$ because we are moving towards the complete graph. We have indeed that the density of the graphs increases as long as greater probabilities are considered.

Finally, graphs have been simulated by using WS model with different rewiring probabilities p. As well-known, intermediate values of p result in small-world networks that share properties of both regular and random graphs. In [26], the authors show that these networks have small mean path lengths and high clustering coefficients. There is indeed a broad interval of p over which the average path is almost as small as random yet the clustering coefficient is significantly greater than random. These small-world networks result from the immediate drop in average path caused by the introduction of few long-range

	q=0.1				q=0.9			
n	$NEE(G)$	r(10)	r(9)	r(12)	$NEE(G)$	r(10)	r(9)	r(12)
4	5.3414	14.7282%	10.5879%	9.5649%	4.5547	0	0	0
5	6.6073	16.6991%	14.6301%	13.8304%	5.6685	2.9025%	2.5585%	2.0332%
6	7.7763	16.7360%	14.3140%	13.9214%	6.6355	2.4206%	2.2596%	2.1703%
7	8.4997	12.2785%	11.7944%	11.5183%	7.5599	1.3736%	1.3162%	1.27981%
8	9.9938	15.5196%	14.3868%	14.1672%	8.4664	0.2785%	0.2708%	0.2653%
9	11.0383	14.5423%	13.8300%	13.6702%	9.4702	0.3917%	0.3837%	0.3778%
10	12.5449	16.8940%	15.8599%	15.7231%	10.4541	0.2735%	0.2692%	0.2659%
20	23.8531	14.4989%	14.1869%	14.1557%	20.4488	0.2645%	0.2637%	0.2630%
30	34.8955	12.9249%	12.7815%	12.7693%	30.4424	0.1876%	0.1874%	0.1872%
50	54.7998	8.0688%	8.0399%	8.0370%	50.4274	0.0977%	0.0976%	0.0976%
100	104.7347	4.1646%	4.1608%	4.1604%	100.4293	0.0562%	0.0561%	0.0561%

Table 2. Lower bounds for $NEE(G)$ and relative errors for graphs generated respectively by $ER(n, 0.1)$ and $ER(n, 0.9)$ models.

edges. In particular, we analyze the behaviour of bounds in this interval by considering graphs generated with a rewiring probability in the range $p \in (0.01, 0.1)$. At this regard, Table 3 reports bounds evaluated by considering $p = 0.1$. In this case, we observe greater relative errors especially for large graphs. Probably, being these networks very far from complete graphs, bounds tend to assure a weaker approximation. Similar results have been obtained by simulating WS graphs choosing different values of p that belong to the interval.

n	$NEE(G)$	bound (10)	bound (9)	bound (12)	r(10)	r(9)	r(12)
4	5.0862	4.5547	4.6783	4.7112	10.4488%	8.0184%	7.3717%
5	6.3276	5.5040	5.6002	5.6389	13.0165%	11.4961%	10.8843%
6	7.5967	6.4749	6.5492	6.5856	14.7666%	13.7886%	13.3087%
7	8.8273	7.4560	7.6023	7.6273	15.5347%	13.8778%	13.5948%
8	10.1431	8.4428	8.5646	8.5878	16.7630%	15.5621%	15.3339%
9	11.3946	9.4331	9.5349	9.5568	17.2145%	16.3209%	16.1287%
10	12.6329	10.4256	10.5736	10.5917	17.4727%	16.3005%	16.1573%
20	25.2327	20.3947	20.5345	20.5442	19.1737%	18.6195%	18.5813%
30	37.7967	30.3853	30.5175	30.5240	19.6086%	19.2590%	19.2418%
50	63.2448	50.3782	50.5227	50.5268	20.3442%	20.1157%	20.1092%
100	126.4764	100.3729	100.5201	100.5222	20.6390%	20.5226%	20.5209%

Table 3. Lower bounds for $NEE(G)$ and relative errors for graphs generated by $WS(n, 0.1)$ model.

5.1.2 Normalized Laplacian energy

We compare here bounds proposed in Section 3.2 for $NE(G)$ with the following upper bounds proposed in [11]:

$$NE(G) \leq 2\left\lfloor \frac{n}{2} \right\rfloor, \tag{25}$$

$$NE(G) \leq \sqrt{\frac{15}{28}}(n+1). \tag{26}$$

Table 4 reports main results derived for graphs generated by a $ER(n, 0.5)$ model. We observe how both bounds (18) and (19) are tighter than those proposed in [11]. The improvement increases for greater number of vertices.

n	$NE(G)$	bound (25)	bound (26)	bound (18)	bound (19)
4	3.00	4	3.66	3.12	3.05
5	2.55	4	4.39	2.70	2.61
6	3.15	6	5.12	3.87	3.62
7	3.81	6	5.86	4.51	4.27
8	4.32	8	6.59	4.69	4.47
9	3.90	8	7.32	4.34	4.14
10	3.58	10	8.05	4.00	3.83
20	5.01	20	15.37	5.68	5.56
30	5.60	30	22.69	6.43	6.33
50	7.31	50	37.33	8.44	8.36
100	9.59	100	73.92	11.13	11.08

Table 4. Upper bounds for $NE(G)$ for graphs generated by $ER(n, 0.5)$ model.

Considering instead WS networks, derived as in Section 5.1.1 by assuming a rewiring probability equal to 0.1, we observe in Table 5 greater values of $NE(G)$. In this case, bound (26) gives better results than those observed for ER graphs. However it is confirmed the best approximation when bound (19) is used.

n	$NE(G)$	bound (25)	bound (26)	bound (18)	bound (19)
4	2	4	3.66	2.72	2.41
5	3.24	4	4.39	3.45	3.37
6	4	6	5.12	4.15	4.08
7	4.49	6	5.86	4.87	4.63
8	5.12	8	6.59	5.57	5.33
9	5.76	8	7.32	6.27	6.03
10	6.47	10	8.05	6.99	6.75
20	11.97	20	15.37	13.67	13.42
30	19.24	30	22.69	21.16	20.90
50	31.79	50	37.33	35.27	34.99
100	63.21	100	73.92	70.22	69.93

Table 5. Upper bounds for $NE(G)$ for graphs generated by $WS(n, 0.1)$ model.

5.2 Bounds based on Randić Index

We now consider an example based on a specific degree sequence of type (5) in order to explain the details of the procedure used to bound $NEE(G)$ via Randić Index. In the next we will extend the results to several degree sequences of type (5).

Example 1. Let us consider the class C_π of graphs with the following degree sequence:

$\pi = (7, 6, 5, 4, 4, 4, 3, 3, 3, 3, 3, 3, 2, 2, 2, 2, 1, 1, 1, 1)$

We have $n = 20$, $m = 30$ and $h = 4$ pendant nodes. Since $\tilde{a} > n$, the minimal element (8) is:

$$\mathbf{x}_*(G) = \left[\underbrace{\frac{8}{7}, \ldots, \frac{8}{7}}_{4}, \underbrace{\frac{54}{91}, \ldots, \frac{54}{91}}_{16} \right].$$

Replacing these values in (4), we find $L_1 = 2.56$, while $\frac{n}{2d_1} = 1.43$.

The bounds for $NEE(G)$ are figured out in Table 6. Furthermore, in order to test how these bounds behave, the exact value of $NEE(G)$ is also needed. Having a huge number[1] of graphs $G \in C_\pi$, we randomly generate one million of different graphs belonging to the class C_π. The average value, the minimum and maximum values of the index are also reported in Table 6.

Reference	Bound
Theorem 3.5 of [23]	20.12
(23)	20.23
Min($NEE(G)$)	20.51
Mean($NEE(G)$)	23.25
Max($NEE(G)$)	25.52

Table 6. Lower bounds for $NEE(G)$.

Considering instead the upper bound, since $a^* < n$, we compute $k = 12 > h = 4$ and we have that the maximal element (7) is:

$$\mathbf{x}^*(G) = \left[\underbrace{\frac{3}{2}, \ldots, \frac{3}{2}}_{4}, \underbrace{1, \ldots, 1}_{8}, \frac{31}{42}, \underbrace{\frac{31}{42}, \ldots, \frac{31}{42}}_{17} \right],$$

leading to $U_1 = 4.96$, while $\frac{n}{2d_n} = 10$.

Upper bounds and values of $NEE(G)$ are summarized in Table 7.

Reference	Bound
Theorem 3.5 of [23]	$1.7 * 10^8$
(23)	7541.32
Min($NEE(G)$)	20.51
Mean($NEE(G)$)	23.25
Max($NEE(G)$)	25.52

Table 7. Upper bounds for $NEE(G)$.

Finally, if we know the value of Randić Index, we can directly use it to compute (23). For example, considering a random graph $G \in C_\pi$, we obtain $R_{-1}(G) = 3.0376$ deriving a better approximation (i.e. $20.27 \leq NEE(G) \leq 177.15$).

[1] We estimate the total number of graphs with the degree sequence π by using the importance sampling algorithm proposed in [8]. Authors show robust results by applying the algorithm with 100.000 trials. In this case we derive a total number of graphs equal to roughly $1.20 \cdot 10^{20}$ with a standard error of $4 \cdot 10^{17}$. However it is noteworthy that also graphs belonging to the same isomorphism class are considered in this value. For the computation of the average values in Tables 6 and 7, we take into account only graphs with a different $NEE(G)$.

We now evaluate these bounds by randomly generating several degree sequences of type (5). For this aim, $ER(n,p)$ model has been used to derive different random graphs, where we disregard graphs whose degree sequence does not belong to the set (6). The number of pendant vertices h varies according to the specific degree sequence obtained. Results have been compared to those analyzed in previous Section 5.1.1. In particular, we report in Table 8 bound (10) and bound $(23d_1)$ proposed in [23], where bound $(23d_1)$ has been derived by using in (23) the lower bound $\frac{n}{2d_1}$ of $R_{-1}(G)$. These bounds have been compared with bound (9) and bound (12) already analysed in previous section and with bound $(23L_1)$ and bound $(23R_{-1})$ evaluated by using the first left inequality of (23) and by considering respectively the value of L_1 or by assuming to know the value of Randić Index $R_{-1}(G)$.

We further observe that bound (12) based on value of Q and R shows the tighter lower bound in all cases by allowing a best approximation respect to bounds based on inequality (23). Furthermore, when inequality (23) is considered, L_1 leads to a better bound than $\frac{n}{2d_1}$ used in [23]. Finally, considering the exact value of Randić Index we only get a slight improvement.

n	m	d_1	$NEE(G)$	bound (10)	bound $(23d_1)$	bound (9)	bound (12)	bound $(23L_1)$	bound $(23R_{-1})$
4	4	3	4.8846	4.5547	4.1657	4.6466	4.6718	4.2797	4.2840
5	5	3	6.2381	5.5040	5.2075	5.6002	5.6389	5.3288	5.3651
6	9	5	6.8224	6.4749	6.1022	6.4977	6.5099	6.1841	6.1952
7	11	5	7.9613	7.4560	7.1182	7.4774	7.4901	7.1933	7.2062
8	12	6	9.2439	8.4428	8.0967	8.4667	8.4817	8.2018	8.2463
9	14	4	10.4376	9.4331	9.1872	9.4722	9.4843	9.2432	9.2490
10	15	8	11.2359	10.4256	10.0706	10.4435	10.4522	10.1687	10.1977
20	30	7	23.3079	20.3947	20.1166	20.4401	20.4465	20.2346	20.2914
30	45	7	34.8334	30.3853	30.1255	30.4342	30.4385	30.2355	30.2914
50	75	6	58.8047	50.3782	50.1563	50.4387	50.4416	50.2535	50.3259
100	150	8	117.1121	100.3729	100.1199	100.4310	100.4325	100.2397	100.3214

Table 8. Lower bounds for $NEE(G)$.

On the same graphs upper bounds have been also evaluated by using the right part of inequality (23). We observe in Table 9 a huge approximation, especially for large graphs, when we apply formula proposed in [23] based on the upper bound $\frac{n}{2d_n}$ of Randić Index $R_{-1}(G)$ (see bound $(23d_n)$). By considering the upper bound based on U_1 we are able to improve the results, but for large graphs we derive useless bounds in this case too. We have indeed that even when we directly use the value of $R_{-1}(G)$ we derive bounds significantly larger for graphs with a great number of vertices.

Bounds proposed for $\ell EE(G)$ have been also compared to the following bounds presented in [22]:

$$\ell EE(G) > ne, \tag{27}$$

n	m	d_1	$NEE(G)$	bound ($23d_n$)	bound ($23U_1$)	bound ($23R_{-1}$)
4	4	3	4.8846	21.72	5.09	4.86
5	5	3	6.2381	56.97	7.62	7.62
6	9	5	6.8224	151.55	8.15	6.65
7	11	5	7.9613	407.35	10.32	8.16
8	12	6	9.2439	1,101.36	16.72	10.86
9	14	4	10.4376	2,986.50	14.15	13.19
10	15	8	11.2359	8,109.45	43.95	12.78
20	30	7	23.3079	1.78E+08	8,371.34	236.01
30	45	7	34.8334	3.93E+12	1.42E+06	4.04E+03
50	75	6	58.8047	1.91E+21	5.44E+09	7.70E+06
100	150	8	117.1121	9.89E+42	2.25E+22	5.79E+13

Table 9. Upper bounds for $NEE(G)$.

$$\ell EE(G) > 2 + \sqrt{n(n-1)e^2 - 6n + 4}, \tag{28}$$

$$\ell EE(G) > \sqrt{n(n-1)e^2 + 4R_{-1}(G) + 5n}. \tag{29}$$

We observe in Table 10 how the proposed bounds significantly improve those in [22].

n	m	d_1	$\ell EE(G)$	bound (27)	bound (28)	bound (29)	bound (15)	bound (16)	bound (24)
4	4	3	13.278	10.873	6.173	10.599	12.631	12.699	11.633
5	5	3	16.957	13.591	7.636	13.333	15.223	15.328	14.485
6	9	5	18.545	16.310	7.991	15.975	17.663	17.696	16.810
7	11	5	21.641	19.028	9.265	18.692	20.326	20.360	19.553
8	12	6	25.128	21.746	10.173	21.422	23.015	23.056	22.295
9	14	4	28.372	24.465	12.482	24.138	25.748	25.781	25.126
10	15	8	30.542	27.183	12.059	26.834	28.388	28.412	27.642
20	30	7	63.358	54.366	24.421	54.043	55.562	55.579	55.003
30	45	7	94.687	81.548	36.926	81.222	82.729	82.740	82.189
50	75	6	159.848	135.914	66.935	135.598	137.107	137.114	136.603
100	150	8	318.344	271.828	133.313	271.509	273.000	273.004	272.480

Table 10. Lower bounds for $\ell EE(G)$.

Considering instead the upper bounds, we compare our results with the following one in [22]:

$$\ell EE(G) < e^n + R_{-1}(G) + \frac{n}{2}(3-n) - 1. \tag{30}$$

As reported in Table 11, upper bound (24) allows a better approximation than (30). Also in this case, the upper bounds do not show a good behaviour for large graphs.

n	m	d_1	$\ell EE(G)$	bound (30)	bound (24)
4	4	3	13.28	52.51	13.83
5	5	3	16.96	143.66	20.73
6	9	5	18.55	394.31	22.15
7	11	5	21.64	1,082.65	28.06
8	12	6	25.13	2,961.24	45.46
9	14	4	28.37	8.08E+03	38.46
10	15	8	30.54	2.20E+04	119.46
20	30	7	63.36	4.85E+08	2.28E+04
30	45	7	94.69	1.07E+13	3.87E+06
50	75	6	159.85	5.18E+21	1.48E+10
100	150	8	318.34	2.69E+43	6.11E+22

Table 11. Upper bounds for $\ell EE(G)$.

6 Conclusions

By using an approach for localizing some relevant graph topological indices based on the optimization of Schur-convex or Schur-concave functions, we derive some new bounds for normalized Laplacian Estrada index and for normalized Laplacian energy. The proposed bounds can be computed by using additional information on the localization of first and second eigenvalue of normalized Laplacian matrix. A numerical section shows how this approach allows to derive tighter bounds than those provided in the literature. In particular, bound derived directly via majorization technique appear sharper than those depending by the Randić Index. According to the latter ones, it is noteworthy that we analyzed only the results for a specific type of degree sequence, while different bounds could be derived for other suitable degree sequences.

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