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Bounding the Sum of Powers of Normalized Laplacian Eigenvalues of Graphs through Majorization Methods

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Abstract

Given a simple connected graph G, this paper presents a new approach for localizing the graph topological indices given by the sum of the α-th power of the non zero normalized Laplacian eigenvalues. Through this method, old and new bounds are derived, showing how former results in the literature can be improved.

1 Introduction

Among the various indices in mathematical Chemistry, the Kirchhoff index $K(G)$ and a close relative of it, the degree-Kirchhoff index $K^*(G)$, have received a great deal of attention recently. For a connected undirected graph $G = (V, E)$ with vertex set $\{1, 2, \ldots, n\}$ and edge set E, the Kirchhoff index was defined by Klein and Randić [1] as

$$K(G) = \sum_{i<j} R_{ij}$$

where R_{ij} is the effective resistance of the edge ij. We refer the reader to references [3],[6] and [12], and their bibliographies, to get a taste of the variety of approaches used to study this descriptor. The degree-Kirchhof index was proposed by Chen and Zhang in [6], defined as

$$K^*(G) = \sum_{i<j} d_i d_j R_{ij}$$

where d_i is the degree of the vertex i. The index $K^*(G)$ was studied in [13], [12] and [16] , where a number of bounds for the index and an expression of it in terms of the eigenvalues of the normalized Laplacian were found.

This latter expression was the source of inspiration for a whole new family of descriptors, in terms of the sum of α powers of the eigenvalues of the normalized Laplacian, defined by Bozkurt and Bozkurt in [4]. These authors found a number of bounds for arbitrary α and particularly for $\alpha = -1$, which is the case of the degree Kirchhoff index. It is worth pointing out that their bound given in Corollary 3.4 was published slightly earlier (in electronic form) and arrived at with a different technique in [3].

It is the purpose of this note to continue using this fruitful technique of majorization and Schur-convex functions on this new family of descriptors, in order to obtain some better bounds.

2 Notations and preliminaries

In this section we recall some basic notions on majorization and graph theory. For more details refer to [9] and [11].

Definition 1 *Given two vectors* $\mathbf{y}$, $\mathbf{z} \in D = \{\mathbf{x} \in \mathbb{R}^n : x_1 \geq x_2 \geq ... \geq x_n\}$, *the majorization order* $\mathbf{y} \trianglelefteq \mathbf{z}$ *means:*

$$\begin{cases} \langle \mathbf{y}, \mathbf{s^k} \rangle \leq \langle \mathbf{z}, \mathbf{s^k} \rangle, \ k = 1, ..., (n-1) \\ \langle \mathbf{y}, \mathbf{s^n} \rangle = \langle \mathbf{z}, \mathbf{s^n} \rangle \end{cases}$$

where $\langle \cdot, \cdot \rangle$ *is the inner product in* $\mathbb{R}^n$ *and* $\mathbf{s^j} = [\underbrace{1, 1, \cdots, 1}_{j}, \underbrace{0, 0, \cdots 0}_{n-j}], \quad j = 1, 2, \cdots, n.$

Given a closed subset $S \subseteq \Sigma_a = D \cap \{\mathbf{x} \in \mathbb{R}^n_+ : \langle \mathbf{x}, \mathbf{s^n} \rangle = a\}$, where $a \in \mathbb{R}$, $a > 0$, let us consider the following optimization problem

$$\text{Min}_{\mathbf{x} \in S} \ \phi(\mathbf{x}) \tag{1}$$

If the objective function ϕ is Schur-convex, i.e. $\mathbf{x} \trianglelefteq \mathbf{y}$ implies $\phi(\mathbf{x}) \leq \phi(\mathbf{y})$, and the set S has a minimal element $\mathbf{x}_*(S)$ with respect to the majorization order, then $\mathbf{x}_*(S)$ solves problem (1) and

$$\phi(\mathbf{x}) \geq \phi(\mathbf{x}_*(S)) \quad \text{for all } \mathbf{x} \in S.$$

It is worthwhile to notice that if $S' \subseteq S$ the following inequality holds $\mathbf{x}_*(S) \trianglelefteq \mathbf{x}_*(S')$ and thus

$$\phi(\mathbf{x}) \geq \phi(\mathbf{x}_*(S')) \geq \phi(\mathbf{x}_*(S)) \text{ for all } \mathbf{x} \in S'. \tag{2}$$

On the other hand, if the objective function ϕ is Schur-concave, i.e. $-\phi$ is Schur-convex, then

$$\phi(\mathbf{x}) \leq \phi(\mathbf{x}_*(S')) \leq \phi(\mathbf{x}_*(S) \text{ for all } \mathbf{x} \in S'. \tag{3}$$

A very important class of Schur-convex (Schur-concave) functions can be built adding convex (concave) functions of one variable. Indeed, given an interval $I \subset \mathbb{R}$, and a convex function $g : I \to \mathbb{R}$, the function $\phi(\mathbf{x}) = \sum_{i=1}^{n} g(x_i)$ is Schur-convex on $I^n = \underbrace{I \times I \times \cdots \times I}_{n-times}$. The corresponding result holds if g is concave on I^n.

In [1] the authors derived the maximal and minimal elements, with respect to the majorization order, of the set

$$S_a = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M_i \geq x_i \geq m_i, i = 1, \cdots, n\}$$

where $M_1 \geq M_2 \geq \cdots \geq M_n$, $m_1 \geq m_2, \cdots \geq m_n$.

In the sequel we will work choosing M_i and m_i in a suitable way. In particular we will make use of the following results

Corollary 2 *(see [1], Corollary 14) Let us consider the set*

$$S_1^{[h]} = \Sigma_a \cap \left\{\mathbf{x} \in \mathbb{R}^n : x_i \geq \alpha,\ i = 1, \cdots, h,\ 1 \leq h \leq n,\ 0 < \alpha \leq \frac{a}{h}\right\} \tag{4}$$

Then

$$x_*(S_1^{[h]}) = \begin{cases} \dfrac{a}{n}\mathbf{s^n} & \text{if } \alpha \leq \dfrac{a}{n} \\ \alpha \mathbf{s^h} + \rho \mathbf{v^h} \text{ with } \rho = \dfrac{a - \alpha h}{n - h} & \text{if } \alpha > \dfrac{a}{n} \end{cases}.$$

Corollary 3 *For $n \geq 3$, let us fix $m_1 \geq m_2 such that m_1 + m_2 \leq a$ and consider the set*

$$S_2 = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : x_1 \geq m_1,\ x_2 \geq m_2\}$$

If the following condition hold

$$\begin{cases} nm_1 & > a \\ m_1 + m_2(n-1) & > a \end{cases}$$

then $x_*(S_2) = \left[m_1, m_2, \underbrace{\frac{a - m_1 - m_2}{n-2}, \cdots, \frac{a - m_1 - m_2}{n-2}}_{n-2} \right].$

Proof. The result follows easily by Theorem 8 in [2] noticing that the first integers satisfying the assumptions of the theorem are $d = 0$ and $k = 2$. ■

Let now $G = (V, E)$ be a simple, connected, undirected graph where $V = \{1, ..., n\}$ is the set of vertices and $E \subseteq V \times V$ the set of edges. We consider graphs with fixed order $|V| = n$ and fixed size $|E| = m$. Denote by $\pi = (d_1, d_2, .., d_n)$ the degree sequence of G, where d_i is the degree of vertex i, arranged in non increasing order $d_1 \geq d_2 \geq \cdots \geq d_n$. 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 $\mu_1 \geq \mu_2 \geq ... \geq \mu_n$ be the set of (real) eigenvalues of $L(G)$ and $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$ be the (real) eigenvalues of $\mathcal{L}(G)$. The following properties of spectra of $L(G)$ and $\mathcal{L}(G)$ hold:

$$\sum_{i=1}^{n} \mu_i = \text{tr}(L(G)) = 2m; \;\; \mu_1 \geq 1 + d_1 \geq \frac{2m}{n}; \;\; \mu_n = 0, \;\; \mu_{n-1} > 0.$$

$$\sum_{i=1}^{n} \lambda_i = \text{tr}(\mathcal{L}(G)) = n; \;\; \sum_{i=1}^{n} \lambda_i^2 = \text{tr}(\mathcal{L}^2(G)) = n + 2 \sum_{(i,j) \in E} \frac{1}{d_i d_j}; \;\; \lambda_n = 0; \lambda_1 \leq 2.$$

For any square matrix M of order n let $\mu(M) = \frac{\text{tr}(M)}{n}$ and $\sigma^2(M) = \frac{\text{tr}(M^2)}{n} - \left(\frac{\text{tr}(M)}{n}\right)^2$. If M admits real eigenvalues $\rho_1 \geq \rho_2 \geq ... \geq \rho_n$, the inequalities below are well-known (see [14]):

$$\mu(M) - \sigma(M)\sqrt{\frac{i-1}{n-i+1}} \leq \rho_i \leq \mu(M) + \sigma(M)\sqrt{\frac{i-1}{n-i+1}}, \;\; i = 1, \cdots, n. \tag{5}$$

and, in particular, more binding inequalities hold for the smallest and biggest eigenvalue, i.e.

$$\rho_1 \geq \mu(M) + \frac{\sigma(M)}{\sqrt{n-1}} \tag{6}$$

and

$$\rho_n \leq \mu(M) - \frac{\sigma(M)}{\sqrt{n-1}}$$

In case of the normalized Laplacian we get

$$\sigma^2(\mathcal{L}(G)) = \left(\frac{2}{n}\right) \sum_{(i,j)\in E} \frac{1}{d_i d_j},$$

and inequality (6) gives

$$\lambda_1 \geq 1 + \sqrt{\frac{2}{n(n-1)} \sum_{(i,j)\in E} \frac{1}{d_i d_j}} \tag{7}$$

Notice that for every connected graph of order n we have (see [3])

$$1 > \sigma(\mathcal{L}(G)) \geq \frac{1}{\sqrt{n-1}},$$

and the right inequality is attained for the complete graph $G{=}K_n$.

3 Bounds for the sum of powers of normalized Laplacian eigenvalues

Most of the topological indices of graphs are formulated by Schur-convex (Schur-concave) functions of the degree sequence as well as the eigenvalues of $A(G)$ or $L(G)$. The corresponding bounds are generally expressed in terms of size and order of G but they can also take into account the degrees of one or more vertices of G. With respect to the eigenvalues of $L(G)$, let

$$s_\alpha(G) = \sum_{i=1}^{n-1} \mu_i^\alpha, \alpha \neq 0, 1$$

be the index given by the sum of the α-th powers of the non zero Laplacian eigenvalues (see [15]).

In [2], taking into account the Schur-convexity or Schur-concavity of the functions $s_\alpha(G)$ for $\alpha > 1$ and $\alpha < 0$ or $0 < \alpha < 1$ respectively, the same bounds as in [15], Theorem 3 and 5, have been easily derived. Furthermore, considering additional information on the localization of the eigenvalues, the previous bounds have been improved.

The same approach can be applied to obtain and improve the bounds for the topological index:

$$s^*_\alpha(G) = \sum_{i=1}^{n-1} \lambda_i^\alpha, \alpha \neq 0, 1$$

given by the sum of the α-th powers of the non zero normalized Laplacian eigenvalues, first introduced by Bozkurt and Bozkurt in [4].

Let $\Sigma_n' = \{\lambda \in \mathbb{R}^{n-1} : \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq 0,\ \sum_{i=1}^{n-1} \lambda_i = n\}$ and define the set

$$S_{\mathcal{L}} = \Sigma_n' \cap \{\lambda \in \mathbb{R}^{n-1} : \lambda_1 \geq P\},$$

where $P \geq \frac{n}{n-1}$.

By Corollary 2 it follows that, for $n \geq 3$, the minimal element of $S_{\mathcal{L}}$ is

$$x_*(S_{\mathcal{L}}) = \left[P, \underbrace{\frac{n-P}{n-2}, \cdots, \frac{n-P}{n-2}}_{n-2} \right].$$

By the Schur-concavity or Schur-convexity of the function $s_\alpha^*(G)$, the following result holds

Theorem 4 *Let G be a simple connected graph with $n \geq 3$ vertices*

1. *if $\alpha < 0$ or $\alpha > 1$ then*
$$s_\alpha^*(G) \geq P^\alpha + \frac{(n-P)^\alpha}{(n-2)^{\alpha-1}}$$

2. *if $0 < \alpha < 1$ then*
$$s_\alpha^*(G) \leq P^\alpha + \frac{(n-P)^\alpha}{(n-2)^{\alpha-1}}.$$

Furthermore, in case of a bipartite graph, we know that $\lambda_1 = 2$. Since the minimal element of the set

$$S = \{(\lambda_2, \lambda_3, \cdots \lambda_{n-1}) : 0 \leq \lambda_{n-1} \leq \cdots \lambda_2 \leq 2, \sum_{i=2}^{n-1} \lambda_i = n-2\}$$

is $x_*(S) = \left[\underbrace{1, \cdots, 1}_{n-2} \right]$, by the Schur-concavity or Schur-convexity of the function $s_\alpha^*(G)$, we get the following result

Theorem 5 *Let G be a simple connected bipartite graph, with $n \geq 3$*

1. *if $\alpha < 0$ or $\alpha > 1$ then $s_\alpha^*(G) \geq 2^\alpha + (n-2)$;*

2. *if $0 < \alpha < 1$ then $s_\alpha^*(G) \leq 2^\alpha + (n-2)$.*

In particular, in what follows, we consider

$$P = 1 + \sqrt{\frac{2}{n(n-1)} \sum_{(i,j) \in E} \frac{1}{d_i d_j}}. \tag{8}$$

In virtue of (7) we get $\lambda_1 \geq P$.

Let us point out that in Theorem 4 and 5, making use of (8) we recover the same bounds as in Theorem 3.3 and 3.7 in [4] throughout a different approach based on majorization techniques.

Notice that for the complete graph K_n the spectra of $\mathcal{L}$ is given by

$$spec(\mathcal{L}) = \left\{ \frac{n}{n-1}, \cdots, \frac{n}{n-1}, 0 \right\}$$

which implies

$$s^*_\alpha(K_n) = \frac{n^\alpha}{(n-1)^\alpha} .$$

Being $P = \dfrac{n}{n-1}$, by easy computation we get that bounds in Theorem 4 are attained for $G = K_n$.

Now we show how the above mentioned bounds in [4] can be improved taking into account additional information on the localization of the eigenvalues.

In the following we consider a non complete graph. If we know that

$$\lambda_2 \geq \beta$$

with $\beta \leq P$, Corollary 3 allows us to compute the minimal element of the set

$$S^1_{\mathcal{L}} = \Sigma'_n \cap \{\lambda \in \mathbb{R}^{n-1} : \lambda_1 \geq P,\ \lambda_2 \geq \beta\}$$

To this aim, since the condition $(n-1)P > n$ is always satisfied, if

$$P + \beta(n-2) > n$$

the minimal element of $S^1_{\mathcal{L}}$ is given by

$$x_*(S^1_{\mathcal{L}}) = \left[P, \beta, \underbrace{\frac{n-P-\beta}{n-3}, \ldots, \frac{n-P-\beta}{n-3}}_{n-3} \right]$$

By the Schur-concavity or Schur-convexity of the function $s^*_\alpha(G)$, we get the following bounds

Theorem 6 *Let G be a simple connected graph with $n \geq 4$ vertices which is not complete and $\lambda_2 \geq \beta$ with $P + \beta(n-2) > n$.*

1. *If $\alpha > 1$ or $\alpha < 0$ then $s^*_\alpha(G) \geq P^\alpha + \beta^\alpha + \frac{(n-P-\beta)^\alpha}{(n-3)^{\alpha-1}}$*

2. If $0 < \alpha < 1$ then $s^*_\alpha(G) \leq P^\alpha + \beta^\alpha + \frac{(n-P-\beta)^\alpha}{(n-3)^{\alpha-1}}$

Furthermore, in case of a bipartite graph we know that $\lambda_1 = 2$. If we have an additional information like $\lambda_2 \geq \beta$, with $\beta > 1$, Corollary 2 entails that

$$\left[2, \beta, \underbrace{\frac{n-2-\beta}{n-3}, \ldots, \frac{n-2-\beta}{n-3}}_{n-3}\right]$$

is the minimal element of the set

$$S^2_{\mathcal{L}} = \Sigma'_n \cap \{\lambda \in \mathbb{R}^{n-1} : \lambda_1 = 2,\ \lambda_2 \geq \beta\}$$

and the following result holds

Theorem 7 *Let G be a simple connected bipartite graph with $n \geq 4$ and $\lambda_2 \geq \beta$ with $\beta > 1$.*

1. *If $\alpha > 1$ or $\alpha < 0$ then $s^*_\alpha(G) \geq 2^\alpha + \beta^\alpha + \frac{(n-2-\beta)^\alpha}{(n-3)^{\alpha-1}}$*

2. *If $0 < \alpha < 1$ then $s^*_\alpha(G) \leq 2^\alpha + \beta^\alpha + \frac{(n-2-\beta)^\alpha}{(n-3)^{\alpha-1}}$*

Notice that, thanks to the inequalities (2) and (3), the bounds in the previous theorem perform equal or better than (16) and (17) in [4].

The following example deals with a class of graphs to which Theorem 7 can be applied.

Example 8 *The Cheeger constant h_G of a graph is a well studied parameter and has been related to λ_{n-1} as follows*

$$\frac{h_G^2}{2} \leq \lambda_{n-1}(\mathcal{L}) \leq 2h_G$$

(see [7]). Let us now consider a full binary tree of depth $d > 1$. It has $n = 2^{d+1} - 1$ vertices, $m = 2^{d+1} - 2$ edges. By Example 3.3 in [8] for such a tree $h_G = \frac{1}{2^{d+1}-3}$, and we get the bound

$$\lambda_{n-1}(\mathcal{L}) \leq \frac{2}{2^{d+1} - 3}. \tag{9}$$

Since a tree is a bipartite graph, we know that $\lambda_2(\mathcal{L}) = 2 - \lambda_{n-1}(\mathcal{L})$ and $\lambda_1(\mathcal{L})$ =2. Thus

$$\lambda_2(\mathcal{L}) \geq 2 - \frac{2}{2^{d+1} - 3}.$$

Since for $d > 1$ we have $1 < 2 - \frac{2}{2^{d+1}-3} < 2$, we can apply Theorem 7 with $\beta = 2 - \dfrac{2}{2^{d+1} - 3}$. Observe that, thanks to the inequalities (2) and (3) as well as to a straight comparison between bounds 1. and 2. and those in Theorem 3.7 in [5] , by easy calculation, it follows that our bounds perform always better.

4 Bounds for the Kirchhoff index

Notice that bounds for the Kirchhoff index

$$K(G) = n\sum_{i=1}^{n-1}\frac{1}{\mu_i} = ns_{-1}(G)$$

can be easily derived taking into account bounds for $s_\alpha(G)$ wit $\alpha = -1$.

The same occurs for the degree Kirchhoff index (see [6])

$$K^*(G) = 2m\sum_{i=1}^{n-1}\frac{1}{\lambda_i}\ .$$

By Theorem 4 and 5 for $\alpha = -1$, we get

Theorem 9 *(see Corollary 3.4 and 3.8 in [4]) Let G be a simple connected graph. Then*

$$K^*(G) \geq \frac{2m}{P} + \frac{2m(n-2)^2}{n-P} \tag{10}$$

Furthermore, if G is bipartite

$$K^*(G) \geq m(2n-3) \tag{11}$$

Bound (10) was firstly proved in [3], while bound (11) was firstly given in [16] and also in [12].

It must also be pointed out that in [13], through electrical considerations, the following lower bound is provided:

$$K^*(G) \geq 2m\left(n-2+\left(\frac{1}{D+1}\right)\right) \tag{12}$$

where D is the largest degree of the graph. We mentioned in [3] that (10) is better than (12) in case there is a vertex with maximal degree $n-1$. However, it is not difficult to find examples where (12) beats (10). For instance, attach to every vertex of a complete graph K_N a single vertex with a single edge; this "snowflake" graph has $n = 2N$ vertices and enough symmetry to make computations easy. Indeed the exact degree-Kirchhoff index is given by $2N^3 + 2N^2 - 2N - 1$, and the lower bound (12) is given by $2N^3 - N$. Thus, for $N = 5$ we obtain that (12) becomes 245, whereas (10) becomes 243. Likewise, for $N = 20$ the figures are, respectively, 1990 and 1985. Therefore, these two lower bounds are not comparable.

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