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More Inequalities for Laplacian Indices by Way of Majorization

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ABSTRACT

The n-tuple of Laplacian characteristic values of a graph is majorized by the conjugate sequence of its degrees. Using that result we find a collection of general inequalities for a number of Laplacian indices expressed in terms of the conjugate degrees, and then with a maximality argument, we find tight general bounds expressed in terms of the size of the vertex set n and the average degree $d_G = 2|E|/n$. We also find some particular tight bounds for some classes of graphs in terms of customary graph parameters.

1. INTRODUCTION

Let $G = (V, E)$ be a finite simple connected graph with vertex set $V = \{1, 2, \dots, n\}$, degrees $d_1 \geq d_2 \geq \cdots \geq d_n$, and $d_G = \frac{2|E|}{n}$ the average degree. Let A be the adjacency matrix of G, D the diagonal matrix having the degrees of G in its diagonal and $L = D - A$ the Laplacian matrix of G, with characteristic values $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n = 0$. There exist many indices in Mathematical Chemistry expressed in terms of these characteristic values that we shall look at; among them the *Laplacian energy like invariant* put forward in [13]:

$$LEL(G) = \sum_{i=1}^{n-1} \sqrt{\lambda_i}, \tag{1}$$

and its generalization (see [4], [7])

$$LEL_\beta(G) = \sum_{i=1}^{n-1} \lambda_i^\beta \tag{2}$$

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for arbitrary $\beta \neq 0{,}1$; we shall also be concerned with the Kirchhoff index (see [12]) $R(G) = \sum_{i<j} R_{ij}$, where R_{ij} represents the effective resistance, as computed by Ohm's and Kirchhoff's laws, between the vertices i and j, and equal also to (see [8] and [18])

$$R(G) = n\sum_{i=1}^{n-1} \frac{1}{\lambda_i}. \tag{3}$$

We shall also discuss the Laplacian energy put forward in [9] as

$$LE(G) = \sum_{i=1}^{n} |\lambda_i - d_G|. \tag{4}$$

And finally we will consider the Laplacian Resolvent Energy of a graph, proposed by Cafure et al. in [3] as an alternative to the Resolvent Energy (see [11]) defined as

$$RL(G) = \sum_{i=1}^{n} \frac{1}{n+1-\lambda_i}. \tag{5}$$

The main ideas around majorization (for more details the reader is referred to [14]) may be briefly exposed thus: for any n-tuples $x = (x_1, \dots, x_n)$ and $y = (y_1, \dots, y_n)$ with $x_1 \geq x_2 \geq \dots \geq x_n$ and $y_1 \geq y_2 \geq \dots \geq y_n$, x majorizes y, written $x \succ y$, if

$$\sum_{i=1}^{k} x_i \geq \sum_{i=1}^{k} y_i, \tag{6}$$

for $1 \leq k \leq n-1$ and

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i, \tag{7}$$

A real function $\Phi : \mathbb{R}_n \to \mathbb{R}$ is a Schur-convex function in case it maintains the majorization inequality, that is, if $\Phi(x) \geq \Phi(y)$ whenever $x \succ y$. Similarly, a Schur-concave function inverts the inequality: $\Phi(x) \leq \Phi(y)$ whenever $x \succ y$. A Schur-convex (resp.Schur-concave) function can be simply constructed considering $\Phi(x) = \sum_{i=1}^{n} f(x_i)$, for any one-dimensional convex (resp. concave) real function $f : \mathbb{R} \to \mathbb{R}$.

The main idea for finding bounds through majorization for a molecular index is to express such index as a Schur-convex or Schur-concave function, and then to identify maximal and minimal elements, x^* and x_* respectively, that is, elements in the subspace of interest of the n-dimensional real space (which can be a set of n-tuples of degrees of vertices, or eigenvalues, or effective resistances, etc.) such that $x^* \succ x \succ x_*$, for all n-tuples x in the subspace of interest, and then if Φ is Schur-convex we will have $\Phi(x^*) \geq \Phi(x) \geq \Phi(x_*)$, for all x, having thus found the upper and lower bounds of interest, $\Phi(x^*)$ and $\Phi(x_*)$, respectively. A similar conclusion follows, exchanging the words ''upper" and "lower", if Φ is Schur-concave.

Several indices in Mathematical Chemistry such as (1), (2), (3), (4) and (5) are con-structed using Schur-convex or Schur-concave functions, and this fact has been used in a collection of articles (such as [2], [6], [13], [15], [16], for example) to find a cornucopia of upper and lower bounds for the indices. Specifically, in [15] we used the fact that the Laplacian eigenvalue sequence majorizes the degree sequence, i.e.:

$$(\lambda_1, \lambda_2, \dots, \lambda_n) \succ (d_1 + 1, d_2, \dots, d_n - 1), \tag{8}$$

with the purpose of finding lower (resp. upper) bounds, expressed in terms of the degree sequence, for descriptors defined through Schur-convex (resp. concave) functions.

Interestingly enough, there is a companion formula for (8), perhaps not so well known, where the eigenvalue sequence is majorized by another set of numbers, the conjugate degree sequence. In general, given a finite sequence $a_1, a_2, \ldots, a_n$ of non-negative numbers, its conjugate sequence a $a'_1, a'_2, \ldots, a'_n$ is defined by $a'_j = |\{i : a_i \geq j\}|$.

The conjugate sequence does not depend on the order of the original sequence and it is always a decreasing sequence, with $a'_1 \leq n$ and $a'_j = 0$ for $j > max\{a_1, \ldots, a_n\}$. For the sequence of degrees $d_1, \ldots, d_n$ of any graph G it should be noted that we have $d'_1 = n$ and $d'_n = 0$. For more details on conjugate sequences, the reader can consult [14].

Here is the important fact that was conjectured by Grone and Merris in [7] and that was finally proven by Bai in [1]:

Lemma 1. Given an arbitrary G we have

$$(d'_1, \ldots, d'_n) \succ (\lambda_1, \ldots, \lambda_n) \tag{9}$$

It is clear that equation (9) (incidentally, since $d'_n = \lambda_n = 0$ this equation can be rewritten as $(d'_1, \ldots, d'_{n-1}) \succ (\lambda_1, \ldots, \lambda_{n-1})$) can be used to find upper (resp. lower) bounds, in terms of the conjugate degree sequence, for Laplacian descriptors defined through Schur- convex (resp. concave) functions. This is precisely what Das et al. did in [5], where they worked with the Laplacian descriptors $LE(G)$ and $LEL(G)$, among other descriptors, and found some bounds in terms of the d'_is. In this article we will obtain additional bounds for the other Laplacian descriptors mentioned here in terms of the conjugate degree sequence, and then with a maximality argument used in majorization, we will find tight general bounds expressed in terms of the size of the vertex index n and the average degree d_G. We will also find some particular tight bounds given in terms of usual graph parameters.

2. THE INEQUALITIES

We begin with the general inequalities in the following

Proposition 1. For any G and $\{\mathrm{d}'_i\}$ its conjugate degree sequence we have

$$LEL(G) \geq \sum_{i=1}^{n} \sqrt{d'_i}, \tag{10}$$

$$LEL_\beta(G) \leq \sum_{i=1}^{n-1} (d'_i)^\beta, \quad \text{for } \beta > 1 \text{ or } \beta < 0 \tag{11}$$

$$LEL_\beta(G) \geq \sum_{i=1}^{n-1} (d'_i)^\beta, \quad \text{for } 0 < \beta < 1 \tag{12}$$

$$R(G) \leq n \sum_{i=1}^{n-1} \frac{1}{d_i'}, \tag{13}$$
$$LE(G) \leq \sum_{i=1}^{n-1} \left| d_i' - d_G \right| + d_G, \tag{14}$$
$$RL(G) \leq \sum_{i=1}^{n-1} \frac{1}{n+1-d_i'} + \frac{1}{n+1}. \tag{15}$$

Proof. Apply (9) and the facts that $R(G)$, $LE(G)$, $LEL_\beta(G)$ for $\beta < 0$ or $\beta > 1$ and $RL(G)$ are Schur-convex, while $LEL(G)$ and $LEL_\beta(G)$ for $0 < \beta < 1$ are Schur-concave.

Inequality (10) was proven in [5]. One may ask how informative these inequalities are. For example, if any of the d_i's are zero, (13) provides no information. On the other hand, from the trivial observation that $d_i' \leq n$, for $1 \leq i \leq n-1$, we can prove with a straightforward argument - worth comparing with the methods used in [17] and [3] to prove these facts - a couple of maximal results in the next

Proposition 2. For arbitrary G the following holds

$$LEL_\beta(G) \leq LEL_\beta(K_n) = (n-1)n^\beta \quad \text{for} \quad \beta > 0, \tag{16}$$

and

$$RL(G) \leq RL(K_n) = n - 1 + \frac{1}{n+1}. \tag{17}$$

Proof. Since the real functions $f(x) = x^\beta$ for $\beta > 0$ and $f(x) = \frac{1}{n+1-x}$ are increasing we obtain from (11) and (15) that $LEL_\beta(G) \leq \sum_{i=1}^{n-1} (d_i')^\beta \leq \sum_{i=1}^{n-1} n^\beta = (n-1)n^\beta$, and $RL(G) \leq \sum_{i=1}^{n-1} \frac{1}{n+1-d_i'} + \frac{1}{n+1} \leq \sum_{i=1}^{n-1} 1 + \frac{1}{n+1} = n - 1 + \frac{1}{n+1}$.

Since the Laplacian eigenvalues of the complete graph K_n are 0 and n with multiplicity $n-1$, it is readily seen that the equalities in (16) and (17) are attained by K_n.

We present now the following result, found in section 2.3 of [2] (corollary 2.3.2) as a lemma which will be used in the next proposition

Lemma 2. Let S_a be the set of real n-tuples $x = (x_1, x_2, \ldots, x_n)$ such that $x_1 \geq x_2 \geq \ldots \geq x_n$ and $\sum_{i=1}^{n} x_i = a$, which additionally satisfy $M \geq x_i \geq m$. Then the maximal element x^* of S_a, that is, the element such that for any other x we have $x^* \succ x$, is given by $x^* = (M, M, \ldots, M, \theta, m, m, \ldots, m)$, where M appears k times, m appears $n-k-1$ times, $k = \lfloor \frac{a-nm}{M-m} \rfloor$ and $\theta = a - Mk - m(n-k-1)$.

Now we can prove our main result in the following

Proposition 3. For any G we have

$$LEL(G) \geq \left(\lfloor d_G \rfloor + \sqrt{d_G - \lfloor d_G \rfloor} \right) \sqrt{n}, \tag{18}$$

$$LEL_\beta(G) \leq [\lfloor d_G \rfloor + (d_G - \lfloor d_G \rfloor^\beta]n^\beta, \quad \text{for} \quad \beta > 1 \; or \; \beta < 0 \tag{19}$$

$$\mathrm{LEL}_\beta(G) \geq [\lfloor d_G \rfloor + (d_G - \lfloor d_G \rfloor^\beta]n^\beta, \quad \text{for} \; 0 < \beta < 1 \tag{20}$$

$$RL(G) \leq \lfloor d_G \rfloor + \frac{1}{n(1-d_G+\lfloor d_G \rfloor)+1} + \frac{n-\lfloor d_G \rfloor -1}{n+1}, \tag{21}$$

$$LE(G) \leq 2\lfloor d_G \rfloor(n - d_G) \quad if \;\; d_G \geq n(d_G - \lfloor d_G \rfloor). \tag{22}$$

$$LE(G) \leq 2d_G(n - \lfloor d_G \rfloor - 1) \quad if \;\; d_G \leq n(d_G - \lfloor d_G \rfloor). \tag{23}$$

All the equalities in (18) through (22) are attained by the complete graph K_n

Proof. We prove only (22), since all the other inequalities have a similar proof. Consider the set $S_{2|E|}$ of all n-tuples $x = (x_1, x_2, \ldots x_n)$ of non-negative numbers such that $\sum_i x_i = 2|E|$ and $n \geq x_i \geq 0$. With the notation of the lemma, $M = n$ and $m = 0$. Then $k = \lfloor \frac{2|E|}{n} \rfloor = \lfloor d_G \rfloor$ and $\theta = n(d_G - \lfloor d_G \rfloor)$. That means that the maximal element of $S_{2|E|}$ is $x^* = (n, n, \ldots, n, n(d_G - \lfloor d_G \rfloor), 0, \ldots, 0)$, where the coordinate n appears $\lfloor d_G \rfloor$ times. Since $x^* \succ (d_1', \ldots, d_n')$ and the function that defines $LE(G)$ is Schur-convex, the following holds:

$$\begin{aligned} LE(G) &\leq \textstyle\sum_{i=1}^{n} |d_i' - d_G| \leq \sum_{i=1}^{\lfloor d_G \rfloor}(n - d_G) + |n(d_G - \lfloor d_G \rfloor) - d_G| + \sum_{i=\lfloor d_G \rfloor+2}^{n} d_G \\ &= (n - d_G)\lfloor d_G \rfloor + |n(d_G - \lfloor d_G \rfloor) - d_G| + (n - \lfloor d_G \rfloor - 1)d_G \\ &= (\mathrm{n} - \mathrm{d_G})\lfloor \mathrm{d_G} \rfloor + d_G - n(d_G - \lfloor d_G \rfloor) + (n - \lfloor d_G \rfloor - 1)d_G \\ &= 2\lfloor d_G \rfloor(n - d_G). \end{aligned}$$

The reader may verify for the case of the complete graph K_n that both the value of $LE(K_n)$ and the upper bound are equal to $2(n - 1)$.

The following corollary is immediate from the previous proposition, but worth being expressed explicitly.

Corollary 1. If the average degree d_G is an integer then

$$LEL(G) \geq d_G\sqrt{n}, \tag{24}$$

$$LEL_\beta(G) \leq d_G n^\beta, \quad \text{for} \; \beta > 1 \; or \; \beta < 0, \tag{25}$$

$$LEL_\beta(G) \geq d_G n^\beta, \quad \text{for} \; 0 < \beta < 1, \tag{26}$$

$$RL(G) \leq \frac{n(d_G + 1)}{n+1}. \tag{27}$$

$$LE(G) \leq 2d_G(n - d_G). \tag{28}$$

Remarks. The corollary holds, in particular, if the graph is d-regular. The proof of the lower bound (24), valid for all G, can be tracked down to [10]. Notice that our bound (18) is stronger than (24) in general, since

$$d_G\sqrt{n} = (\lfloor d_G \rfloor + d_G - \lfloor d_G \rfloor)\sqrt{n} \leq (\lfloor d_G \rfloor + \sqrt{d_G - \lfloor d_G \rfloor})\sqrt{n},$$

because $0 \leq d_G - \lfloor d_G \rfloor \leq 1$. The same is valid for (20)–(22) with respect to (26)–(28). Of all these, perhaps the only one worth a couple of lines is the proof that (21) is always better than (27), and this, after some algebra is equivalent to proving that

$$\frac{1}{n^2(1-\alpha)\alpha + n + 1} \leq \frac{1}{n+1}, \tag{29}$$

for $\alpha = d_G - \lfloor d_G \rfloor$, which satisfies $0 \leq \alpha \leq 1$, and makes the truth of (29) obvious. As for (19), it is better than (25) only for $\beta > 1$.

In the next propositions, we explore other ways to handle the n-tuple of conjugate degrees that yield inequalities in terms of the usual graph parameters for certain classes of graphs.

Proposition 4. For a graph possessing k vertices with maximal degree $n - 1$ we have

$$LEL_\beta(G) \leq n^\beta + (n-2)k^\beta \quad \text{for } \beta < 0, \text{ and } R(G) \leq 1 + \frac{n(n-2)}{k}. \tag{30}$$

The equalities in both cases are attained by the star graph S_n and the complete graph K_n.

Proof. We prove only the second half of (30) as the other proof is similar. We know that $d_1' = n$, and by the hypothesis $d_i' \geq k$ for $2 \leq i \leq n-1$. Given that the function $f(x) = \frac{1}{x}$ decreases in the interval $(0, \infty)$, by (13) we can write $R(G) \leq n\left(\frac{1}{n} + \sum_{i=2}^{n-1}\frac{1}{k}\right) = 1 + \frac{n(n-2)}{k}$. In the case of the star graph it is well known that $R(S_n) = (n-1)^2$ which coincides with the upper bound when $k = 1$; in the case of the complete graph it is also well known that $R(K_n) = n - 1$ which coincides with the value of the upper bound when $k = n$.

Proposition 5. If G has k pendent vertices then

$$LEL_\beta(G) \leq n^\beta + (n-2)(n-k)^\beta \text{ for } \beta > 1 \text{ and } RL(G) \leq 1 + \frac{n-2}{k+1} + \frac{1}{n+1}. \tag{31}$$

The equalities are attained by the star graph S_n

Proof. We prove the second half of (31). The hypothesis implies that $d_i' \leq n - k$ for $2 \leq i \leq n-1$. Also the real function $f(x) = \frac{1}{n+1-x}$ is increasing, and therefore $RL(G) \leq \sum_{i=1}^{n}\frac{1}{n+1-d_i'} = 1 + \sum_{i=2}^{n-1}\frac{1}{n+1-d_i'} + \frac{1}{n+1} \leq 1 + \sum_{i=2}^{n-1}\frac{1}{n+1-(n-k)} + \frac{1}{n+1}$. Now for the n-star graph S_n its eigenvalues are $n, 1$ with multiplicity $n-2$ and 0 and therefore $RL(S_n) = 1 + \frac{n-2}{n} + \frac{1}{n+1}$, which coincides with the upper bound when $k = n - 1$.

Proposition 6. If G is a chemical graph then

$$LEL_\beta(G) \leq 4n^\beta, \text{ for } \beta > 1 \text{ and } RL(G) \leq 4 + \frac{n-4}{n+1}. \quad (32)$$

The equalities are attained by the complete graph K_5.

Proof. We prove the second half of (32). The hypothesis implies that $d_i' \leq n$ for $1 \leq i \leq 4$ and $d_i' = 0$ for $i > 4$. Therefore, with the same arguments as in the previous proposition $RL(G) \leq \sum_{i=1}^{n} \frac{1}{n+1-d_i'} \leq \sum_{i=1}^{4} 1 + \sum_{i=5}^{n} \frac{1}{n+1} = 4 + \frac{n-4}{n+1}$. Combining the hypotheses of the last two propositions we obtain the next proposition with an obvious proof.

Proposition 7. If G is a chemical graph with k pendent vertices then

$$LEL_\beta(G) \leq n^\beta + 3(n-k)^\beta, \text{ for } \beta > 1 \text{ and } RL(G) \leq 1 + \frac{3}{k+1} + \frac{n-4}{n+1}.$$

The equalities are attained by the star graph S_5 .

3. CONCLUSIONS

The fact that the n-tuple of Laplacian eigenvalues of a graph is majorized by the conjugate sequence of its degrees allows to find easily general bounds for some Laplacian descriptors in terms of the conjugate sequence. We have shown here how to handle the conjugate sequence with a maximality argument, in order to express these bounds in terms of n and the average degree d_G , and with basic arguments for graphs with vertices of maximal or minimal degrees, in order to exhibit bounds given in terms of the number of these special vertices. We expect that in the future, as more relationships are uncovered for the conjugate sequence of the degrees of a graph, better bounds will be obtained in a similar way to those found here.

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