**MATCH**
*Communications in Mathematical and in Computer Chemistry*

MATCH Commun. Math. Comput. Chem. **77** (2017) 189-194

ISSN 0340 - 6253

# Some Inequalities for Laplacian Descriptors via Majorization

**José Luis Palacios**
*Electrical and Computer Engineering Department,*
*The University of New Mexico, Albuquerque, NM 87131, USA*
jpalacios@unm.edu

(Received December 11, 2015)

**Abstract**

The $n$-tuple of Laplacian eigenvalues of a graph majorizes the $n$-tuple of its degrees. This simple fact allows us to obtain a set of inequalities - some known, some new - for several descriptors given in terms of the Laplacian eigenvectors, in a unified manner.

## 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*. We consider $A$ to be the adjacency matrix of $G$, $D$ the diagonal matrix whose diagonal elements are the degrees of $G$ and $L = D - A$ the Laplacian matrix of $G$, with eigenvalues $\lambda_1 \geq \dots \geq \lambda_{n-1} \geq \lambda_n = 0$. There are several descriptors in Mathematical Chemistry defined in terms of these eigenvalues; among them we will work with the *the Laplacian energy like invariant* introduced in [8]:

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

and its generalization

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

for an arbitrary real number $\beta \neq 0, 1$; we will also look at the Kirchhoff index $R(G)$, introduced in [7] and defined by

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

where $R_{ij}$ is the effective resistance between the vertices $i$ and $j$, but which can be written as (see [4] and [14])

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

and finally we will look at the Laplacian energy defined first in [5] as

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

The main ideas around majorization can be summarized thus: given two $n$-tuples $\mathbf{x} = (x_1, \ldots, x_n)$ and $\mathbf{y} = (y_1, \ldots, y_n)$ with $x_1 \geq x_2 \ldots \geq x_n$ and $y_1 \geq y_2 \ldots y_n$, we say that $\mathbf{x}$ majorizes $\mathbf{y}$ and write $\mathbf{x} \succ \mathbf{y}$ in case

$$\sum_{i=1}^{k} x_i \geq \sum_{i=1}^{k} y_i, \tag{5}$$

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

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i. \tag{6}$$

A Schur-convex function $\Phi : \mathbb{R} \to \mathbb{R}$ keeps the majorization inequality, that is, if $\Phi$ is Schur-convex then $\mathbf{x} \succ \mathbf{y}$ implies $\Phi(\mathbf{x}) \geq \Phi(\mathbf{y})$. Likewise, a Schur-concave function reverses the inequality: for this type of function $\mathbf{x} \succ \mathbf{y}$ implies $\Phi(\mathbf{x}) \leq \Phi(\mathbf{y})$. A simple way to construct a Schur-convex (resp. Schur-concave) function is to consider

$$\Phi(\mathbf{x}) = \sum_{i=1}^{n} f(x_i),$$

where $f : \mathbb{R} \to \mathbb{R}$ is a convex (resp. concave) one-dimensional real function. For more details on majorization the reader is referred to [9].

Many descriptors in Mathematical Chemistry, as (1), (2), (3) and (4), are defined with Schur-convex or Schur-concave functions, and this fact has been exploited in several works (see [2], [11], and their references) in order to find a variety of upper and lower bounds for the descriptors. In this article we use these ideas of majorization, and instead of looking for minimal or maximal elements of appropriate subsets of $\mathbb{R}^n$, we use the basic knowledge that the $n$-tuple of Laplace eigenvalues majored the $n$-tuple of degrees in order to find in a unified manner, with almost trivial proofs, a number of inequalities found in the literature, as well as some new ones.

## 2 The inequalities

Here is a fact that is presented in the nice review [1] and that deserves to be better known:

**Lemma 1** *For any $G$ we have*

*(i)* $(\lambda_1, \dots, \lambda_n) \succ (d_1, \dots, d_n)$;

*(ii)* $(\lambda_1, \dots, \lambda_n) \succ (d_1 + 1, d_2, \dots, d_{n-1}, d_n - 1)$.

Part (ii) of the previous lemma implies the following one. Notice the subtle difference that whereas in the previous one the vectors are in $\mathbb{R}^n$, in the next the vectors are in $\mathbb{R}^{n-1}$.

**Lemma 2** *If $G$ has at least one pendant vertex then we have*

*(iii)* $(\lambda_1, \dots, \lambda_{n-1}) \succ (d_1 + 1, d_2, \dots, d_{n-1})$.

Now we apply (i), (ii) and (iii) to the descriptors in the introduction. Starting with the Laplacian energy like invariant, which is defined with a Schur-concave function, we have that (i) implies that for all $G$

$$LEL(G) = \sum_{i=1}^{n} \sqrt{\lambda_i} \leq \sum_{i=1}^{n} \sqrt{d_i}.$$

Now using the Cauchy-Schwarz inequality we can bound the above with

$$\sqrt{\sum_{i=1}^{n} d_i \sum_{i=1}^{n} 1} = \sqrt{2|E|n}.$$

Also, applying (iii) we obtain that for any $G$ with at least one pendant vertex we have

$$LEL(G) = \sum_{i=1}^{n-1} \sqrt{\lambda_i} \leq \sqrt{d_1 + 1} + \sum_{i=2}^{n-1} \sqrt{d_i}.$$

Applying the Cauchy-Schwartz inequality once more, we can bound the above with

$$\sqrt{\left(d_1 + 1 + \sum_{i=2}^{n-1} d_i\right) \sum_{i=1}^{n-1} 1} = \sqrt{2|E|(n-1)}. \tag{7}$$

We see that in this case majorization produces a weak result, because the bound (7) is known to hold for any $G$, not just for graphs with some pendant vertex (see [8]). Likewise, when we apply (i) to $LEL_\beta(G)$ we reach the conclusion, via Hölder's inequality, that for any $G$ and $0 < \beta < 1$ we have

$$LEL_\beta(G) \leq (2|E|)^\beta n^{1-\beta}. \tag{8}$$

Also, using (iii) and Hölder's inequality, we have that that for any $G$ with at least one pendant vertex and and $0 < \beta < 1$ we have

$$LEL_\beta(G) \leq (2|E|)^\beta (n-1)^{1-\beta}. \tag{9}$$

We notice that (8) and (9) compare favorably with the inequality in [12] that states that for all $\beta > 0$

$$LEL_\beta(G) \leq (n-1)n^\beta,$$

although we require the more restrictive condition that $0 < \beta < 1$. The inequality (9) also recovers one of the inequalities in theorem 3.2 in [3] (setting $k = 1$), although we need that the graph have a pendant vertex.

We look now at $R(G)$. Recall that the *inverse degree* of a graph is defined as $I(G) = \sum_{i=1}^{n} \frac{1}{d_i}$. The we can prove the following

**Proposition 1** *For a graph with a least one pendant vertex we have*

$$R(G) \geq n\left(I(G) - 1 - \frac{1}{d_1} + \frac{1}{d_1+1}\right). \tag{10}$$

*The equality is attained by the star graph $S_n$.*

**Proof.** Since the real function $f(x) = \frac{1}{x}$, $x \geq 0$, is convex, the function defining $R(G)$ in (3) is Schur-convex, and applying (iii) we have

$$R(G) = n\sum_{i=1}^{n-1} \frac{1}{\lambda_i} \geq n\left(\frac{1}{d_1+1} + \sum_{i=2}^{n-1} \frac{1}{d_i}\right) = n\left(I(G) - 1 - \frac{1}{d_1} + \frac{1}{d1+1}\right).$$

In the case of the star graph $S_n$, $d_1 = n-1$, $R(S_n) = (n-1)^2$ and $I(S_n) = n-1+\frac{1}{n-1}$. A bit of algebra shows that the right hand side of (9) also equals $(n-1)^2$•

The proposition above also yields a weak result for $R(G)$ , because in [13] it was shown that for all $G$ one has

$$R(G) \geq -1 + (n-1)I(G),$$

and this bound is *always* better than (10), as can be shown with some calculations and the fact (see [6]) that for all $G$

$$I(G) \leq n - 1 + \frac{1}{n-1}.$$

Finally for the Laplace energy we can show

**Proposition 2** *For any $G$ we have*

$$LE(G) \geq 2 + \sum_{i=1}^{n} |d_i - d_G|. \tag{11}$$

**Proof.** The function $f(x) = |x - d_G|$ is convex, and thus the function defining $LE(G)$ is Schur-convex. Using (ii) we have that

$$LE(G) = \sum_{i=1}^{n} |\lambda_i - d_G| \geq |d_1 + 1 - d_G| + \sum_{i=2}^{n-1} |d_i - d_G| + |d_n - 1 - d_G|$$

$$= 2 + \sum_{i=1}^{n} |d_i - d_G| \bullet$$

The bound (11) improves the one found in [10], which we could have obtained, had we used (i) instead of (ii). It should be noted that applying (iii) would not improve (11) for graphs with pendant vertices. There are not many lower bounds in the literature for the Laplacian energy; in [5] it is found that

$$LE(G) \geq 2\sqrt{|E| + \frac{1}{2}\sum_{i=1}^{n}(d_i - d_G)^2}, \tag{12}$$

which looks like a relative of (11), but in fact these bounds are not comparable. Notice that for a regular graph we obtain $LE(G) \geq 2$ when using (11) and $LE(G) \geq 2\sqrt{|E|}$ when using (12). On the other hand, for the star graph $S_n$ the bound obtained with (12) is

$$2\sqrt{(n-1) + \frac{1}{2}n(n-1)\left(1 - \frac{2}{n}\right)} \sim \sqrt{2}n,$$

whereas the bound obtained with (11) is

$$2n - 4 + \frac{4}{n}.$$

# References


[1] R. B. Bapat, The Laplacian matrix of a graph, *Math. Student* **65** (1996) 214–223.

[2] M. Bianchi, A. Cornaro, J. L. Palacios, A. Torriero, Localization of graph topological indices via majorization technique, in: M. Dehmer, F. Emmert-Streib (Eds.), *Quantitative Graph Theory*, CRC Press, Boca Raton, 2015, pp. 35–79.

[3] K. C. Das, K. Su, M. Liu, Sums of powers of eigenvalues of the Laplacian, *Lin. Algebra Appl.* **439** (2013) 3561–3575.

[4] I. Gutman, B. Mohar, The quasi-Wiener and the Kirchhoff indices coincide, *J. Chem. Inf. Comput. Sci.* **36** (1996) 982–985.

[5] I. Gutman, B. Zhou, Laplacian energy of a graph, *Lin. Algebra Appl.* **414** (2006) 29–37.

[6] Y. Hu, X. Li, Y. Shi, T. Xu, Connected $(n, m)$-graphs with minimum and maximum zeroth-order general Randić index, *Discr. Appl. Math.* **155** (2007) 1044–1054.

[7] D. J. Klein, M. Randić, Resistance distance, *J. Math. Chem* **12** (1993) 81-95.

[8] J. Liu, B. Liu, A Laplacian-energy like invariant of a graph, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 355–372.

[9] A. W. Marshall, I. Olkin, *Inequalities–Theory of Majorization and its Applications*, Academic Press, London, 1979.

[10] W. So, M. Robbiano, N. M. M. de Abreu, I. Gutman, Applications of a theorem by Ky Fan in the theory of graph energy, *Lin. Algebra Appl.* **432** (2010) 2163–2169.

[11] Y. Yang, On a new cyclicity measure of graphs – The global cyclicity index. *Discr. Appl. Math.* **172** (2014) 88–97.

[12] B. Zhou, On a sum of powers of the Laplacian eigenvalues of a graph, *Lin. Algebra Appl.* **429** (2008) 2239–2246.

[13] B. Zhou, N. Trinajstić, A note on Kirchhoff index, *Chem. Phys. Lett.* **455** (2008) 120–123.

[14] H. Y. Zhu, D. J. Klein, I. Lukovits, Extensions of the Wiener number, *J. Chem. Inf. Comput. Sci.* **36** (1996) 420–428.