Iranian J. Math. Chem. 9 (2) June (2018) 113 – 120

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

Some Remarks on the Arithmetic–Geometric Index

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ARTICLE INFO

Article History:

Received: 21 July 2017
Accepted: 30 August 2017
Published online 30 May 2018
Academic Editor: Tomislav Došlić

Keywords:

Arithmetic-geometric index
Majorization
Global cyclicity index

ABSTRACT

Using an identity for effective resistances, we find a relationship between the arithmetic-geometric index and the global cyclicity index. Also, with the help of majorization, we find tight upper and lower bounds for the arithmetic-geometric index.

1. INTRODUCTION

Let G=(V,E) be a finite simple graph with vertex set V={1, 2, ..., n}, edge set E and degrees $d_1 \geq d_2 \geq \cdots \geq d_n$. The arithmetic-geometric index of a graph, proposed by Vukičević and Furtula (see[19]), is defined by

$$GA(G) = \sum_{(i,j)\in E} \frac{2\sqrt{d_i d_j}}{d_i + d_j} \tag{1}$$

This index has attracted considerable attention and, through a variety of inequalities, it has been compared to a number of other indices, such as the ABC index, the first and second Zagreb indices, the general Randić index, the modified Narumi-Katayama index and the harmonic and sum-connectivity indices, among others. Different upper and lower bounds have been found for $GA(G)$ either through the connections to these other indices, or from first principles, see [5 – 8, 12, 15 – 18] for details.

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DOI: 10.22052/ijmc.2017.96064.1309

In this note we present two additional contributions to the study of $GA(G)$. First, we use notions of electric circuits in order to prove a relationship, to the best of our knowledge not explored yet, between $GA(G)$ and the global cyclicity index, introduced by Klein and Ivanciuc (see [10]) and defined by

$$C(G) = \sum_{(i,j)\in E} \frac{1}{R_{ij}} - |E| \tag{2}$$

where R_{ij} denote the effective resistance between the vertices i and j, that is, the voltage drop between vertices i and j when a battery is installed between those two vertices such that a unit current flows between them. This index has further been studied in [2, 21–23].

We also apply majorization techniques in order to find tight upper and lower bounds for $GA(G)$. Majorization has been applied extensively to find bounds and extremal values for a variety of descriptors .We point out the book chapters [1] and [3] and the recent articles [9, 13, 21] for a sample of the variety of scenarios covered with this approach.

Here is a brief summary of majorization (for more details the reader is referred to [11]): given two n-tuples $x = (x_1, x_2, \dots, x_n)$ and $y = (y_1, y_2, \dots, y_n)$ with $x_1 \geq x_2 \geq \cdots \geq x_n$ and $y_1 \geq y_2 \geq \cdots \geq y_n$, we say that x majorizes y and write $x \succ y$ in case

$$\sum_{i=1}^{k} x_i \geq \sum_{i=1}^{k} y_i, \tag{3}$$

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

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i. \tag{4}$$

A Schur-convex function $\Phi : R \rightarrow R$ keeps the majorization inequality, that is, if Φ is Schur-convex then $x \succ y$ implies $\Phi(x) \geq \Phi(y)$. Likewise, a Schur-concave function reverses the inequality: for this type of function $x \succ y$ implies $\Phi(x) \leq \Phi(y)$. A simple way to construct a Schur-convex (resp. Schur-concave) function is to consider $\Phi(x) = \sum_{i=1}^{n} f(x_i)$, where $f\colon \mathbb{R} \rightarrow \mathbb{R}$ is a convex (resp. concave) one-dimensional real function.

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.

2. EFFECTIVE RESISTANCES AND THE GEOMETRIC-ARITHMETIC INDEX

The following lemma is fundamental for what follows.

Lemma 1. For any G and (i,j) ∈ E we have

$$R_{ij} \geq \frac{\delta}{\delta+1}\left(\frac{1}{d_i}+\frac{1}{d_j}\right) \tag{5}$$

Proof. We prove that

$$\frac{d_i+d_j-2}{d_id_j-1} \geq \frac{\delta}{\delta+1}\left(\frac{1}{d_i}+\frac{1}{d_j}\right) \tag{6}$$

Without loss of generality, let us assume that $d_i = \max\{d_i,d_j\}$ and $d_j = \min\{d_i,d_j\}$. Then $\delta \leq d_j$ and since the real function $f(x) = \frac{x}{x+1}$ is increasing, in order to prove (6) it is enough to prove that

$$\frac{d_i+d_j-2}{d_id_j-1} \geq \frac{d_j}{d_j+1}\left(\frac{1}{d_i}+\frac{1}{d_j}\right) \tag{7}$$

But it is an easy computation to see that the truth of (7) is equivalent to the statement $(d_i-1)(d_i-d_j) \geq 0$. And now we can apply a result in [14] stating that for (i,j) ∈ E $R_{ij} \geq \frac{d_i+d_j-2}{d_id_j-1}$ finishing the proof .With this lemma we can prove now the following

Proposition 2. For any graph G we have

$$GA(G) \geq \frac{2\delta}{\Delta(\delta+1)}\left(C(G)+|E|\right) \tag{8}$$

Proof. For any G we have

$$GA(G) = \sum_{(i,j)\in E}\frac{2\sqrt{d_id_j}}{d_i+d_j} \geq \frac{2}{\Delta}\sum_{(i,j)\in E}\left(\frac{1}{d_i}+\frac{1}{d_j}\right)^{-1}$$
$$\geq \frac{2\delta}{\Delta(\delta+1)}\sum_{(i,j)\in E}\frac{1}{R_{ij}} = \frac{2\delta}{\Delta(\delta+1)}(C(G)+|E|).$$

The previous proposition yields as corollaries many lower bounds for GA(G) and upper bounds for C(G). For example,

Corollary 3. For any G with $n \geq 3$ we have

$$GA(G) \geq \frac{2\delta|E|^2}{\Delta(\delta+1)(n-1)} \tag{9}$$

For any d-regular G we have

$$C(G) \leq \frac{nd(d-1)}{4} \tag{10}$$

Proof. It is shown in [21] that, for $n \geq 3$, $C(G) \geq \frac{|E|(|E|-n+|1)}{n-1}$. Inserting into (8) finishes the proof of (a). For (b), it is immediate from the definition that if G is regular, then GA(G) = |E| and inserting this into (8) gives us the desired result .

Remarks4. The inequality (9) attains the equality for K_n, but not for other regular graphs, and it is not comparable to the bound found in [5]:

$$GA(G) \geq \frac{2|E|\sqrt{\Delta\delta}}{\Delta+\delta} \tag{11}$$

as can be seen taking G to be K_{n-1} together with an extra vertex attached with a single edge to any of the vertices of the K_{n-1} . For this graph the bound (11) is of order $n^{3/2}$ whereas (9) is of order n^2 . We will improve slightly the bound (9) below. Also, the bound (10) recovers a result in [21], with a totally different proof.

3. MAJORIZATION AND THE GEOMETRIC-ARITHMETIC INDEX

We present the following results, found in Section 2.3 of [1] (Corollary 2.3.2 and Theorem 2.3.2) as a lemma which will be used below.

Lemma 1. Let Σ_a be the set of real n – tuples $x = (x_1, x_2, \dots, x_n)$ such that $x_1 \geq x_2 \geq \dots \geq x_n$ and $\sum_{i=1}^{n} x_i = a$. Let S_a be the set of n-tuples belonging to Σ_a which additionally satisfy $M \geq x_i \geq m$. Then

(i) The minimal element of Σ_a is $(\frac{a}{n}, \dots, \frac{a}{n})$

(ii) If the minimal element in (i) belongs to S_a , then it is also the minimal element of S_a;

(iii) the maximal element of S_a is $(M,M,\dots,M,\theta,m,m,\dots,m)$, where M appears k times, m appears $n-k-1$ times, $k = [\frac{a-nm}{M-m}]$ and $\theta = a - Mk - m(n-k-1)$.

Lemma 2. For all G we have

$$\frac{2}{\Delta}\sum_{(i,j)\in E}\frac{1}{A_{ij}} \leq GA(G) \leq \frac{2}{\delta}\sum_{(i,j)\in E}\frac{1}{A_{ij}} \ , \tag{12}$$

where $A_{ij} = \frac{1}{d_i} + \frac{1}{d_j}$.

Proof. Write

$$\sum_{(i,j)\in E}\frac{2\sqrt{d_i d_j}}{d_i + d_j} \geq \frac{2}{\Delta}\sum_{(i,j)\in E}\frac{d_i d_j}{d_i + d_j} = \frac{2}{\Delta}\sum_{(i,j)\in E}\frac{1}{A_{ij}}$$

The other inequality proceeds similarly. Now we will apply majorization to the summation $\sum_{(i,j)\in E}\frac{1}{A_{ij}}$, by looking at the function $\Phi(x) = \sum_{i=1}^{|E|}\frac{1}{x_i}$ on the set of |E|-tuples $x = (x_1, x_2, \dots, x_n)$. Specifically we will show the following:

Proposition 3. For any G we have

$$\frac{2}{\Delta}\frac{|E|^2}{n} \le GA(G) \le \frac{2}{\delta}\left(\frac{2k}{3} + \frac{1}{\theta} + (|E| - k - 1)\frac{n-1}{2}\right) \tag{13}$$

where

$$k = \left\lfloor \frac{n - |E|\frac{2}{n-1}}{\frac{3}{2} - \frac{2}{n-1}} \right\rfloor, \theta = n - \frac{3}{2}k - \frac{2}{n-1}(|E| - k - 1).$$

The lower bound is attained by any regular graph. The upper bound is attained by the complete graph.

Proof. We notice that the numbers A_{ij} satisfy

$$\frac{2}{n-1} \le A_{ij} \le \frac{3}{2} \tag{14}$$

And

$$\sum_{(i,j)\in E} A_{ij} = \sum_{i=1}^{n} \frac{d_i}{d_i} = n \tag{15}$$

The right inequality in (14) is clear because in any edge (i,j) of a connected graph G with n > 2, if $d_i = 1$ then $d_j \ge 2$.

Let us consider the subset of $\mathbb{R}^{|E|}$ defined as

$$\Sigma_n = \{x \in \mathbb{R}^{|E|} : x_1 \ge x_2 \ge \cdots \ge x_{|E|} ; \sum_{j=1}^{|E|} x_j = n\}$$

and S_n the subset of Σ_n such that its |E|-tuples satisfy $\frac{3}{2} \ge x_i \ge \frac{2}{n-1}$ for $1 \le i \le |E|$. By Lemma 1 we can find explicitly the minimal element of S_n , that is, an |E|-tuple x_* such that $x \succ x_*$ for $x \in S_n$, indeed $x_* = (\frac{n}{|E|}, \frac{n}{|E|}, \dots, \frac{n}{|E|})$.

Notice that x_* belongs to S_n because the coordinates of x_* , which are all equal to $\frac{n}{|E|}$ Satisfy $m = \frac{1}{2(n-1)} \le \frac{n}{|E|} \le \frac{n}{n-1} \le \frac{3}{2} = M$, as long as $n \ge 3$. Also, since $f(x) = \frac{1}{x}$, for $x > 0$, is convex, then $\Phi(x) = \sum_{i=1}^{|E|} \frac{1}{x_i}$ is Schur-convex, and $\Phi(x) \ge \Phi(x_*) = \frac{|E|^2}{n}$, and since the |E|-tuple of numbers A_{ij} over the edges of the graph, properly arranged in decreasing order, belongs to the set S_n on account of facts (14) and (15), we have that $\sum_{(i,j)\in E} A_{ij} \ge \frac{|E|^2}{n}$, and this together with (12) of lemma 2 ends the proof of the lower bound in (13).

Analogously for the upper bound, by Lemma 2 we can identify explicitly the maximal element of S_n , that is, the |E|-tuple x^* such that $x^* \succ x$ for all $x \in S_n$, indeed $x^* = \left(\frac{3}{2}, \frac{3}{2}, \dots, \frac{3}{2}, \theta, \frac{2}{n-1}, \frac{2}{n-1}, \dots, \frac{2}{n-1}\right)$, where $\frac{3}{2}$ appears k times, $\frac{2}{n-1}$ appears $|E| - k - 1$ times and $k = \left\lfloor \frac{n - |E|\frac{2}{n-1}}{\frac{3}{2} - \frac{2}{n-1}} \right\rfloor, \theta = n - \frac{3}{2}k - \frac{2}{n-1}(|E| - k - 1)$. Therefore

$$\sum_{(i,j)\in E} A_{ij} \leq \Phi(x^*) = (\frac{2k}{3} + \frac{1}{\theta} + (|E| - k - 1)\frac{n-1}{2}),$$

and this together with (12) gives us the upper bound in (13).

For any Δ-regular graph G the lower bound becomes |E|, which coincides with the value of GA(G). For the complete graph K_n , k = 0, $\theta = \frac{2}{n-1}$ and the upper bound becomes $\frac{n(n-1)}{2}$, which is precisely the value of GA(K_n) = |E|.

Remarks 4. The versatility of majorization can be seen in this theorem, where the quantities to be majorized are neither degrees, nor eigenvalues, nor effective resistances, as is usually the case in the literature, but the numbers A_{ij} , which perhaps do not have a clear-cut graph significance. The lower bound in (13) is always better than (8) on account of the fact that δ ≤ n − 1. We point out that this lower bound could have been obtained without majorization, by using the harmonic mean-arithmetic mean inequality. The real strength of the method in this case seems to be in the upper bound, which can be improved if we restrict somewhat the degrees of the vertices in the graph, as in the following three propositions.

Proposition 5. For any G without pendent vertices we have

$$GA(G) \leq \frac{2}{\delta}(k + \frac{1}{\theta} + (|E| - k - 1)\frac{n-1}{2})$$

Where $k = [\frac{n(n-1)-2|E|}{n-1}]$,$\theta = n - k - \frac{2}{n-1}(|E| - k - 1)$. The equality is attained by the cycle graph C_n and the complete graph K_n .

Proof. In the absence of pendent vertices we can get the upper bound $A_{ij} \leq 1$ and the proof in the previous proposition applies, replacing everywhere 3/2 with 1. For the complete graph we obtain k = 0, $\theta = \frac{2}{n-1}$ and the upper bound becomes $\frac{n(n-1)}{2}$, which is the precise value of GA(K_n) = |E|. For the cycle graph, where |E| = n, we get k = n and $\theta = \frac{2}{n-1}$, and the upper bound becomes n, which is the value GA(C_n) = |E|.

Recall that a chemical graph is one where $d_i \leq 4$ for all i. For this sort of graph we can prove the following.

Proposition 6. For any chemical graph G we have

$$GA(G) \leq \frac{2}{\delta}\left(\frac{2k}{3} + \frac{1}{\theta} + 2(|E| \pm k - 1)\right),$$

Where $k = [n - \frac{|E|}{2}]$, $\theta = n - \frac{3}{2}k - \frac{1}{2}(|E| - k - 1)$. The equality is attained by any 4-regular graph.

Proof. In this case we can get the lower bound $A_{ij} \geq \frac{1}{2}$ and the proof in proposition 2 applies, replacing everywhere $\frac{2}{n-1}$ with $\frac{1}{2}$. For any 4-regular graph we have k = 0 and $\theta = \frac{1}{2}$, and thus the upper bound becomes 2n, which is precisely the value of GA(G) = |E|. Combining the two hypotheses, we obtain a more compact statement in the following

Proposition 7. For any chemical graph G without pendent vertices we have

$$GA(G) \leq \frac{2}{\delta}(3|E| - 2n)$$

The equality is attained by the cycle graph C_n and any 4-regular graph.

Proof. In this case we obtain that k = 2n−|E| and $\theta = \frac{1}{2}$, making the computations, similar to those in the previous propositions, very simple .

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