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Note

Extremal graphs for the geometric–arithmetic index with given minimum degree

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ABSTRACT

Let $G(k, n)$ be the set of connected simple n-vertex graphs with minimum vertex degree k. The geometric–arithmetic index $GA(G)$ of a graph G is defined by $GA(G) = \sum_{uv} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$, where $d(u)$ is the degree of vertex u and the summation extends over all edges uv of G. In this paper we find for $k \geq \lceil k_0 \rceil$, with $k_0 = q_0(n-1)$, where $q_0 \approx 0.088$ is the unique positive root of the equation $q\sqrt{q} + q + 3\sqrt{q} - 1 = 0$, extremal graphs in $G(k, n)$ for which the geometric–arithmetic index attains its minimum value, or we give a lower bound. We show that when k or n is even, the extremal graphs are regular graphs of degree k.

1. Introduction

The geometric–arithmetic (GA) index is a newly proposed graph invariant in mathematical chemistry. Motivated by the definition of the Randić connectivity index [13], Vukičević and Furtula [14] proposed the geometric–arithmetic index. Let G be a simple graph with the vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, d_u denotes the degree of the vertex u in G. The geometric–arithmetic index $GA(G)$ of a graph G is defined as in [14] by

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v},$$

where the summation extends over all edges uv of G. It is noted in [14] that the predictive power of GA for physico-chemical properties (boiling point, entropy, enthalpy and standard enthalpy of vaporization, enthalpy of formation, acentric factor) is somewhat better than the predictive power of the Randić connectivity index. In [14] Vukičević and Furtula gave the lower and upper bounds for GA, and identified the trees with the minimum and the maximum GA indices, which are the star and the path respectively. In [15] Yuan, Zhou and Trinajstić gave the lower and upper bounds for the GA index for molecular graphs using the numbers of vertices and edges. They also determined the n-vertex molecular trees with the minimum, the second-minimum and the third-minimum, as well as the second-maximum and the third-maximum, GA indices.

In fact, this index belongs to a wider class of so-called *geometric–arithmetic general* topological indices. A class of geometric–arithmetic general topological indices is defined in [7]:

$$GA_{\text{general}}(G) = \sum_{uv \in E(G)} \frac{2\sqrt{Q_u Q_v}}{Q_u + Q_v},$$

where Q_u is some quantity that (in a unique manner) can be associated with the vertex u of the graph G. It is easy to recognize that GA is the first representative of this class obtained by setting $Q_u = d_u$. The second member of this class was considered

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by Fath-Tabar et al. [7] by setting Q_u to be the number n_u of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of the graph G:

$$GA_2(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_u n_v}}{n_u + n_v}.$$

In [7] the main properties of GA_2 were established, including lower and upper bounds. Zhou et al. [16] proposed a third member of the class of GA_{general} by setting Q_u to be the number m_u of the edges of G lying closer to vertex u than to vertex v.

The Randić connectivity index has been studied by chemists and mathematicians, and there are a lot of papers about it [1–3,8,13]. Several books are devoted to the Randić index [9]. Recently, the geometric–arithmetic index has attracted the attention of mathematicians also, but there are few papers about it dedicated to molecular graphs [6,10]. In [5], the authors collected all hitherto obtained results on class GA indices.

In this paper we consider extremal values for the first geometric–arithmetic index for graphs in the class $G(k, n)$. We find extremal graphs for which this index attains its minimum value, or we give a lower bound. We use an approach similar to one introduced for the first time in [4], and later in [12].

2. A linear programming model of the problem

First, we will give some linear equalities and inequalities that must be satisfied in any graph in $G(k, n)$. Let $x_{i,j}$ denote the number of edges joining vertices of degrees i and j. The mathematical description of the problem P of determining $\min\{GA(G) = \sum_{k \le i \le j \le n-1} \frac{2\sqrt{ij}}{i+j} x_{i,j} \mid G \in G(k, n)\}$ is

$$\min \sum_{k \le i \le j \le n-1} \frac{2\sqrt{ij}}{i+j} x_{i,j},$$

subject to

$$\begin{array}{l} 2x_{k,k} + x_{k,k+1} + x_{k,k+2} + \cdots + x_{k,n-1} = kn_k, \\ x_{k,k+1} + 2x_{k+1,k+1} + x_{k+1,k+2} + \cdots + x_{k+1,n-1} = (k+1)n_{k+1}, \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ x_{k,n-1} + x_{k+1,n-1} + x_{k+2,n-1} + \cdots + 2x_{n-1,n-1} = (n-1)n_{n-1}, \end{array} \tag{1}$$

$$n_k + n_{k+1} + n_{k+2} + \cdots + n_{n-1} = n, \tag{2}$$

$$x_{i,j} \ge 0, \quad k \le i \le j \le n-1, \qquad n_i \ge 0, \quad k \le i \le n-1. \tag{3}$$

Variables $x_{i,j}$ and n_i are integers. (1)–(3) define a linear programming optimization problem.

3. The main results

Theorem 1. *If $k \ge \lceil k_0 \rceil$, where $k_0 = q_0(n-1)$, and $q_0 \approx 0.088$ is the unique positive root of the equation $q\sqrt{q}+q+3\sqrt{q}-1 = 0$, and if $G \in G(k, n)$, then*

$$GA(G) \ge \frac{kn}{2}.$$

If k or n is even, this value is attained by regular graphs of degree k.

Proof. We will consider the problem

$$\min \sum_{k \le i \le j \le n-1} \frac{2\sqrt{ij}}{i+j} x_{i,j},$$

subject to (1)–(3). This is a problem of linear programming. The basic variables are n_i, $k \le i \le n-1$ and $x_{k,k}$. This means that we will solve equalities (1) and (2) with n_i and $x_{k,k}$. We have

$$n_i = \frac{x_{k,i} + x_{k+1,i} + \cdots + 2x_{i,i} + \cdots + x_{i,n-1}}{i}, \quad k+1 \le i \le n-1. \tag{4}$$

From (2) we get

$$n_k = n - \sum_{i=k+1}^{n-1} n_i = n - \sum_{i=k+1}^{n-1} \frac{1}{i} x_{k,i} - \sum_{k+1 \le i \le j \le n-1} \left(\frac{1}{i} + \frac{1}{j}\right) x_{i,j}. \tag{5}$$