Abstract

Let $G$ be a graph and $d_u$ the degree of its vertex $u$. The geometric-arithmetic (GA) index of $G$ is defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$ and the summation runs over all edges of $G$. Let $G(1,n)$ be the set of connected simple graphs of order $n$ with minimum degree 1. In this paper, we use linear programming formulation to find graphs on which the geometric-arithmetic index attains minimum and maximum value.

Keywords: Geometric-Arithmetic index, Extremal graphs, Linear programming.

1 Introduction

A topological index is a numerical descriptor of the molecular structure derived from the corresponding molecular graph. There are numerous topological descriptors that have found some applications in theoretical chemistry, especially in QSAR/QSPR research [8].

Let $G$ be a connected simple graph with the vertex set $V(G)$ and edge set $E(G)$. The geometric-arithmetic index (GA) is one of the new topological indices motivated by the definition of Randić connectivity index [9, 2], defined as

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

where $Q_u$ is some quantity that in a unique manner can be associated with the vertex $u$ of the graph $G$.

The first member of this class was considered by Vukicević and Furtula [9] by setting $Q_u$ to be the degree $d_u$ of the vertex $u$ of the graph $G$:

$$GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$ (1)

For physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and acentric factor, it is noted in [9] that the predictive power of $GA$ index is somewhat better than predictive power of Randić connectivity index.

Let $G(k,n)$ be the set of connected simple graphs have $n$ vertices and the minimum degree of vertices is $k$. Pavlović and Gutman [6] used linear programming formulation and calculated the minimum value of Randić index for $G(1,n)$ . For $k=2$ the minimum value of Randić index was obtained in [5]. Li et al. [3] studied the famous conjecture of minimum Randić index for $G(k,n)$, however, faced with a serious problem [4]. Recently [9, 10, 11], lower and upper bounds have been studied for $GA_1$ index in the special cases.

Divnić et al. [1] considered the extremal values for the first geometric-arithmetic index for graphs in the class $G(k,n)$. They used linear programming formulation and found extremal graphs, for which, this index attains its minimum value when $k \geq k_0$, where $k_0 = q_0(n-1), q_0 \approx 0.088$ and left the case $k < k_0$ as an open problem.

In this paper, we use linear programming formulation and characterize the extremal graphs with the minimum value of geometric-arithmetic index among all graphs of $G(1,n)$.

2 Main results
Let $G$ be a connected simple graph on $n$ vertices and $n \geq 2$. The maximum possible vertex degree in such a graph is $n-1$. Denote by $n_i$ the number of vertices of degree $i$ in $G$, and by $x_{i,j}$ ($x_{i,j} \geq 0$) the number of edges joining the vertices of degrees $i$ and $j$ in $G$. Clearly, $x_{i,j} = x_{j,i}$ and $n_0 = 0$. Then, the geometric-arithmetic index Eq.1 can be written as

$$GA_i = \sum_{i=1, j=1, i \neq j}^{n} \frac{2\sqrt{ij}}{i+j} x_{i,j}.$$  

(2)

Now we find the minimum and maximum value of (2) under the following constraints:

$$2x_{1,1} + x_{1,2} + x_{1,3} + \ldots + x_{1,n-1} = n_1$$

$$x_{1,2} + 2x_{2,2} + x_{2,3} + \ldots + x_{2,n-1} = 2n_2$$

$$x_{1,3} + x_{2,3} + 2x_{3,3} + \ldots + x_{3,n-1} = 3n_3$$

$$\vdots$$

$$x_{1,n-1} + x_{2,n-1} + x_{3,n-1} + \ldots + 2x_{n-1,n-1} = (n-1)n_{n-1}$$

(3)

and,

$$n_1 + n_2 + n_3 + \ldots + n_{n-1} = n.$$  

(4)

2.1 Lower bound of $GA_1$

Consider the first and last equations of system (3) and the equation (4). We solve a system of three linear equations in the unknowns $n_1, n_{n-1}$, and $x_{1,n-1}$.

$$n_1 - x_{1,n-1} = 2x_{1,1} + \sum_{i=2}^{n-1} x_{i,j}$$

$$(n-1)n_{n-1} - x_{1,n-1} = 2x_{n-1,n-1} + \sum_{i=2}^{n-2} x_{i,j}$$

$$n_1 + n_{n-1} = n - \sum_{i=2}^{n-1} n_i$$

For $i=2,3,\ldots,n-2$, each $n_i$ is directly expressed from system (3),

$$n_i = \frac{1}{i} (x_{1,i} + x_{2,i} + \ldots + x_{i-1,i} + 2x_{i,j} + x_{i+1,j} + \ldots + x_{i,n-1})$$

On the other hand,

$$\sum_{i=2}^{n-1} n_i = n_2 + \ldots + n_{n-2} = \frac{n-1}{2} (x_{1,2} + x_{1,3} + \ldots + x_{1,n-1}) + \sum_{2 \leq i \neq j \leq n-2} \frac{1}{i+j} x_{i,j}.$$  

Then,

$$n_1 = n-1 + \frac{2x_{1,1}}{n} + \sum_{i=2}^{n-1} \frac{n-1}{i} x_{1,j} - \sum_{i=2}^{n-1} \frac{n-1}{i} x_{i,n-1} - \sum_{2 \leq i \neq j \leq n-2} \frac{n-1}{i+j} x_{i,j},$$

$$n_{n-1} = 1 + \frac{2x_{n-1,n-1}}{n} - \sum_{i=1}^{n-2} \frac{1}{i+1} x_{1,i} + \sum_{i=2}^{n-1} \frac{1}{i} x_{i,n-1} - \sum_{2 \leq i \neq j \leq n-2} \frac{1}{i+j} x_{i,j},$$

$$x_{1,n-1} = n-1 - \sum_{i=2 \leq i \neq j \leq n-1} \frac{n-1}{i} x_{1,j}.$$  

After substitution of $x_{1,n-1}$ into the $GA_i$ index, we have
\[ GA_i(G) = \sum_{1 \leq i,j \leq n-1} 2^{\Delta i,j} x_{i,j} = \frac{2\sqrt{n-1}}{n} x_{i,1} + \sum_{1 \leq i,j \leq n-1}^{(i,j) \neq (1,1)} 2^{\Delta i,j} x_{i,j} \]
\[ = \frac{2\sqrt{n-1}}{n} \left[ n-1 - \sum_{1 \leq i,j \leq n-1}^{(i,j) \neq (1,1)} \frac{n-1}{n} \left( \frac{1}{i} + \frac{1}{j} \right) x_{i,j} \right] + \sum_{1 \leq i,j \leq n-1}^{(i,j) \neq (1,1)} 2^{\Delta i,j} x_{i,j} \]
\[ = \frac{2(n-1)\sqrt{n-1}}{n} + \sum_{1 \leq i,j \leq n-1}^{(i,j) \neq (1,1)} f_{i,j} x_{i,j}. \]

Where
\[ f_{i,j} = \frac{2\sqrt{j}}{i+j} - \frac{2(n-1)\sqrt{n-1}}{n^2} \left( \frac{1}{i} + \frac{1}{j} \right). \]

Graph \( G \) is connected and for \( n \geq 3 \), \( x_{1,1} = 0 \), so we can consider \( (i,j) \neq (1,1) \). Now we prove that all functions \( f_{i,j} \geq 0 \), for \( i=1,2,\ldots,n-1 \) and \( j=i+1,\ldots,n-1 \). Since \( j \geq i \), we have
\[ \frac{\partial f_{i,j}}{\partial i} = -\frac{j(j-i)}{\sqrt{j(i+j)^2}} + \frac{2(n-1)\sqrt{n-1}}{n^2} \geq 0, \]
and therefore \( f_{i,j} \leq f_{i+1,j} \). On the other hand,
\[ f_{i,j} = \frac{2\sqrt{j}}{i+j} - \frac{2(n-1)\sqrt{n-1}}{n^2} \left( \frac{1}{i} + \frac{1}{j} \right), \]
and for \( j=2,3,\ldots,n-1 \) we have \( f_{i,j} \geq 0 \), because
\[ f_{i,j} \geq 0 \Leftrightarrow n^4 j^3 - (n-1)^4 (1+j)^4 \geq 0 \]
\[ \Leftrightarrow (n-j-1)((n^3 - 3n^2 j) + (n^3 - 3n^2 j) + (6n^3 - 4n^2 j + 2n - 1)) \]
\[ + (7nj - 3j) + (8nj^2 - 3j^2) + (3nj^3 - j^3) + (2\sqrt{3n^3 - 6n^2 j^2}) \geq 0. \]

Simple operations show that the last inequality is true for \( n \geq 12 \), then \( f_{i,j} \geq 0 \) for \( n \geq 12 \). And by numerical checking, we can see that \( f_{i,j} \geq 0 \) for small \( n \). Then \( f_{i,j} \geq 0 \) for \( i=1,2,\ldots,n-1 \) and \( j=i+1,\ldots,n-1 \). Consequently, the right-hand side of Eq. (5) will attain its minimal possible value if \( x_{i,j} = 0 \) for all \( 1 \leq i \leq j \leq n-1 \), except for \( i=1 \) and \( j=n-1 \).

So, the minimum value of \( GA_i \) index is \( \frac{2(n-1)\sqrt{n-1}}{n} \) and in the extremal graph we have
\( n_1 = n - 1, n_2 = n_3 = \cdots = n_{n-2} = 0, n_{n-1} = 1, x_{1,n-1} = n - 1 \) and all other \( x_{i,j} \) and \( x_{i,1} \) are equal to 0, which lead us to the following theorem:

**Theorem 1** Let \( G \) be a simple connected graph with \( n \) vertices, then
\[ \frac{2(n-1)\sqrt{n-1}}{n} \leq GA_i(G), \]
and lower bound is achieved if and only if \( G \) is a star.

### 2.2 Upper bound of \( GA_i \)

Consider the last equation of system (3) and the equation (4). At first, we solve a system of two linear equations in the unknowns \( n_{n-1} \) and \( x_{n-1,n-1} \).
\[ n_{n-1} = n - \sum_{i=1}^{n-2} x_{i,n-1} - \sum_{1 \leq i,j \leq n-2}^{(i,j) \neq (1,1)} \left( \frac{1}{i} + \frac{1}{j} \right) x_{i,j}. \]
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\[ x_{n-1,n-1} = \frac{n(n-1)}{2} - \sum_{1 \leq i < j \leq n-1} \frac{n-1}{2} \left( \frac{1}{i} + \frac{1}{j} \right) x_{i,j}. \]

After substitution of \( x_{n-1,n-1} \) into the \( GA_i \) index, we have

\[ GA_i = \sum_{1 \leq i < j \leq n-1} 2\sqrt{ij} x_{i,j} = x_{n-1,n-1} + \sum_{1 \leq i < j \leq n-1} 2\sqrt{ij} x_{i,j}, \]

\[ = \frac{n(n-1)}{2} + \sum_{1 \leq i < j \leq n-1} g_{i,j} x_{i,j}, \]

where

\[ g_{i,j} = \frac{2\sqrt{ij}}{i+j} - \frac{n-1}{2} \left( \frac{1}{i} + \frac{1}{j} \right). \]

Now we prove that \( g_{i,j} \leq 0 \), for \( i=1,2,...,n-1 \) and \( j=i+1,...,n-1 \). Note that

\[ g_{i,j} = \frac{2\sqrt{ij}}{i+j} - \frac{n-1}{2} \left( \frac{1}{i} + \frac{1}{j} \right) \leq 0 \Leftrightarrow \]

\[ \Leftrightarrow \frac{(i+j)^2(n-1)}{4ij} \geq 1 \]

\[ \Leftrightarrow \frac{n-1}{4} \cdot i + j \cdot \frac{i + j}{ij} \geq 1. \]

The last inequality is true because, \( \frac{i + j}{ij} \geq 2 \) for \( i, j \in N \), and \( \frac{i + j}{ij} = \frac{1}{i} + \frac{1}{j} \geq \frac{2}{n-1} \).

We obtained that \( g_{i,j} \leq 0 \), for \( i=1,2,...,n-1 \) and \( j=i+1,...,n-1 \), except for \( i=j=n-1 \). Consequently, the right-hand side of Eq. (6) will be maximized if and only if, \( x_{i,j} = 0 \) for all \( i, j \), \( 1 \leq i \leq j \leq n-1 \), except for \( i \neq n-1 \) and \( j \neq n-1 \). Therefore, the maximum value of the geometric-arithmetic index is \( \frac{n(n-1)}{2} \) which is related to the complete graph. In the special case of minimum degree 1, we will prove the following theorem:

**Theorem 2** The maximum value of the geometric-arithmetic index of \( G \in G(1,n) \) is:

\[ GA_1(G) = \left( \frac{n-2}{2} \right) \left( n-3 \right) + \frac{2\sqrt{n-1}}{n} + \frac{2(n-2)(n-3)}{2n-3}. \]

The value is attained on the graph with \( n_1 = 1, n_{n-1} = 1, n_{n-2} = n-2, n_2 = n_3 = \ldots = n_{n-3} = 0, x_{1,n-2} = 1, x_{n-1,n-2} = n-2, x_{n-2,n-3} = \frac{(n-2)(n-3)}{2} \) and all other \( x_{i,j} \) and \( x_{j,i} \) being equal to zero.

**Proof:**
By proposition 1 in [10], if \( G \) be a graph with \( m \) edges, then \( GA_1(G) \leq m \) and increasing the number edges of a graph, will increase the geometric-arithmetic index. Therefore we can consider \( n_1 = 1 \) and \( n_{n-1} = 1 \), so by (4) we have

\[ n_{n-2} = n - 2 - \sum_{i=2}^{n-3} n_i. \]

Using two last constraints of (3), we find,

\[ x_{n-2,n-1} = n - 2 - \sum_{i=2}^{n-3} x_{i,n-1}, \]

\[ 2x_{n-2,n-2} = (n-2)n_{n-2} - x_{n-2,n-1} - \sum_{i=2}^{n-3} x_{i,n-2}. \]

On the other hand it is easy to find \( n_i \) by Eq. 3 for \( i=2,3,...,n-3 \):
\[ n_i = \frac{1}{i} (x_{1,i} + x_{2,i} + \cdots + x_{i-1,i} + 2x_{i,j} + x_{i,j+1} + \cdots x_{i,n-1}), \]

and

\[ \sum_{i=2}^{n-3} n_i = \sum_{i=2}^{n-3} \frac{1}{i} x_{1,i} + \sum_{i=2}^{n-3} \frac{1}{i} x_{i+1,i} + \sum_{2 \leq j \leq n-3} \left( \frac{1}{i} + \frac{1}{j} \right) x_{i,j}. \]  

By substitution (7), (8) and (10) in (9), we have:

\[ x_{n-2,n-2} = \frac{(n-2)(n-3)}{2} + \sum_{i=2}^{n-3} \left( \frac{1}{i} - \frac{n-2}{2i} \right) x_{i,n-1} - \sum_{i=2}^{n-3} \left( \frac{1}{2i} + \frac{n-2}{2i} \right) x_{i,n-2} \]

\[ - \sum_{2 \leq j \leq n-3} \left( \frac{n-2}{2j} + \frac{n-2}{2j} \right) x_{i,j} - \sum_{i=2}^{n-3} \frac{n-2}{2i} x_{i,n-2}. \]

It is easy to see \( x_{1,i} = 0, \) for \( i = 1, 2, \ldots, n-2, \) \( x_{n-1,n-1} = 0, \) and \( x_{i,n-1} = 1, \) because \( n_1 = 1 \) and \( n_{n-1} = 1. \) Then,

\[ GA_i(G) = 2\sqrt{n-1} x_{1,n-1} + 2\sqrt{(n-2)(n-1)} x_{n-2,n-1} + x_{n-2,n-2} \]

\[ + \sum_{i=2}^{n-3} \frac{2i}{n-i+1} x_{i,n-1} + \sum_{i=2}^{n-3} \frac{2i}{n-i+2} x_{i,n-2} + \sum_{2 \leq j \leq n-3} \frac{2ij}{i+j} x_{i,j} \]

After substitution \( x_{n-2,n-1} \) and \( x_{n-2,n-2} \) by (8) and (11), and \( x_{1,n-1} = 1 \) into \( GA_i(G), \) we have:

\[ GA_i(G) = \frac{(n-2)(n-3)}{2} + \frac{2\sqrt{n-1}}{n} + \frac{2(n-2)\sqrt{(n-2)(n-1)}}{2n-3} \]

\[ + \sum_{i=2}^{n-3} F_i x_{i,n-1} + \sum_{i=2}^{n-3} K_i x_{i,n-2} + \sum_{2 \leq j \leq n-3} H_{i,j} x_{i,j}, \]

where,

\[ F_i = \frac{2\sqrt{i(n-1)}}{n-1+i} - \frac{2\sqrt{(n-2)(n-1)}}{2n-3} + \frac{1}{2} - \frac{n-2}{2i}, \]

\[ K_i = \frac{2\sqrt{i(n-2)}}{n-2+i} - \frac{1}{2} - \frac{n-2}{2i}, \]

\[ H_{i,j} = \frac{2\sqrt{ij}}{i+j} - \frac{n-2}{2j}. \]

Now we show that \( F_i, K_i \) and \( H_{i,j} \) are non positive for \( i = 2, 3, \ldots, n-3 \) and \( j = i+1, \ldots, n-3. \) Note that

\[ \frac{\partial F_i}{\partial i} = \frac{(n-1)(n-i-1)}{(n-1+i)^2} \frac{1}{2i^2} > 0. \]

Therefore \( F_i \) is increasing on \( i, \) and on the other hand

\[ F_{n-3} = \frac{2\sqrt{(n-3)(n-1)}}{2n-4} - \frac{2\sqrt{(n-2)(n-1)}}{2n-3} + \frac{1}{2} - \frac{n-2}{2(n-3)} \]

\[ = 2\sqrt{n-1} - \left( \frac{\sqrt{n-3}}{2n-4} - \frac{\sqrt{n-2}}{2n-3} \right) - \frac{1}{2n-3} \leq 0. \]

The last inequality is true, because

\[ \frac{\sqrt{n-3}}{2n-4} - \frac{\sqrt{n-2}}{2n-3} < 0 \iff -3n + 5 \leq 0. \]

Consequently, \( F_i \leq 0 \) for \( i = 2, 3, \ldots, n-3. \) Also note that

\[ \frac{\partial K_i}{\partial i} = \frac{(n-2)(n-i-2)}{(n-2+i)^2} \frac{n-2}{2i^2} > 0, \]

which means the function \( K_i \) is increasing on \( i, \) and
\[ K_{n-3} = \frac{2\sqrt{(n-3)(n-2)}}{2n-5} - \frac{1}{2} \frac{n-2}{2(n-3)} \leq 0 \]

\[ \Leftrightarrow 2\sqrt{(n-3)(n-2)} \frac{2n-5}{2n-5} \leq 0 \]

\[ \Leftrightarrow -16n^3 + 120n^2 - 296n + 239 \leq 0. \]

Simple calculation shows that the last inequality is true for \( n \geq 3 \). So, \( K \) is non positive for \( i=2,3,...,n-3 \).

Finally, we show that \( H_{i,j} \leq 0 \) for \( i=2,3,...,n-3 \) and \( j=i,i+1,...,n-3 \). Note that \( i \leq j \) and then we have

\[ \frac{\partial H_{i,j}}{\partial i} = \frac{j(j-i)}{(i+j)^2j} + \frac{n-2}{2i^2} > 0. \]

Therefore, function \( H_{i,j} \) is increasing on \( i \), and it is sufficient to show that \( H_{n-3,j} \leq 0 \). Note that

\[ H_{n-3,j} = \frac{2\sqrt{j(n-3)}}{n-3+j} - \frac{(n-2)(n-3+j)}{2j(n-3)} \leq 0 \Leftrightarrow \frac{(n-2)(n-3+j)^2}{4j(n-3)\sqrt{j(n-3)}} \geq 1. \]

The last inequality is true, because \( \frac{(n-3+j)^2}{\sqrt{j(n-3)}} \geq 2 \) and \( \frac{1}{j} + \frac{1}{n-3} = \frac{(n-3+j)}{j(n-3)} \geq \frac{2}{n-2} \). Consequently, the right-hand side of Eq. (12) will be maximized if and only if, \( x_{i,j} = 0 \) for \( i=2,3,...,n-3 \) and \( j=i,i+1,...,n-1 \). Then, for any graph \( G \in G(1,n) \), the maximum value of the geometric-arithmetic index is:

\[ GA(G) = \frac{(n-2)(n-3)}{2} + \frac{2\sqrt{n-1}}{n} + \frac{2(n-2)\sqrt{(n-2)(n-1)}}{2n-3}. \]

References


