Sum Geometric Arithmetic Means Index of Graphs

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ABSTRACT

In this paper, the concept of sum geometric arithmetic means index of a graph G, denoted by SGAM(G) is introduced and sum geometric arithmetic means index SGAM(G)of few families of graphs is computed. Further, we establish the bounds for sum geometric arithmetic means index.

General Terms

AMS, Subject Classification 05C07; 92E10

Keywords

Graph, Molecular graph, Sum geometric arithmetic means index of a graph ${\cal G}$

1. INTRODUCTION

Graph theory began in 1736 when Leonhard Euler (1707 - 1783) solved the well-known Konigsberg bridge problem. This problem asked for a circular walk through the town of Konigsberg (now Kaliningrad) in such a way as to cross over each of the seven bridges spanning the river Pregel once, and only once [13], for more details, see [11].

Graph theory is one of the branches of modern mathematics having experienced a most impressive development in recent years. In the beginning, graph theory was only a collection of recreational or challenging problems like Euler tours or the four coloring of a map, with no clear connection among them, or among techniques used to attach them [21].

Algebraic graph theory is the branch of mathematics that studies graphs by using algebraic properties of associated matrices. More in particular, spectral graph theory studies the relation between graph properties and the spectrum of the adjacency matrix or Laplace matrix [4].

The origins of topological graph theory can be traced back to the 19^{th} century, largely with the four colour problem and its

extension to higher-order surfaces – the Heawood map problem. With the explosive growth of topology in the early 20^{th} century, mathematicians like Veblen, Rado and Papakyriakopoulos provided foundational results for understanding surfaces combinatorially and algebraically. Kuratowski, MacLane and Whitney in the 1930s approached the four colour problem as a question about the

structure of graphs that can be drawn without edge-crossings in the plane [3].

The concept of geometric-arithmetic index was introduced in the chemical graph theory recently [19]. The study of topological indices is a subject of increasing interest, both in pure and applied mathematics [19]. Topological indices are interesting since they capture some of the properties of a molecule (or a graph) in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener in which he used the sum of all shortest-path distances of a molecular graph for modeling physical properties of alkanes [19].

In this paper, a simple graph G = (V; E), that is nonempty, finite, having no loops, no multiple and directed edges are considered. Let n and m be the number of its vertices and edges, respectively. The elements of V(G) are called vertices (points, nodes, junctions, or 0-simplexes) and elements of E(G) are called edges (lines, arcs, branches or 1-simplexes). The set V(G) is known as the vertex set of G and E(G) as the edge set of G.

For a vertex $v \in V(G)$, we denote a set of neighbours of v by N(v). Degree is denoted by deg(v) and defined as deg(v) = |N(v)|, is the number of the vertices adjacent to v.

A molecular graph is a simple graph whose vertices correspond to the atoms and whose edges correspond to the bonds. It can be described in different ways, such as by a drawing, a polynomial, a sequence of numbers, a matrix or by a derived number called a topological index. The topological index is a numeric quantity

associated with a graph, which characterizes the topology of the graph and is invariant under a graph automorphism. Some major types of topological indices of graphs are degree-based topological indices, distance-based topological indices and counting-related

topological indices. The degree-based topological indices, the atom-bond connectivity ABC and geometric – arithmetic G_A indices, are of great importance, with a significant role in chemical

graph theory [1]. In chemical graph theory, we have many different topological index of arbitrary molecular graph G.

A topological index of graphs is a member related to a graph which is invariant under graph automorphisms obviously, every topological index defines a counting polynomial and vice versa [14].

The first geometric- arithmetic index of a graph G was defined as

$$GA_1 = \sum \left(\frac{\sqrt{deg(v_i)deg(v_j)}}{\frac{deg(v_i) + deg(v_j)}{2}} \right)$$

with summation going over all pairs of adjacent vertices [23]. In 2011, K. Ch. Dasa, I. Gutman, and B. Furtula obtained lower and upper bounds on GA_1 and characterize graphs for which these bounds are best possible [5].

In 2015, Sehgehalli et al. [20] proposed the arithmetic-geometric index of a graph G, Vukicevic and Furtula defined a new

topological index the arithmetic-geometric index of a graph G [23], denoted by GA(G) and defined by

$$GA = GA(G) = \sum_{uv \in E(G)} \left(\frac{2\sqrt{deg(u)deg(v)}}{deg(u) + deg(v)} \right),$$

where uv is an edge of the graph G connecting the vertices u and v, also deg(u) stands for the degree of the vertex u, and where the summation goes over all edges of G.

Recently, Graovac defined the fifth version of geometric- arithmetic index of a graph G as

$$GA_5(G) = \sum_{uv \in G} \frac{2\sqrt{S_u S_v}}{S_u + S_v},$$

where S_u the sum of degrees of all neighbors of vertex u in the graph G. In 2016 Mehdi Alaeiyan, Mohammad Reza Farahani and Muhammad Kamran Jamil computed the fifth geometric arithmetic index of Polycyclic Aromatic Hydrocarbons [2].

Details on the properties of geometric-arithmetic indices of graphs can be found in [6, 7]. For history and further results on this family of topological indices, please refer to [8, 9, 10, 15, 23, 24].

2. MAIN RESULTS

DEFINITION 1. Sum geometric arithmetic means index of any graph G, denoted by SGAM(G) and defined by

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right).$$

2.1 Calculate the index by using the edge partition of G on the basis of the degrees of the end vertices of each edge method.

EXAMPLE 1. For the complete bipartite graph $K_{p,q}$, because, it is vertex set can be partitioned into two subsets, namely X and *Y* such that $\forall u \in X$, deg(u) = q and $\forall v \in Y$, deg(v) = p, where $|E(K_{p,q})| = pq$, then the number of edges of $K_{p,q}$ on the basis of the degrees of the vertices of each edge is such that deg(u) = q, and deg(v) = p is equal to the number of edges of $K_{p,q}$.

EXAMPLE 2. For the complete graph K_n , because, $\forall u \in K_n$, deg(u) = n - 1, where $|E(K_n)| = \frac{n(n-1)}{2}$, then the number of edges of K_n on the basis of the degrees of the vertices of each edge is such that deg(u) = n - 1 is equal to the number of edges of K_n .

THEOREM 2. For the complete graph K_n , the SGAM index is equal to the following

$$SGAM(K_n) = n(n-1)^2.$$

PROOF. Since K_n is regular graph of order n - 1 and the edge partition of K_n on the basis of the degrees of the end vertices of each edge, and because its vertex set cannot be partitioned into subsets, and so has only one set, then the number of edges of K_n on the basis of the degrees of the vertices of each edge is equal to

the number of edges of K_n , and because

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right),$$

then

$$SGAM(K_n) = \frac{n(n-1)}{2} \left(\sqrt{(n-1)^2} + \frac{n-1+n-1}{2} \right)$$

= $\frac{n(n-1)}{2} \left(n-1+n-1 \right) = \frac{n(n-1)}{2} (2n-2)$
= $n(n-1)^2$.

THEOREM 3. For the complete bipartite graph $K_{p,q}$, the SGAM index is equal to the following

$$SGAM(K_{p,q}) = (pq)^{\frac{3}{2}} + \frac{pq(p+q)}{2}$$

PROOF. By using the edge partition of $K_{p,q}$ on the basis of the degrees of the vertices of each edge (see example 1 above), and hecause

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right),$$

this implies that

$$SGAM(K_{p,q}) = pq\left(\sqrt{pq} + \frac{p+q}{2}\right) = (pq)^{\frac{3}{2}} + \frac{pq(p+q)}{2}.$$

THEOREM 4. For the star graph $K_{1,n-1}$, the SGAM index is equal to the following

$$SGAM(K_{1,n-1}) = (n-1)^{\frac{3}{2}} + \frac{n(n-1)}{2}$$

PROOF. Let $V(K_{1,n-1}) = \{v_0, v_1, v_2, \dots, v_{n-1}\}, and$ $E(K_{1,n-1}) = \{e_0, e_1, e_2, \dots, e_{n-1} : e_i = v_0 v_i (1 \le i \le n-1)\},\$ in every edge in $K_{1,n-1}$, $deg(v_0) = n - 1$, $deg(v_i) = 1(1 \le 1)$ $i \leq n-1$). Thus the number of edges of $K_{1,n-1}$ on the basis of the degrees of the vertices of each edge is equal to be the number of edges of $K_{1,n-1}$, and because

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right),$$
 then

then

$$SGAM(K_{1,n-1}) = (n-1)\left(\sqrt{n-1} + \frac{n-1+1}{2}\right)$$
$$= (n-1)^{\frac{3}{2}} + \frac{n(n-1)}{2}.$$

DEFINITION 5. [16] The crown graph S_p^0 for an integer $p \ge 2$ is the graph with vertex set $\{u_1, u_2, \ldots, u_p, v_1, v_2, \ldots, v_p\}$ and edge set $\{u_i v_i : 1 \le i, j \le p, i \ne j\}$. S_p^0 is therefore equivalent to the complete bipartite graph $K_{p,p}$ with horizontal edges removed.

THEOREM 6. For the crown graph S_p^0 , $p \ge 2$, the SGAM index is equal to the following

$$SGAM(S_p^0) = 2p(p-1)^2.$$

PROOF. Suppose that

 $V(S_p^0) = \{u_1, u_2, \ldots, u_p, v_1, v_2, \ldots, v_p\}$ and edge set $E(S_p^0) = \{u_i v_j : 1 \le i, j \le p, i \ne j\}$. In every edge in S_p^0 , $deg(u_i) = p - 1, deg(v_j) = 1(1 \le i, j \le p - 1)$. Since in every edge e_{ij} in S_p^0 has $deg(u_i) = deg(v_j) = p - 1$. Thus the edge partition of S_n^0 on the basis of the degrees of the vertices can not be partitioned into more one subset and is equal to the number of edges of S_p^0 , and because

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right)$$

therefore

$$SGAM(S_p^0) = p(p-1)\left(\sqrt{(p-1)^2} + \frac{p-1+p-1}{2}\right)$$

= $p(p-1)(p-1+p-1) = p(p-1)(2p-2)$
= $p(p-1)\left(2(p-1)\right) = 2p(p-1)^2.$

DEFINITION 7. [22] The cycle graph $C_n, n \ge 3$, consists of n vertices v_1, v_2, \ldots, v_n and edges $\{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n, v_nv_1\}$.

THEOREM 8. For the cycle graph C_n , $n \ge 3$, the SGAM index is equal to the following

$$SGAM(C_n) = 4n.$$

PROOF. Since C_n is regular graph of order 2, the number of edges is n, and because its vertex set cannot be partitioned into subsets, and so has only one set, then the number of edges of C_n on the basis of the degrees of the vertices of each edge is equal to the number of edges of C_n , and because

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right)$$

then

$$SGAM(C_n) = n\left(\sqrt{2^2} + \frac{2+2}{2}\right) = n(2+2) = 4n.$$

DEFINITION 9. [22] The graph obtained from the cycle graph $C_n, n \ge 3$, by removing an edge is called the path graph of n vertices, it is denoted by P_n .

THEOREM 10. For the path graph $P_n, n \ge 3$, the SGAM index is equal to the following

$$SGAM(P_n) = 2\sqrt{2} + 4n - 9.$$

PROOF. Suppose that $V(P_n) = \{u_1, u_2, \ldots, u_n\}$, $E(P_n) = \{e_1, e_2, \ldots, e_{n-1}, e_i = u_i u_{i+1} \ (1 \le i \le n-1\}$. The number of edges of P_n is n-1 in which, there are two types of edges, in the first one

$$deg(u) = 1, deg(v) = 2,$$

and number of edges is 2 and in the second type

$$deg(u) = deg(v) = 2,$$

and number of edges is n - 3 and because

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right)$$

so

$$SGAM(P_n) = 2\left(\sqrt{2} + \frac{3}{2}\right) + (n-3)\left(\sqrt{4} + \frac{4}{2}\right)$$

= $2\sqrt{2} + 3 + 4(n-3) = 2\sqrt{2} + 3 + 4n - 12$
= $2\sqrt{2} + 4n - 9.$

DEFINITION 11. [22] The wheel graph W_n is obtained when an additional vertex to the cycle C_{n-1} , for $n \ge 4$, and connect this new vertex to each of the n-1 vertices in C_{n-1} , by new edges.

THEOREM 12. For the wheel graph $W_n, n \ge 4$, the SGAM index is equal to the following

$$SGAM(W_n) = (n-1)\left(\sqrt{3(n-1) + \frac{n+2}{2}} + 6\right)$$

PROOF. Let $V(W_n) = \{v_1, v_2, \dots, v_n\},\$

 $E(P_n) = \{e_1, e_2, \dots, e_{2n-2}\}$. By using the edge partition of W_n on the basis of the degrees of the vertices of each edge, there are two types of edges, in the first one

$$deg(u) = 3, deg(v) = n - 1$$

and number of edges is n - 1 and in the second

$$deg(u) = deg(v) = 3,$$

and number of edges is n - 1 and because

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right),$$

this implies that

$$SGAM(W_n) = (n-1)\left(\sqrt{3(n-1) + \frac{n+2}{2}}\right) + (n-1)\left(\sqrt{9} + \frac{6}{2}\right)$$
$$= (n-1)\left(\sqrt{3(n-1) + \frac{n+2}{2}} + 3 + 3\right)$$
$$= (n-1)\left(\sqrt{3(n-1) + \frac{n+2}{2}} + 6\right).$$

DEFINITION 13. [17] A friendship graph F_r for an integer $r \ge 2$, is the graph constructed by joining r copies of K_3 graph with common vertex. F_r graph has n = 2r + 1 vertices and has m = 3r edges.

THEOREM 14. For the friendship graph F_r for an integer $r \ge 2$, the SGAM index is equal to the following

$$SGAM(F_r) = 2r^2 + 6r + 4r\sqrt{r}.$$
 (1)

PROOF. By using the edge partition of F_r on the basis of the degrees of the vertices of each edge, there are two types of edges, in the first one

$$deg(u) = deg(v) = 2,$$

and number of edges is r and in the second

$$deg(u) = 2, deg(v) = 2r,$$

and number of edges is 2r and because

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right)$$

this implies that

$$SGAM(F_r) = r(2+2) + 2r\left(2\sqrt{r} + \frac{2(r+1)}{2}\right)$$

= $4r + 2r\left(2\sqrt{r} + r + 1\right)$
= $4r + 4r\sqrt{r} + 2r^2 + 2r = 2r^2 + 6r + 4r\sqrt{r}.$

DEFINITION 15. [12] The double star graph $S_{p,q}$ is the graph constructed from $K_{1,p-1}$ and $K_{1,q-1}$ by joining their centers v_0 and u_0 . A vertex set $V(S_{p,q}) = V(K_{1,p-1}) \bigcup V(K_{1,q-1}) = \{v_0, v_1, \ldots, v_{p-1}, u_0, u_1, \ldots, u_{q-1}\}$ and edge set $E(S_{p,q}) = \{v_0 u_0, v_0 v_i, u_0 u_j | 1 \le i \le p-1, 1 \le j \le q-1\}.$

THEOREM 16. For the double star graph $S_{p,q}$ for an integer $p, q \ge 3$, the SGAM index is equal to the following

$$SGAM(S_{p,q}) = (p-1)\sqrt{p} + (q-1)\sqrt{q} + \sqrt{pq} + \frac{p^2 + q + q^2 + q - 2}{2}$$

PROOF. By using the edge partition of $S_{p,q}$ on the basis of the degrees of the vertices of each edge, there are three types of edges, in the first one

$$deg(u_0) = p, deg(u_1) = 1,$$

and number of edges is p - 1, in the second

$$deg(v_0) = q, deg(v_1) = 1,$$

and number of edges is q - 1 and in the third

$$deg(u_0) = p, deg(v_0) = q,$$

and number of edges is 1 and because

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right)$$

then

$$SGAM(S_{p,q}) = (p-1)(\sqrt{p} + \frac{p+1}{2}) + (q-1)(\sqrt{q} + \frac{q+1}{2}) + \sqrt{pq} + \frac{p+q}{2} \times 1 = (p-1)\sqrt{p} + (q-1)\sqrt{q} + \sqrt{pq} + \frac{p^2 + p + q^2 + q - 2}{2}.$$

3. APPLICATION THE SUM GEOMETRIC ARITHMETIC MEANS INDEX OF A GRAPH IN CHEMISTRY.

SGAM Index of Cycloalkenes

We denote a cycloalkene having n carbon atoms and 2n-2 hydrogen atoms by C_n^{2n-2} .

The molecular graphs of them are obtained by attaching 2n-2

pendant vertices corresponding to hydrogen atoms to vertices of a cycle corresponding to carbon atoms as shown in Fig. 1.



Figure 1: A cycloalkene and its graph model

THEOREM 17. For $n \geq 3$, the SGAM index is equal to the following

$$SGAM(C_n^{2n-2}) = 17n + 6\sqrt{3} - 25.$$

PROOF. The cycloalkene molecular graph C_n^{2n-2} has 3n-2 vertices including two vertices (namely, C_1 and C_2) of degree three, n-2 vertices C_3, C_4, \ldots, C_n of degree four and correspond to the carbon atoms of cycloalkenes and the remaining 2n-2 vertices (namely, H's) are end vertices and they correspond to hydrogen atoms of cycloalkenes. Thus we have the following: on the basis of degrees of the vertices we divide the edge set into a partition

$$E_{1} = \{uv \in E(C_{n}^{2n-2}) \mid deg(u) = deg(v) = 4, \};$$

$$E_{2} = \{uv \in E(C_{n}^{2n-2}) \mid deg(u) = deg(v) = 3\};$$

$$E_{3} = \{uv \in E(C_{n}^{2n-2}) \mid deg(u) = 3, deg(v) = 4\};$$

$$E_{4} = \{uv \in E(C_{n}^{2n-2}) \mid deg(u) = 1, deg(v) = 3\};$$

$$E_{4} = \{uv \in E(C_{n}^{2n-2}) \mid deg(u) = 1, deg(v) = 3\};$$

 $E_5 = \{uv \in E(C_n^{2n-2}) \mid deg(u) = 1, deg(v) = 4\}.$ So there are five types of edges, where $|E_1| = n - 3$,

 $|E_2| = 1, |E_3| = 2, |E_4| = 2, |E_5| = 2n - 4.$ Because

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right),$$

then

$$\begin{aligned} SGAM(C_n^{2n-2}) &= (n-3)(\sqrt{16} + \frac{4+4}{2}) + 1 \times (\sqrt{9} + \frac{3+3}{2}) \\ &+ 2(\sqrt{12} + \frac{4+3}{2}) + 2(\sqrt{3} + \frac{1+3}{2}) \\ &+ (2n-4)(\sqrt{4} + \frac{1+4}{2}) \\ &= 8(n-3) + 6 + 4\sqrt{3} + 7 + 2\sqrt{3} + 4 \\ &+ 2(2n-4) + 5(n-2) = 8n - 24 + 17 + 6\sqrt{3} \\ &+ 4n - 8 + 5n - 10 = 17n + 6\sqrt{3} - 25. \end{aligned}$$

THEOREM 18. For any graph G of order n = |V(G)| and size m = |E(G)| with δ and Δ the minimum and maximum degree of the graph, respectively. Then

$$2\delta m \le SGAM(G) \le 2\Delta m$$

PROOF. Since

$$\delta \leq \sqrt{deg(u)deg(v)} \leq \Delta, \delta \leq \frac{\sqrt{deg(u) + deg(v)}}{2} \leq \Delta,$$

then

$$2\delta \le \sqrt{deg(u)deg(v)} + \frac{\sqrt{deg(u) + deg(v)}}{2} \le 2\Delta,$$

because

$$SGAM(G) = \sum_{uv \in E(G)} \left(\sqrt{deg(u)deg(v)} + \frac{deg(u) + deg(v)}{2} \right)$$

hence

$$\sum_{uv \in E(G)} 2\delta \leq SGAM(G) \leq \sum_{uv \in E(G)} 2\Delta,$$

as |E(G)| = m, Thus

$$2\delta m \le SGAM(G) \le 2\Delta m.$$

4. CONCLUSION

In this paper, we have computed the concept of sum geometric arithmetic means index of some standard graphs. Also, sum geometric arithmetic means index of a graph in chemistry is given. The sum geometric arithmetic means index of several other families of graphs is an open problem.

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