Difference Arithmetic Geometric Mean Index – Study Of Some Graphs

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ABSTRACT

In this paper, the concept of difference arithmeticgeometric mean index of a graph G denoted by DAGM (G) is introduced and the difference arithmetic geometric mean index DAGM(G) of few families of graphs is computed. Further, we establish Correlation and regression of physical-chemical properties of isomers of octane using difference arithmetic geometric index are investigated.

Keywords: Molecular graph, isomers of octane, correlation, Difference arithmeticgeometric index of graphs.

1. INTRODUCTION

Graph theory is one of the branches of Mathematics having most magnificent development in recent years. It is the study of relationship between vertices and edges. It provides a helpful tool for quantifying and simplifying the many moving parts of dynamic systems. Studying graphs through a framework provides answers to many arrangements, networking, optimization, matching and operational problems. Graphs can be used to model many types of relations and processes in physical, biological, social and information systems, and it has a wide range of useful applications.

2. Preliminaries

Some known definitions and results related to difference arithmetic geometric mean index ofgraphs for ready reference to go through the work presented in this paper are discussed in this section.

Def 2.1: Let G = (V, E) be a graph with vertex sets V(G) and edge sets E(G). The geometric – arithmetic mean index is defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$ where d_u and d_v are the degrees of end-vertices of an edge uv

Def 2.2: Let G = (V,E) be a graph with vertex sets V(G) and edge sets E(G). The arithmetic geometric mean index is defined as $AG(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}}$ where d_u and d_v are the degrees of end-vertices of an edge uv

Def 2.3: Let G = (V,E) be a graph with vertex sets V(G) and edge sets E(G). The harmonic index of a graph is defined as $H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$ where d_u is the degree of vertices.

Def 2.4: The general Randic index of a graph was proposed by Bollobas and Erdos and is defined as

$$R_\propto(G) = \sum_{uv \in E(G)} (d_u d_v)^\propto$$

Def 2.5: Let G = (V,E) be a graph with vertex sets V(G) and edge sets E(G). The sum connectivity index of a graph is defined as $\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$

3. Difference ArithmeticGeometricMean Index

Motivated by the definition of arithmetic geometric index, Difference arithmetic geometric mean index (DAGM(G)) of a simple graph G is defined. Also, Difference arithmetic geometric mean index of the standard graphs are found.

Definition3.1: Difference arithmetic geometric mean index of graph G, denoted by DAGM (G) is defined as $DAGM(G) = \frac{d_u + d_v}{2} - \sqrt{d_u d_v}$ for all u, v belongs to V(G)

Remark: It is known that, for all the same data Arithmetic Mean = Geometric Mean.

For any k – regular graph G, $d_u = k$, for all u, v belongs to V(G). In this case,

clearly DAGM (G) = 0.
From this remark, it follows that the DAGM(K_n) = 0

Theorem 3.2
For the complete bipartite graph$K_{m,n}$, the DAGM index is
$DAGM (K_{m,n}) = \frac{mn(m+n)}{2} - (mn)^{\frac{3}{2}}$
Proof: Let V $(K_{m,n})$ = $V_1 \cup V_2$ where V_1 and $V_2$are the partitions of V such that every vertex u belongs to
$V_1$is adjacent to every vertex v belongs to $V_2.$ Note that d(u) = n, d(v) = n. Also, $|E (K_{m,n})| = mn$
$DAGM(G) = \frac{d_u + d_v}{2} - \sqrt{d_u d_v}$
$DAGM (K_{m,n}) = \frac{mn(m+n)}{2} - (mn)^{\frac{3}{2}}$
Corollary: For the star graph K $_{1, n-1}$,the DGAM index is $\frac{n(n+1)}{2} - (n-1)^{\frac{3}{2}}$
It follows from the above theorem by replacing m by 1, n by n-1

Theorem 3.3
For the cycle graph C_n, n ≥ 3, the DGAM index is zero.
Proof: Since C_n is a regular graph of order2, For any k – regular graph G, $d_u = k$, for all u, v belongs to
V(G). Obviously DAGM (G) = 0.
$DAGM(G) = \frac{d_u + d_v}{2} - \sqrt{d_u d_v}$
$DAGM(Cn) = 0$

Theorem 3.4
For the path graph P_n , n≥3, the DAGM index is $3 - 2\sqrt{2}$
Proof: Let V(P_n) = {$v_1,v_2,...v_n$} , $|E (Pn) | = n - 1$
Note that d(u_1) = d(u_n) = 1 and d(u_i) = 2 for $2 \leq i \leq n - 1$
$DAGM(G) = \frac{d_u + d_v}{2} - \sqrt{d_u d_v}$
DAGM (P_n) = $3 - 2\sqrt{2}$

Theorem 3.5
For the wheel graph, W_n, (K_1+ Cn), n ≥ 4, the DAGM index is equal to
$\frac{(n-1)(n+2)}{2} - \sqrt{3} (n-1)^{\frac{3}{2}}$
Proof: LetV(W_n) = {$v_1,v_2..... v_n$}and E(P_n) = {$e_1,e_2...... e_{2n-2}$}
By the edge partition of $W_n$on the basis of the degrees of the vertices of each edge, there are two types of
edgesand the number of edges is n – 1 in each type.
$$DAGM(G) = \frac{d_u + d_v}{2} - \sqrt{d_u d_v}$$
$$= (n-1)\left(\frac{3+3}{2} - \sqrt{9}\right) + (n-1)\left(\frac{3+n-1}{2} - \sqrt{3(n-1)}\right)$$
$$= \frac{(n-1)(n+2)}{2} - \sqrt{3} (n-1)^{\frac{3}{2}}$$

Theorem 3.6
For the friendship graph F_n, for an integer n ≥ 2, the DGAM index is
2n (n + 1) - 4n$\sqrt{n}$
Proof: Let V (F_n) = { v_1, v_2, ... v_{2n+1}} with v_1 as the centre vertex.
E (F_n) = { $v_1 v_i$ /2 ≤ i≤ 2n+1} U {$v_{2i} v_{2i+1}$ / 1≤i≤ n}
By using the edge partition of F_n, on the basis of the degrees of the vertices of each edge, there are two
types of edges namely n and 2n
$DAGM(G) = \frac{d_u + d_v}{2} - \sqrt{d_u d_v}$
$DAGM(Fn) =$2n (n + 1) - 4n$\sqrt{n}$

Theorem 3.7

For the double star graph $S_{m,n}$ for an integer m,n $\geq$ 3, the DGAM index is DGAM

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

Proof:. Let V ($K_{1,n,n}$) = {u} $\cup$ {v_1, v_2, . . . , v_n} $\cup$ {w_1, w_2, . . . , w_n}. By using the edge partition of $S_{m,n}$ on the basis of the degrees of the vertices of each edge, there are three types of edges,

d(u_0) = p , d(u_1) = 1, number of edges = p – 1,   d(v_0) = q , d (v_1) = 1, number of edges = q – 1

d(v_0) = P , d (v_o) = q ; number of edges = 1

$$DAGM(G) = \frac{d_u + d_v}{2} - \sqrt{d_u d_v}$$

$$DAGM(S_{m,n}) = (p-1)\left(\frac{p+1}{2} - \sqrt{p}\right) + (q-1)\left(\frac{q+1}{2} - \sqrt{q}\right) + \left(\frac{p+q}{2} - \sqrt{pq}\right)$$

Therefore, $DAGM(S_{m,n}) = \frac{p^2 + q^2 + p + q - 2}{2} - \sqrt{p}(p-1) - \sqrt{q}(q-1) - \sqrt{pq}$

## 4.Applications of the DGAM index of a graph in chemistry

Different organic molecules of organic compounds have different properties based upon their structure such as the Cycloalkanes. Cycloalkanes are the class of hydrocarbons having a ring-like structure. This ring is formed due to their saturated nature, and they have three compounds of alkane present in the structure which helps them in forming a ring. They have the general formula C_nH_{2n}, where n is said to be the number of carbon atoms present in the organic compound.

DAGM index of Octane isomers

In this section, the DAGM index of various octane isomers are calculated. It is compared with the existing boiling point, entropy, density of various octane isomers. The topological indices for 3 – Methyl heptane and 4 – Methyl heptane are same.

Computation of DAGM index with some physical properties of n octane isomers

n	Octane's	Boiling point	Entropy	Density	DAGM(G)
1	n - octane	125.7	111.67	0.703	0.172
2	2 – Methyl heptane	117.6	109.84	0.698	0.673
3	3 – Methyl heptane	118.9	111.26	0.702	0.542
4	4 – Methyl heptane	117.7	109.32	0.705	0.542
5	2, 2 – dimethyl hexane	106.8	103.42	0.695	1.758
6	3, 3 – dimethyl hexane	112	104.74	0.710	1.516
7	2, 3 – dimethyl hexane	115.6	108.02	0.691	2.941
8	2, 4 – dimethyl hexane	109.4	106.98	0.696	1.34
9	2, 5 – dimethyl hexane	109.1	105.72	0.691	1.174
10	3, 4 – dimethyl hexane	117.7	106.59	0.715	0.81
11	2,3,4 trimethyl pentane	113.5	102.39	0.719	1.34
12	2,2,3 trimethyl pentane	109.8	101.31	0.716	1.941
13	2,2,4 trimethyl pentane	99.24	104.09	0.688	1.991
14	2,3,3 trimethyl pentane	114.8	102.06	0.726	1.83
15	2,2,3,3tetramethyl butane	106.5	93.06	0.824	3
16	2-methyl-3-ethyl pentane	115.6	106.06	0.719	0.81
17	3-methyl-3-ethyl pentane	118.3	101.48	0.727	0.274
18	3 – ethyl hexane	118.5	109.43	0.714	0.411

Comparison of DAGM index with Octane isomers
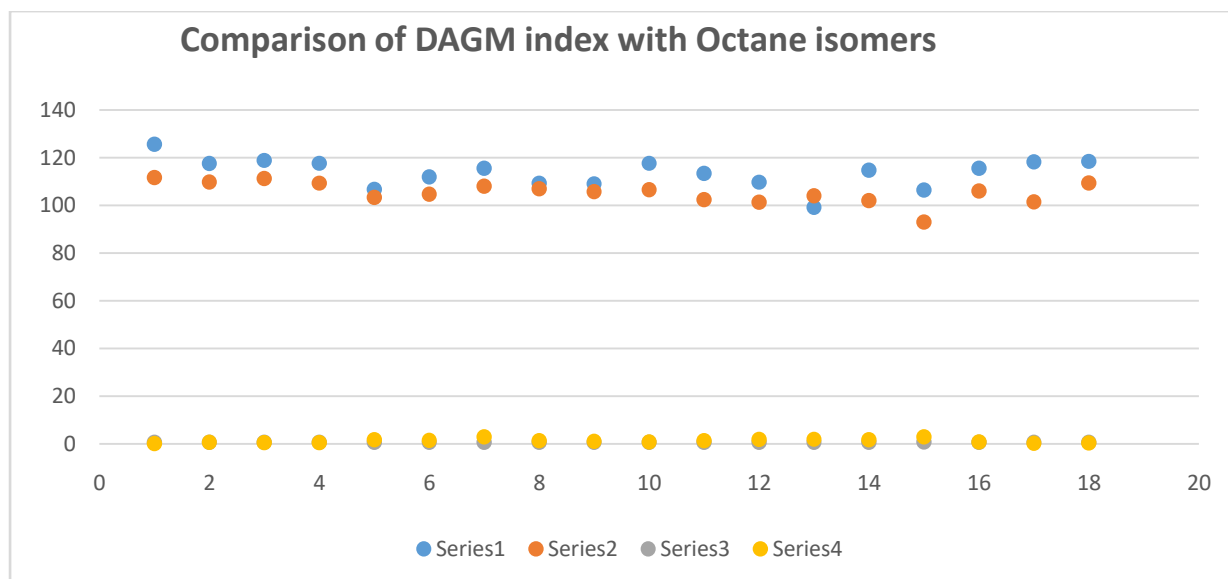
5.DAGM index of cycloalkanes

A cycloalkane has n carbon atoms and 2n-2 hydrogen atoms is denoted 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

Theorem 5.1

For $n \geq 3$, the DAGM index is equal to DAGM $(C_n^{2n-2)} = n + 9 - 6\sqrt{3}$

Proof : The cycloalkane 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 $C_3, C_4, \ldots\ldots\ldots C_n$ of degree 4 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, on the basis of degrees of the vertices, we divide the edge set into partitions.

$E_1 = \{uv \in E(C_n^{2n-2}) / d(u) = d(v) = 4\}$, $E_2 = \{uv \in E(C_n^{2n-2}) / d(u) = d(v) = 3\}$

$E_3 = \{uv \in E(C_n^{2n-2}) / d(u) = 3; d(v) = 4\}$, $E_4 = \{uv \in E(C_n^{2n-2}) / d(u)=1; d(v) = 3\}$

$E_5 = \{uv \in E(C_n^{2n-2}) / d(u) = 1; d(v) = 4\}$

There are 5 types of edges where $|E_1| = n - 3$, $|E_2| = 1$, $|E_3| = 2$, $|E_4| = 2$, $|E_5| = 2n - 4$

$$DAGM(G) = \frac{d_u + d_v}{2} - \sqrt{d_u d_v}$$

$DAGM(C_n^{2n-2}) = n + 9 - 6\sqrt{3}$

6. CONCLUSION

In this paper, the concepts of difference arithmetic geometric means index of some standard graphs are computed. Also, difference arithmetic geometric means index of a graph in chemistry is discussed.

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