International Journal of Advance Research in Science and Engineering
Volume No.07, Special Issue No.(02), March 2018
www.ijarse.com
IJARSE
ISSN: 2319-8354

A Study of Some Topological Indices of Grid

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ABSTRACT

In this paper, computation of the Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index and SK_2 index of grid is carried out without the aid of acomputer.

Keywords: Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, SK_2 index and grid.

I.INTRODUCTION

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [3, 4]. This theory had an important effect on the development of the chemical sciences.

In mathematics chemistry, a molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. And also a connected graph is a graph such that there is a path between all pairs of vertices. Note that hydrogen atoms are often omitted [4].

Let $G= (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [1].

II. COMPUTING THE TOPOLOGICAL INDICES OF GRID.

Motivated by previous research on grid, here we used to four new topological indices and computed their corresponding topological index value of grid [6].

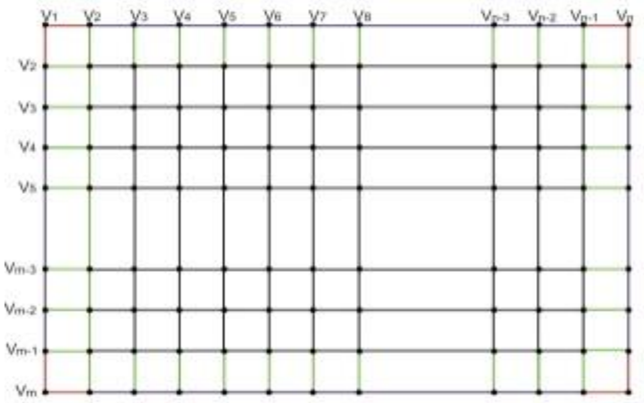

Figure 1

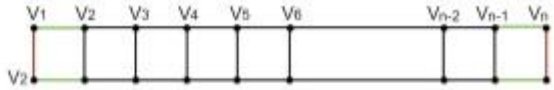

Figure 2

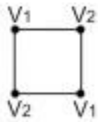

Figure 3

In [5,7,8,9 and 10], Shigehalli and Kanabur have put forward new degree based topological indices viz. arithmetic-geometric index, SK index, SK_1 index and SK_2 index. Which are defined as follows:

Definition 2.1: Arithmetic-Geometric (AG_1) Index

Let $G = (V, E)$ be a molecular graph, and $d_G(u)$ is the degree of the vertex u, then AG_1 index of G is defined as

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u).d_G(v)}}$$

Where, AG_1index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v, where $d_G(u)$ (or $d_G(v)$) denotes the degree of the vertex u (or v).

Definition 2.2: *SK* Index

The SK index of a graph $G = (V, E)$ is defined as $SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u)+d_G(v)}{2}$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

Definition 2.3: SK_1 Index

The SK_1 index of a graph $G = (V, E)$ is defined as $SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}$, where $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G.

Definition 2.4: ***SK₂*** **Index**

The SK_2 index of a graph $G = (V, E)$ is defined as $SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

III.MAIN RESULTS

Theorem3.1: The AG_1 index of grid with *"(m-1)"* rows and *"(n-1)"* columns is given by

$$AG_1(G) = \begin{cases} 2mn - 0.9793m - 0.9793n - 8.0829, & if\ m \succ 2\ \ and\ \ n \succ 2 \\ 3n - 1.9174, & if\ \ m = 2\ \ and\ \ n \succ 2 \\ 4, & if\ \ m = n = 2 \end{cases}$$

Proof: The topological structure of a grid network, denoted by $G(m, n)$, is defined as the Cartesian product $P_m \times P_n$ of undirected paths P_m and P_n. The spectrum of the graph does not depends on the numbering of the vertices. However, here we adopt a particular numbering such that the edges has a pattern which is common for any dimension. We follow the sequential numbering from left to right as shown in the figure1.

Consider a two-dimensional structure of grid with $(m-1)$ rows and $(n-1)$ columns as shown in the figure1. Let $e_{i,j}$ denotes the number of edges connecting the vertices of degrees d_i and d_j.

Table1.

Row	$e_{2,3}$	$e_{3,3}$	$e_{3,4}$	$e_{4,4}$
1	4	n-3	n	n-3
2	0	2	2	2n-5
3	0	2	2	2n-5
4	0	2	2	2n-5
. . .	. . .	. . .	. . .	. . .
m-2	0	2	2	2n-5
m-1	4	n-3	n-2	0
Total	**8**	**2m+2n-12**	**2m+2n-8**	**2mn-5m-5n+12**

Table2.

Row	$e_{2,2}$	$e_{2,3}$	$e_{3,3}$
1	2	4	(3n-8)

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u).d_G(v)}}$$

$$AG_1(G) = e_{2,3}\left(\frac{2+3}{2\sqrt{2.3}}\right) + e_{3,3}\left(\frac{3+3}{2\sqrt{3.3}}\right) + e_{3,4}\left(\frac{3+4}{2\sqrt{3.4}}\right) + e_{4,4}\left(\frac{4+4}{2\sqrt{4.4}}\right)$$

$$=8\left(\frac{5}{2\sqrt{6}}\right) + (2m+2n-12)\,(1) + (2m-2n-8)\left(\frac{7}{2\sqrt{12}}\right) + (2mn-5m-5n+12)\,(1)$$

$$= \frac{20}{\sqrt{6}} + 2m+2n-12 + (m+n-4)\frac{7}{\sqrt{12}} + 2mn-5m-5n+12$$

$$=2mn-3m-3n+\frac{7m}{\sqrt{12}} + \frac{7n}{\sqrt{12}} - \frac{28}{\sqrt{12}}$$

$$= 2mn-0.979m-0.979n-8.0829.$$

Now, we consider the following cases:

Case 1. Ifm>2 and n>2, Grid contains$e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$ only edges. In the figure1 $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$edges are colored in red, blue, green and black respectively. The number of $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$edges in each row is mentioned in the following table1.

The Arithmetic-Geometric index of grid for if m>2 and n>2

$AG_1(G)$= 2mn-0.979m-0.979n-8.0829

Case 2. In this case Grid contains $e_{2,2}$, $e_{2,3}$,and $e_{3,3}$ edges. The edges $e_{2,2}$, $e_{2,3}$,and $e_{3,3}$ are colored in red, blue and black respectively as shown in the figure2. The number of $e_{2,2}$, $e_{2,3}$,and $e_{3,3}$ edges in each row is mentioned in the table2.

If $m=2$ and $n>2$

In this case grid contains $e_{2,2}$, $e_{2,3}$ and $e_{3,3}$ edges.

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u).d_G(v)}}$$

$$AG_1(G) = e_{2,2}\left(\frac{2+2}{2\sqrt{2.2}}\right) + e_{2,3}\left(\frac{2+3}{2\sqrt{2.3}}\right) + e_{3,3}\left(\frac{3+3}{2\sqrt{3.3}}\right)$$

$$=2(1) + 4\left(\frac{5}{2\sqrt{6}}\right) + (3n-8)(1)$$

$$= 2+\frac{20}{\sqrt{6}} + 3n-8$$

$$= 3n-1.9174.$$

Case 3. If $m=n=2$

In this case the number of $e_{2,2}$ edges is as shown in figure3.

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u).d_G(v)}}$$

$$AG_1(G) = e_{2,2}\left(\frac{2+2}{2\sqrt{2.2}}\right)$$

$$=4(1)$$

$$= 4.$$

Theorem3.2: The *SK* index of grid with *"(m-1)"* rows of benzene rings and *"(n-1)"* columns is given by

$$SK(G) = \begin{cases} 8mn-7m+33n+28, & if\ m \succ 2\ \ and\ \ n \succ 2 \\ 9n-10, & if\ \ m=2\ \ and\ \ n \succ 2 \\ 8, & if\ \ m=n=2 \end{cases}$$

Proof: The topological structure of a grid network, denoted by *G (m, n)*, is defined as the Cartesian product $P_m \times P_n$ of undirected paths P_m and P_n. The spectrum of the graph does not depends on the numbering of the vertices. However, here we adopt a particular numbering such that the edges has a pattern which is common for any dimension. We follow the sequential numbering from left to right as shown in the figure1.

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$SK(G) = e_{2,3}\left(\frac{2+3}{2}\right) + e_{3,3}\left(\frac{3+3}{2}\right) + e_{3,4}\left(\frac{3+4}{2}\right) + e_{4,4}\left(\frac{4+4}{2}\right)$$

$$= 8\left(\frac{5}{2}\right) + 2\,(m+n-6)\left(\frac{6}{2}\right) + 2\,(m+n-4)\left(\frac{7}{2}\right) + (2mn-5m-5n+12)\left(\frac{8}{2}\right)$$

$$= 20+6m+6n-12+7m+7n-28+8mn-20m+20n+48$$

$$= 8mn-7m+33n+28$$

Now, we consider the following cases:

Case 1. If m>2 and n>2, Grid contains $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ only edges. In the figure1 $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ edges are colored in red, blue, green and black respectively. The number of $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ edges in each row is mentioned in the following table1.

The SK index of grid for if m>2 and n>2

$AG_1(G)$=8mn-7m+33n+28

Case 2. In this case Grid contains $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ edges. The edges $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ are colored in red, blue and black respectively as shown in the figure2. The number of $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ edges in each row is mentioned in the table2.

If $m=2$ and $n>2$

In this case grid contains $e_{2,2}$, $e_{2,3}$ and $e_{3,3}$ edges.

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$SK(G) = e_{2,2}\left(\frac{2+2}{2}\right) + e_{2,3}\left(\frac{2+3}{2}\right) + e_{3,3}\left(\frac{3+3}{2}\right)$$

$$= 2\left(\frac{4}{2}\right) + 4\left(\frac{5}{2}\right) + (3n-8)\left(\frac{6}{2}\right)$$

$$= 4+10+9n-24$$

= 9n-10.

Case 3. If $m=n=2$

In this case the number of $e_{2,2}$ edges is as shown in figure3.

$$SK(G) = \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$SK(G) = e_{2,2}\left(\frac{2+2}{2}\right)$$

$$=4\left(\frac{4}{2}\right)$$

= 8.

Theorem3.3: The SK_1 index of grid with *"(m-1)"* rows of benzene rings and *"(n-1)"* columns is given by

$$SK_1(G) = \begin{cases} 16mn-19m+61n+18, \ if \ m \succ 2 \ and \ n \succ 2 \\ 13.5n-20, \ if \ m=2 \ and \ n \succ 2 \\ 8, \ if \ m=n=2 \end{cases}$$

Proof: The topological structure of a grid network, denoted by $G(m, n)$, is defined as the Cartesian product $P_m \times P_n$ of undirected paths P_m and P_n. The spectrum of the graph does not depends on the numbering of the vertices. However, here we adopt a particular numbering such that the edges has a pattern which is common for any dimension. We follow the sequential numbering from left to right as shown in the figure1.

$$SK_1(G) = \sum_{u,v\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$SK_1(G) = e_{2,3}\left(\frac{2\times 3}{2}\right)+e_{3,3}\left(\frac{3\times 3}{2}\right)+e_{3,4}\left(\frac{3\times 4}{2}\right)+e_{4,4}\left(\frac{4\times 4}{2}\right)$$

$$=8\left(\frac{6}{2}\right)+2(m+n-6)\left(\frac{9}{2}\right)+2(m+n-4)\left(\frac{12}{2}\right)+(2mn-5m-5n+12)\left(\frac{16}{2}\right)$$

= 24+9m+9n-54+12m+12n-48+16mn-40m+40n+96

= 16mn-19m+61n+18.

Now, we consider the following cases:

Case 1. If m>2 and n>2, Grid contains $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ only edges. In the figure1 $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ edges are colored in red, blue, green and black respectively. The number of $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ edges in each row is mentioned in the following table1.

The SK_1 index of grid for if m>2 and n>2

$SK_1(G)$=16mn-19m+61n+18

Case 2. In this case Grid contains $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ edges. The edges $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ are colored in red, blue and black respectively as shown in the figure2. The number of $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ edges in each row is mentioned in the table2.

If $m= 2$ and $n>2$

In this case grid contains $e_{2,2}$, $e_{2,3}$ and $e_{3,3}$ edges.

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$SK_1(G) = e_{2,2}\left(\frac{2\times 2}{2}\right) + e_{2,3}\left(\frac{2\times 3}{2}\right) + e_{3,3}\left(\frac{3\times 3}{2}\right)$$

$$=2\left(\frac{4}{2}\right)+4\left(\frac{6}{2}\right) + (3n-8)\left(\frac{9}{2}\right)$$

= 4+12+13.5n-36

= 13.5n-20.

Case 3. If $m=n=2$

In this case the number of $e_{2,2}$ edges is as shown in figure3.

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$SK_1(G) = e_{2,2}\left(\frac{2\times 2}{2}\right)$$

$=4\left(\frac{4}{2}\right)$

$= 8.$

Theorem3.4: TheSK_2 index of grid with *"(m-1)"* rows of benzene rings and *"(n-1)"* columns is given by

$$SK_2(G) = \begin{cases} 32mn - 37.5m + 122.5n + 36, & if\ m \succ 2\ \ and\ \ n \succ 2 \\ 27n - 39, & if\ \ m = 2\ \ and\ \ n \succ 2 \\ 16, & if\ \ m = n = 2 \end{cases}$$

Proof: The topological structure of a grid network, denoted by $G(m, n)$, is defined as the Cartesian product $P_m \times P_n$ of undirected paths P_m and P_n. The spectrum of the graph does not depends on the numbering of the vertices. However, here we adopt a particular numbering such that the edges has a pattern which is common for any dimension. We follow the sequential numbering from left to right as shown in the figure1.

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2}\right)^2$$

$$SK_2(G) = e_{2,3}\left(\frac{2+3}{2}\right)^2 + e_{3,3}\left(\frac{3+3}{2}\right)^2 + e_{3,4}\left(\frac{3+4}{2}\right)^2 + e_{4,4}\left(\frac{4+4}{2}\right)^2$$

$$=8\left(\frac{25}{4}\right)+2(m+n-6)\left(\frac{36}{4}\right)+2(m+n-4)\left(\frac{49}{4}\right)+(2mn-5m-5n+12)\left(\frac{64}{4}\right)$$

$= 50+18m+18n-108+24.5m+24.5n-98+32mn-80m+80n+192$

$= 32mn-37.5m+122.5n+36$

Now, we consider the following cases:

Case 1. If m>2 and n>2, Grid contains $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$ only edges. In the figure1 $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$ edges are colored in red, blue, green and black respectively. The number of $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$ edges in each row is mentioned in the following table1.

The SK_2 index of grid for if m>2 and n>2

$AG_1(G)$=32mn-37.5m+122.5n+36

Case 2. In this case Grid contains $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ edges. The edges $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ are colored in red, blue and black respectively as shown in the figure2. The number of $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ edges in each row is mentioned in the table2.

If $m= 2$ and $n>2$

In this case grid contains $e_{2,2}$, $e_{2,3}$ and $e_{3,3}$ edges.

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2$$

$$SK_2(G) = e_{2,2}\left(\frac{2+2}{2}\right)^2 + e_{2,3}\left(\frac{2+3}{2}\right)^2 + e_{3,3}\left(\frac{3+3}{2}\right)^2$$

$$=2\left(\frac{16}{4}\right)+4\left(\frac{25}{4}\right) + (3n-8)\left(\frac{36}{4}\right)$$

$$= 8+25+27n-72$$

$$= 27n-39.$$

Case 3. If $m=n=2$

In this case the number of $e_{2,2}$ edges is as shown in figure3.

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2$$

$$SK_2(G) = e_{2,2}\left(\frac{2+2}{2}\right)^2$$

$$=4\left(\frac{16}{4}\right)$$

$$= 16.$$

IV. CONCLUSION

A generalized formula for Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, SK_2index of Grid is obtained without using computer.

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