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INVESTIGATION ON TOPOLOGICAL INDICES OF LINE GRAPH BASED ON SUBDIVISION APPROACH FOR ABID-WAHEED GRAPH

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ABSTRACT

In chemical graph theory, there is the study of Quantitative Structure Property Relationships (QSPR) and Quantitative Structure Activity Relationships (QSAR) that uses topological in dices which are numerical measures for the structures of molecular graphs. These topological indices are also able to predict the physico-chemical properties of chemical compounds such as boiling points, enthalpy of vaporization and stability. This paper aims to generalize the Randić index, geometric-arithmetic index, atom-bond connectivity index, first Zagreb index and second Zagreb index for a line graph of Abid-Waheed graph and a line graph of subdivision graph of Abid-Waheed graph. An analysis and comparison of the topological indices studied are also computed and shown. This study successfully generalized and compared several topological indices for Abid-Waheed Graph.

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1. INTRODUCTION

In the expansive domain of mathematical sciences, the study of graph theory holds a critical position, focusing on mathematical structures designed to model and analyze pairwise relations between objects. These structures themselves are commonly referred to as graphs. A graph, denoted as G, is fundamentally constituted by numerous distinct points or nodes, formally termed vertices. The connections established between any two vertices are termed edges [1]. The standard notation designates the vertex using the symbol v, and the edge using e.

For a given graph G, the collective set of all vertices is denoted as $V(G)$, and the set of all edges in G is also denoted as $E(G)$. Furthermore, quantitative analysis of the graph structure requires defining its size; the total number of vertices in G is denoted as $|V(G)|$, and the total number of edges is represented by $|E(G)|$. Beyond these foundational counts, a critical structural attribute of an individual vertex is its degree, defined as the total count of edges connected to that specific vertex. For a vertex v, this degree is denoted concisely as d_v. Advanced metrics concerning connectivity can also be established, such as the degree sum of neighbors of the end vertices of each edge in graph G. These foundational definitions are integral to the application of graph theory across various engineering and scientific disciplines. The concepts underlying graph theory and its applications are thoroughly documented [2].

A pivotal development within graph theory is the establishment of topological indices. These are specific numerical values whose primary function is to characterize and facilitate the structural analysis and understanding of graphs based on their inherent properties. Topological indices serve as essential quantitative descriptors, translating complex network topology into measurable, numerical data. The utility of these indices finds particular significance and extensive application in the field of chemical graph theory [3].

Chemical graph theory is a specialized area of study dedicated to investigating the structure and resulting properties of chemical molecules, which are modeled mathematically as graphs where atoms correspond to vertices and chemical bonds correspond to edges. The numerical values derived from topological indices are instrumental in revealing the physicochemical properties of the chemical molecules under investigation. This analytical bridge allows for the theoretical prediction and modeling of chemical behavior directly from structural data [4].

The application of topological indices in chemical graph theory has been evolving for decades. The Hosoya index holds the distinction of being the first index to gain recognition within this field. Hosoya introduced this index in 1971 as a newly proposed quantity designed to characterize the topological indices of structural isomers of saturated hydrocarbons. Since its inception, the field has expanded considerably, leading to the development and widespread exploration of numerous other topological descriptors. Examples of other indices commonly utilized in chemical structure analysis include the Wiener index, the Zagreb index, and the Espada Index, among many others. Comprehensive reviews detailing the theoretical underpinnings and variety of available topological indices are available for further reference [5], [6], [7], [8].

In addition to their foundational role in characterizing molecular structures, topological indices play an indispensable role in advanced computational modeling frameworks [9], [10]. Specifically, these indices are employed extensively in the methodologies known as Quantitative Structure Property Relationships (QSPR) and Quantitative Structure Activity Relationships (QSAR) [11], [12]. These modeling techniques rely on the numerical properties inherent in graph structures to effectively predict the macroscopic properties and biological activities of chemical compounds. For instance, Basak highlighted the essential role of graph invariants as key inputs in QSAR studies, demonstrating their capacity to predict biological activity based purely on structural topology.

The practical application of QSPR and QSAR frameworks utilizing topological indices is significant in pharmaceutical and medical research. These indices have been successfully implemented in QSPR modeling to analyze certain novel drugs specifically used in the treatment of cancer. Furthermore, topological descriptors have been utilized in conjunction with multicriteria decision-making attributes to estimate the physicochemical properties of critical compounds, such as those used as kidney cancer drugs.

Recent scholarly investigations continue to explore the utility and computational aspects of various topological descriptors, continually refining the tools available for structural analysis. Research has involved a geometric approach tailored to exploring the Sombor indices, which are a class of degree-based topological indices. Computational studies have also focused on deriving Zagreb polynomials for complex molecular structures, such as nanostar dendrimers. More recently, detailed investigations have been conducted on the

characteristics of Zagreb indices and Zagreb coindices when applied to line graphs that have been generated through a subdivision process. Furthermore, theoretical studies have established new lower bounds for certain complex descriptors, including a lower bound for the first hyper-Zagreb index in trees possessing a given roman domination number and similarly, establishing a lower bound for the second hyper-Zagreb index in trees under the constraint of a given roman domination number.

Graph theory provides the core mathematical language for understanding complex systems of relationships. The development and application of topological indices translate this structural complexity into actionable quantitative data, serving as the backbone for chemical graph theory and modern predictive frameworks like QSPR and QSAR. The ongoing investigation into new indices and the refinement of existing ones confirms the dynamic and evolving nature of this critical field, which fundamentally bridges abstract mathematical concepts with tangible scientific discovery, from structural chemistry to pharmacological development.

2. RESEARCH METHODS

2.1 Abid Waheed Graph

The Abid-Waheed Graph is a simple, unweighted, and undirected graph that was first introduced by Abid Mahboob and Muhammad Waheed Rasheed [13]. By definition, Abid-Waheed Graphs are denoted as $(AW)_a^b$ which consists of $(ab)+1$ vertices and $a(b+1)$ edges for all $b \geq 3$ and $a \geq 1$. The $(AW)_a^b$ is generated with a-cycles and order of b. In simpler terms, a is the number of branches (edges) coming from a singular center vertex while b is a closed polygon with b number of vertices that meets with the edges from a. Some examples of $(AW)_a^b$ are as shown below in Fig. 1.

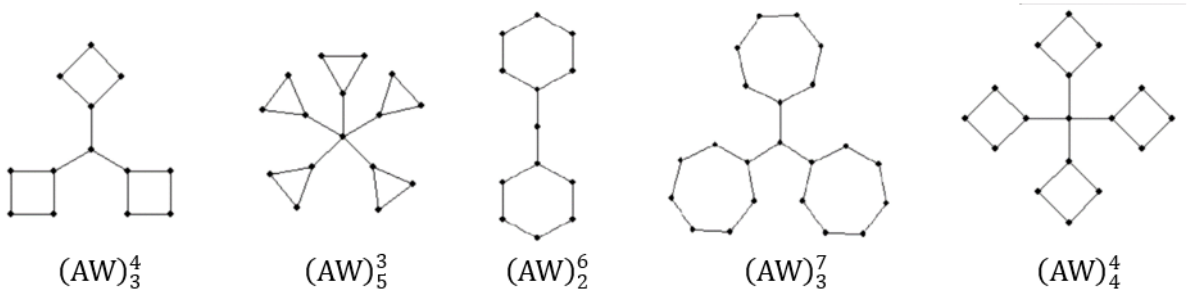


Figure 1. Abid-Waheed Graph, $(AW)_a^b$

A line graph of a graph G, $L(G)$ is another graph that represents adjacent of the edges of the graph G. A line graph is formed by considering each of the edges in G as vertices of $L(G)$. For any two edges in G that has a common vertex, an edge is drawn for the corresponding vertex of $L(G)$ [14]. The line graph of an $(AW)_a^b$ consists of a center that is a complete graph, K_n where n is the number of vertices and $n = a$. Each of the vertex will form a triangle that is further connected to a polygon of b number vertices. Examples for the line graph of $(AW)_a^b$ corresponding to Figure 1 is shown as below in Fig. 2.

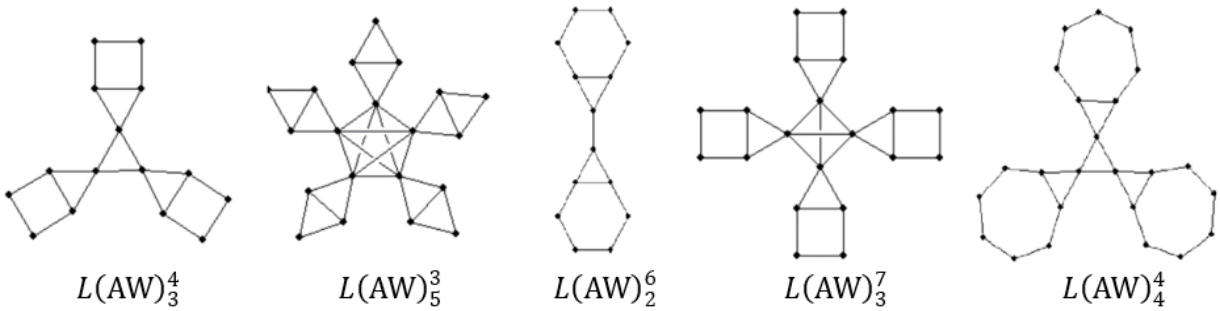


Figure 2. Line Graph of Abid-Waheed Graph, $L(AW)_a^b$

The subdivision of a graph G, $S(G)$ is a graph with its edges subdivided into 2 parts. That is, for an edge e connecting any two vertices u and v in graph G, the subdivision of it contains vertices u, v and w

where the edges are $e_1 = uw$ and $e_2 = wv$. The line graph for a subdivision of a graph G, $L[S(G)]$ is when the process of generating a line graph is applied to the subdivision of the graph G.

For $(AW)_a^b$, the line graph of its subdivision graph, $L[S(AW)_a^b]$ has a complete graph, K_n as its center where $n = a$. It also has n number of polygons of order $2b$ (has $2b$ number of vertices) where two adjacent vertices of each polygon are connected to an extra vertex to form a triangle. Each vertex of the complete graph is then connected to a polygon-triangle hybrid at the extra vertex by a line. The line graph of subdivision of $(AW)_a^b$ corresponding to Fig. 1 is shown as below in Fig. 3.

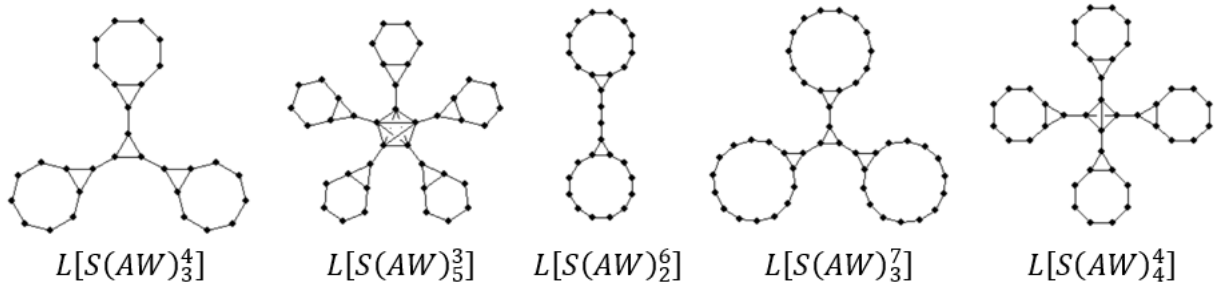


Figure 3. Line Graph of Subdivision Graph of Abid-Waheed Graph, $L[S(AW)_a^b]$

2.2 Topological Indices

In this article, only a simple, undirected, and unweighted graph is taken into consideration. While for topological indices, only some degree based topological indices are taken into account. The Randić Index is the oldest degree based topological index that was first introduced by Milan Randić in the year 1975 [15]. The Randić Index of a graph, G is defined as follows

$$R(G) = \sum_{u,v \in G} (d_u \cdot d_v)^{-1/2}, \tag{1}$$

where d_u and d_v are the degrees of the two vertices u and v respectively.

The Geometric Arithmetic Index was introduced by Vukicevic and Furtula [16] using the Randić Index as a reference point. It has a somewhat better predictive power for some physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and acentric factor [17]. This index is calculated by using the ratios of end vertex degrees of edges as shown below,

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

where d_u and d_v are the degree of the vertex u and v respectively.

The Atom-Bond Connectivity Index was first proposed by Estrada et al. [18] in where it is defined as the sum over all pairs of adjacent vertices u, v, shown as Eq. (3) below.

$$ABC(G) = \sum_{uv \in G} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}} \tag{3}$$

where d_u and d_v are the degree of the vertex u and v respectively. This index has been proven to be very useful in predicting the heat of formation of alkanes and in the study of strain energy in cycloalkanes [19]. Further studies and articles on the ABC Index can be found at [20], [21], [22] .

For the Zagreb Index, only the first and second Zagreb Indices are covered for this article while others such as the modified Zagreb Index is omitted. Trinajstić and Gutman in 1972 [23] came out with a formula that concerns with the total energy of π electrons where the sum squared of valences of the vertices of a molecular graph is calculated. This sum is now called as the first Zagreb Index (M_1). On the other hand, for the second Zagreb Index (M_2), the index is concerned with the sum of the products of the degrees of pairs of adjacent vertices [24]. Thus, the formulas for the first and second Zagreb Index is

$$M_1(G) = \sum_{uv \in G} d_u + d_v \tag{4}$$

$$M_2(G) = \sum_{uv \in G} d_u \cdot d_v \tag{5}$$

where d_u and d_v are the degree of the vertex u and v respectively. The Zagreb Index is important in mathematics as it is used extensively in molecular chemistry, spectral graph theory and many more. For more information on Zagreb Index please refer to [25], [26], [27].

From the above, it is seen that these topological indices are very important in the study of chemicals and their structures and has different uses. For further studies on topological indices on different types of molecular graphs, readers can refer to [28], [29], [30], [31], [32]. Based on paper [14], [15] where the intention was to study more on topological indices for some networks and entropy, this paper have somewhat similar aim to study on topological indices for a graph named the Abid-Waheed graph that will be further explained in the section below.

3. RESULTS AND DISCUSSION

In this research, the general structure for the line graph and the line graph of the subdivision graph of the Abid-Waheed graph is constructed. Next, the Randić, Geometric Arithmetic, Atom-Bond Connectivity, First Zagreb, and Second Zagreb Indices are calculated for the graphs by method of induction. After calculation, an analysis is made to compare the results of each index used for $b = 10$ and $1 \leq a \leq 10$. This part contains the result of the generalization for the topological indices mentioned above for $L(AW)_a^b$ and $L[S(AW)_a^b]$.

Theorem 1. *Let G be the line graph of an Abid-Waheed graph, $L(AW)_a^b$ where $b \geq 3$ and $a \geq 1$. Then the Randić, Geometric Arithmetic, Atom-Bond Connectivity, First Zagreb, and Second Zagreb Indices are as follows:*

RG=$a12b$+26−76+$233a$+1+a−$12a$+1,

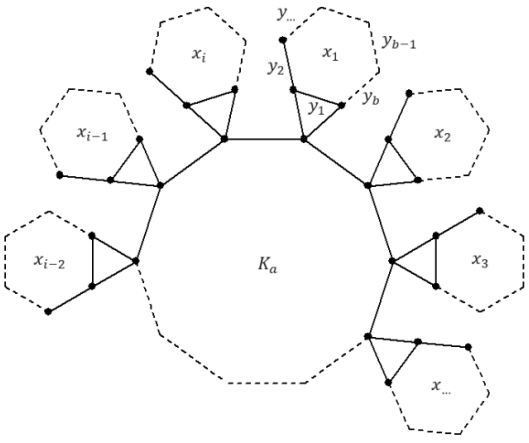
$$GA(G) = a\left[b + \frac{4\sqrt{6}-10}{5} + \frac{4\sqrt{3}\cdot\sqrt{a+1}}{a+4} + \frac{a-1}{2}\right],$$

$$ABC(G) = \frac{2a}{3} + 2a\sqrt{\frac{a+2}{3a+3}} + \frac{a(a-1)\sqrt{2a}}{2a+2},$$

$$M_1(G) = a[4b + 11 + 2a + a^2],$$

$$M_2(G) = a\left[4b + \frac{29}{2} + \frac{11a}{2} + \frac{a^2}{2} + \frac{a^3}{2}\right].$$

Proof. Let G be the line graph of subdivision graph of $(AW)_a^b$ graph, $L(AW)_a^b$ as shown in Fig. 4 below.



$* Note: i = 1, 2, 3, \ldots, a$
$j = 1, 2, 3, \ldots, b$

Figure 4. General Structure for $L(AW)_a^b$

From the figure, it can be noticed that for the graph G, $|V(G)| = a(b+1)$ and $|E(G)| = \frac{a}{2}(3+a+2b)$. It can also be noticed that the possible degrees for each of the vertices of G, d_v are 2, 3, and $a+1$. The vertex degrees are determined by their specific structural placement within the central complete graph K_a and the peripheral attachments. The vertices labeled d_v within the outer hexagonal-like clusters primarily possess a degree of 2, as they form simple paths or cycles within those subgraphs. When these clusters connect to the central core, the vertices at the "neck" of the attachment (forming the small triangles) gain an additional edge, resulting in a degree of 3. Most significantly, each vertex belonging to the central core K_a is connected to every other vertex in that core and is also connected to two external vertices from its respective peripheral cluster, and since there are a such vertices in the core, the sum of these connections leads to a degree of $a+1$. This distribution ensures that every vertex in the entire system falls into one of these three distinct functional roles, creating a highly symmetric but tiered connectivity pattern.

Let (d_u, d_v) be the degree sum of neighbors of end vertices of each edge in graph G, where $uv \in E(G)$. Then finding the edge partition of G based on degree sum of neighbors of end vertices of each edge, we obtain $(2,2)$ with number of edges being $a(b-3)$, $(2,3)$ with number of edges being $2a$, $(3,3)$ with number of edges totaling a, $(3, a+1)$ with number of edges totaling to $2a$ and $(a+1, a+1)$ with number of edges coming to $\frac{(a-1)a}{2}$.

For the Randić index with a formula of $R(G) = \sum_{u,v\in G} (d_u \cdot d_v)^{-1/2}$, when the edge partition is applied into the formula for computation, we obtain $R(G) = a(b-3)[2\cdot 2]^{-\frac{1}{2}} + 2a[2\cdot 3]^{-\frac{1}{2}} + a[3\cdot 3]^{-\frac{1}{2}} + 2a[3\cdot(a+1)]^{-\frac{1}{2}} + \frac{(a-1)a}{2}[(a+1)\cdot(a+1)]^{-\frac{1}{2}}$. After some simplification, we have general formula of the Randić Index,

$$R(G) = a\left[b + \frac{4\sqrt{6}-10}{5} + \frac{4\sqrt{3}\cdot\sqrt{a+1}}{a+4} + \frac{a-1}{2}\right].$$

Next for the Geometric arithmetic index, the same edge partition is used for calculation. Hence after substitution into the formula of Geometric arithmetic index which is $GA(G) = \sum_{uv\in G} \frac{2\sqrt{d_u\cdot d_v}}{d_u+d_v}$, we obtain the following sum,

$$GA(G) = a(b-3)\left[\frac{2\sqrt{2\cdot 2}}{2+2}\right] + 2a\left[\frac{2\sqrt{2\cdot 3}}{2+3}\right] + a\left[\frac{2\sqrt{3\cdot 3}}{3+3}\right] + 2a\left[\frac{2\sqrt{3\cdot(a+1)}}{3+(a+1)}\right] + \frac{(a-1)a}{2}\left[\frac{2\sqrt{(a+1)\cdot(a+1)}}{(a+1)+(a+1)}\right].$$

After simplification is done, the general formula is

$$GA(G) = a\left[b + \frac{4\sqrt{6}-10}{5} + \frac{4\sqrt{3}\cdot\sqrt{a+1}}{a+4} + \frac{a-1}{2}\right].$$

For the Atom-Bond Connectivity index with formula of $ABC(G) = \sum_{uv\in G}\sqrt{\frac{d_u+d_v-2}{d_u\cdot d_v}}$, the edge partition as above is still maintained. The application of the edge partition into the formula of $ABC(G)$ will produce the following,

$$ABC(G) = a(b-3)\left[\sqrt{\frac{2+2-2}{2\cdot 2}}\right] + 2a\left[\sqrt{\frac{2+3-2}{2\cdot 3}}\right] + a\left[\sqrt{\frac{3+3-2}{3\cdot 3}}\right] + 2a\left[\sqrt{\frac{3+(a+1)-2}{3\cdot(a+1)}}\right] + \frac{(a-1)a}{2}\left[\sqrt{\frac{(a+1)+(a+1)-2}{(a+1)\cdot(a+1)}}\right].$$

By simplification, the general formula for $ABC(G)$ is

$$\frac{a(b-1)}{\sqrt{2}} + \frac{2a}{3} + 2a\sqrt{\frac{a+2}{3a+3}} + \frac{a(a-1)\sqrt{2a}}{2a+2}$$

For the Zagreb Index, there is the First Zagreb Index, $M_1(G)$ and Second Zagreb Index, $M_2(G)$. For the computation of both $M_1(G)$ and $M_2(G)$, the same edge partition as above is used. The application of the edge partition into the formula for the First Zagreb Index which is $M_1(G) = \sum_{uv\in G}[d_u + d_v]$ and the Second Zagreb Index which is $M_2(G) = \sum_{uv\in G}[d_u \cdot d_v]$, we will obtain $M_1(G) = a(b-3)[2+2] + 2a[2+3] + a[3+3] + 2a[3+(a+1)] + \frac{(a-1)a}{2}[(a+1)+(a+1)]$ and $M_2(G) = a(b-3)[2\cdot 2] + 2a[2\cdot 3] + a[3\cdot 3] + 2a[3\cdot(a+1)] + \frac{(a-1)a}{2}[(a+1)\cdot(a+1)]$. After some simplification, the general formula for $M_1(G)$ is $= a[4b + 11 + 2a + a^2]$ and the general formula for $M_2(G)$ is $= a\left[4b + \frac{29}{2} + \frac{11a}{2} + \frac{a^2}{2} + \frac{a^3}{2}\right]$.

Theorem 2. *Let G be the line graph of a subdivision of Abid-Waheed graph, $L[S(AW)_a^b]$ where $b \geq 3$ and $a \geq 1$. Then the Randić, Geometric Arithmetic, Atom-Bond Connectivity, First Zagreb, and Second Zagreb Indices are as follows:*

$$R(G) = a\left[b + \frac{\sqrt{6}}{3} + \frac{1}{\sqrt{3a}}\right] - \frac{1}{2},$$

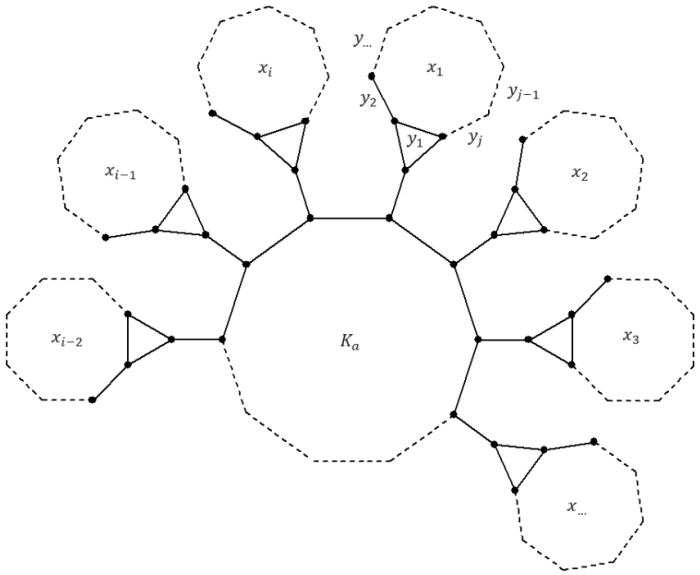
$$GA(G) = a\left[2b + \frac{8\sqrt{6}-5}{10} + \frac{2\sqrt{3a}}{3+a} + \frac{a}{2}\right],$$

$$ABC(G) = a\left[\sqrt{2}b + \frac{4-\sqrt{2}}{2} + \sqrt{\frac{a+1}{3a}} + \frac{(a-1)\left(\sqrt{2a-2}\right)}{2a}\right],$$

$$M_1(G) = a[8b + 19 + a^2],$$

$$M_2(G) = a\left[8b + 27 + 3a - \frac{a^2}{2} + \frac{a^3}{2}\right].$$

Proof. Let G be the line graph of subdivision graph of $(AW)_a^b$ graph, $L[S(AW)_a^b]$ as shown in Fig. 5 below.



$* Note: i = 1, 2, 3, \ldots, a$
$j = 1, 2, 3, \ldots, 2b$

Figure 5. General Structure for $L[S(AW)_a^b]$

From the figure, it can be noticed that for the graph G, $|V(G)| = 2[a(b+1)]$ and $|E(G)| = \frac{a}{2}(5 + a + 4b)$. It can also be noticed that the possible degrees for each of the vertices of G, d_v are 2, 3, and a.

Let (d_u, d_v) be the degree sum of neighbors of end vertices of each edge in graph G, where $uv \in E(G)$. Then finding the edge partition of G based on degree sum of neighbors of end vertices of each edge, we obtain $(2,2)$ with number of edges being $a(2b-3)$, $(2,3)$ with number of edges being $2a$, $(3,3)$ with number of edges totaling $3a$, $(3,a)$ with number of edges totaling to a and (a,a) with number of edges coming to $\frac{(a-1)a}{2}$.

For the Randić index with a formula of $R(G) = \sum_{u,v \in G} (d_u \cdot d_v)^{-1/2}$, when the edge partition is applied into the formula for computation, we obtain

$$R(G) = a(2b-3)\,[2\cdot 2]^{-\frac{1}{2}} + 2a\,[2\cdot 3]^{-\frac{1}{2}} + 3a\,[3\cdot 3]^{-\frac{1}{2}} + a\,[3\cdot a]^{-\frac{1}{2}} + \frac{(a-1)a}{2}\,[a\cdot a]^{-\frac{1}{2}}.$$

After some simplification, we have general formula of the Randić Index,

$$R(G) = a\left[b + \frac{\sqrt{6}}{3} + \frac{1}{\sqrt{3a}}\right] - \frac{1}{2}.$$

Next for the Geometric arithmetic index, the same edge partition is used for calculation. Hence after substitution into the formula of Geometric arithmetic index which is $GA(G) = \sum_{uv\in G} \frac{2\sqrt{d_u \cdot d_v}}{d_u+d_v}$, we obtain the following sum,

$$GA(G) = a(2b-3)\left[\frac{2\sqrt{2\cdot 2}}{2+2}\right] + 2a\left[\frac{2\sqrt{2\cdot 3}}{2+3}\right] + 3a\left[\frac{2\sqrt{3\cdot 3}}{3+3}\right] + a\left[\frac{2\sqrt{3\cdot a}}{3+a}\right] + \frac{(a-1)a}{2}\left[\frac{2\sqrt{a\cdot a}}{a+a}\right].$$

After simplification is done, the general formula is

$$GA(G) = a\left[2b + \frac{8\sqrt{6}-5}{10} + \frac{2\sqrt{3a}}{3+a} + \frac{a}{2}\right].$$

For the Atom-Bond Connectivity index with formula of $ABC(G) = \sum_{uv\in G}\sqrt{\frac{d_u+d_v-2}{d_u\cdot d_v}}$, the edge partition as above is still maintained. The application of the edge partition into the formula of $ABC(G)$ will produce the following,

$$ABC(G) = a(2b-3)\left[\sqrt{\frac{2+2-2}{2\cdot 2}}\right] + 2a\left[\sqrt{\frac{2+3-2}{2\cdot 3}}\right] + 3a\left[\sqrt{\frac{3+3-2}{3\cdot 3}}\right] + a\left[\sqrt{\frac{3+a-2}{3\cdot a}}\right] + \frac{(a-1)a}{2}\left[\sqrt{\frac{a+a-2}{a\cdot a}}\right].$$

By simplification, the general formula for $ABC(G)$ is

$$a\left[\sqrt{2}b + \frac{4-\sqrt{2}}{2} + \sqrt{\frac{a+1}{3a}} + \frac{(a-1)(\sqrt{2a}-2)}{2a}\right].$$

For the Zagreb Index, there is the First Zagreb Index, $M_1(G)$ and Second Zagreb Index, $M_2(G)$. For the computation of both $M_1(G)$ and $M_2(G)$, the same edge partition as above is used. The application of the edge partition into the formula for the First Zagreb Index which is $M_1(G) = \sum_{uv\in G}[d_u + d_v]$ and the Second Zagreb Index which is $M_2(G) = \sum_{uv\in G}[d_u \cdot d_v]$, we will obtain

$$M_1(G) = a(2b-3)[2+2] + 2a[2+3] + 3a[3+3] + a[3+a] + \frac{(a-1)a}{2}[a+a]$$

and

$$M_2(G) = a(2b-3)[2\cdot 2] + 2a[2\cdot 3] + 3a[3\cdot 3] + a[3\cdot a] + \frac{(a-1)a}{2}[a\cdot a]$$

After some simplification, the general formula for $M_1(G)$ is

$$M_1(G) = a[8b + 19 + a^2]$$

and the general formula for $M_2(G)$ is

$$M_2(G) = a\left[8b + 27 + 3a - \frac{a^2}{2} + \frac{a^3}{2}\right].$$

The calculation for all topological indices can directly use Python-based libraries like MathChem or SageMath, which automate the process of analyzing a graph's structure. The calculation follows a straightforward degree-based algorithm. These tools essentially scan the graph's connectivity map to quickly transform the physical shape of a molecule into a single numerical value used to predict its chemical properties.

This section shows the output from the theorems as discussed above for the Abid-Waheed Graph when $b = 10$ and $1 \le a \le 10$. Table 1 shows the output for the line graph of Abid-Waheed Graph while Table 2 shows the output for line graph of subdivision graph of Abid-Waheed Graph.

Table 1. Topological Indices for $L(AW)_a^b$ when $b = 10$ and $1 \le a \le 10$

Index	a									
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
$R(G)$	5.47	10.97	16.43	21.87	27.28	32.67	38.04	43.41	48.77	54.12
$GA(G)$	10.60	21.66	33.16	45.02	57.21	69.68	82.40	95.35	108.50	121.86
$ABC(G)$	7.92	16.43	25.11	33.90	42.76	51.68	60.65	69.64	78.67	87.71
$M_1(G)$	54	118	198	300	430	594	798	1048	1350	1710
$M_2(G)$	61	143	267	466	785	1281	2023	3092	4581	6595

Table 2. Topological Indices for $L[S(AW)_a^b]$ when $b = 10$ and $1 \leq a \leq 10$

Index	a									
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
$R(G)$	10.89	21.95	32.95	43.92	54.87	65.8132	76.74	87.66	98.58	109.49
$GA(G)$	21.96	45.16	69.35	94.38	120.18	146.66	173.78	201.48	229.73	258.49
$ABC(G)$	10.23	21.88	44.48	56.18	67.96	69.79	79.79	91.67	103.59	115.52
$M_1(G)$	100	206	324	460	620	810	1036	1304	1620	1990
$M_2(G)$	110	230	375	572	860	1290	1925	2840	4122	5870

There are also graphical outputs for both tables as shown below in Figs. 6 and 7.

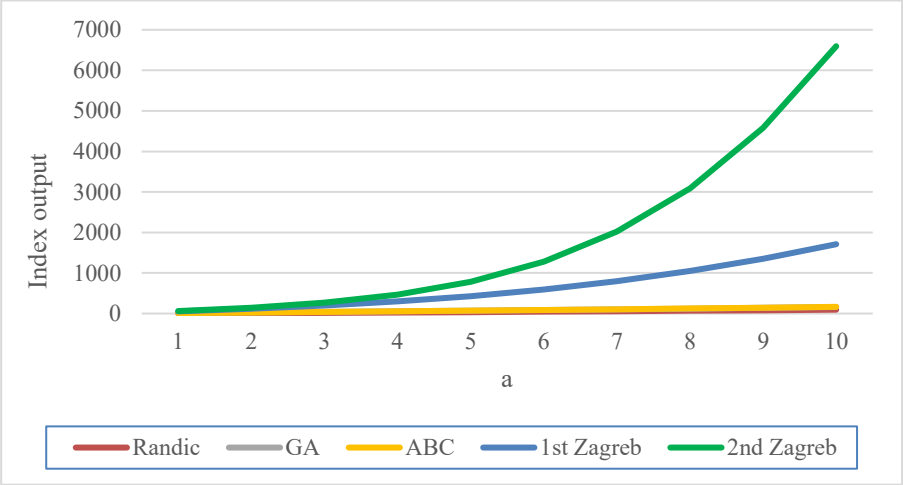


Figure 6. Graph of Topological Index Against a for $L(AW)_a^b$ when $b = 10$

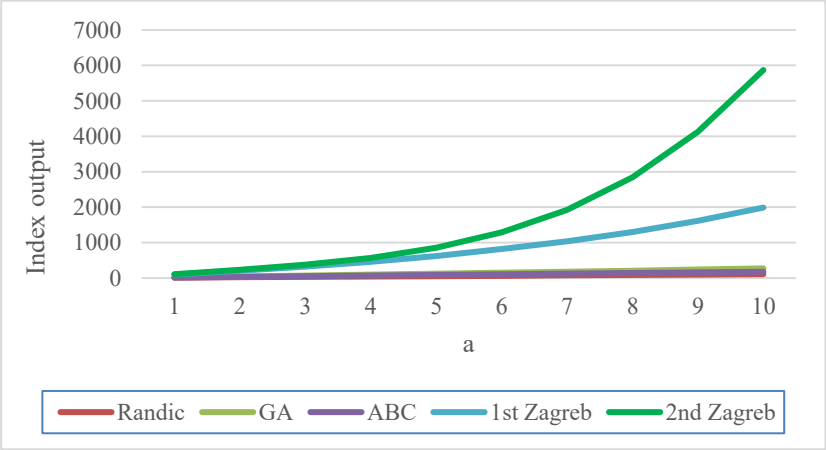


Figure 7. Graph of Topological Index Against a for $L[S(AW)_a^b]$ when $b = 10$

Next, the comparison of Randić Index for $L(AW)_a^b$ and $L[S(AW)_a^b]$ is shown in Fig. 8.

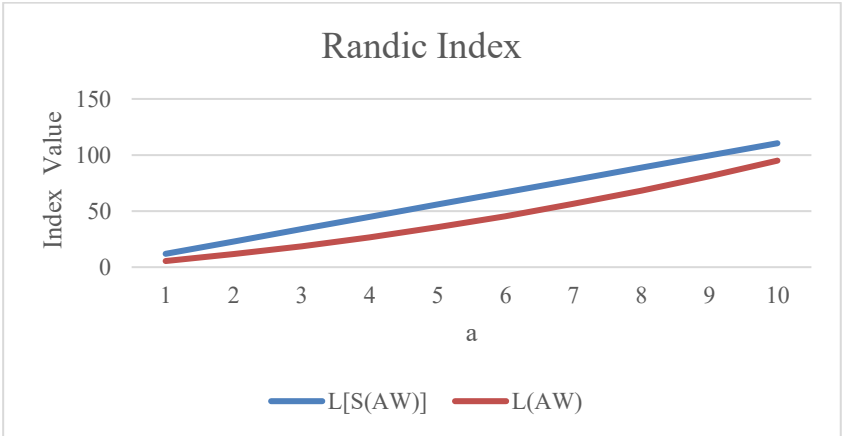


Figure 8. Graph of Randić Index Against a for $L(AW)_a^b$ and $L[S(AW)_a^b]$ when $b = 10$

From the Fig. 8, it can be noticed that the Randić Index for $L(AW)_a^b$ is almost linear while for $L[S(AW)_a^b]$ it is a curve. Thus, for a sufficiently large a, the Randić Index for $L(AW)_a^b > L[S(AW)_a^b]$. Meanwhile, the comparison of Geometric Arithmetic Index for $L(AW)_a^b$ and $L[S(AW)_a^b]$.is shown in Fig. 9.

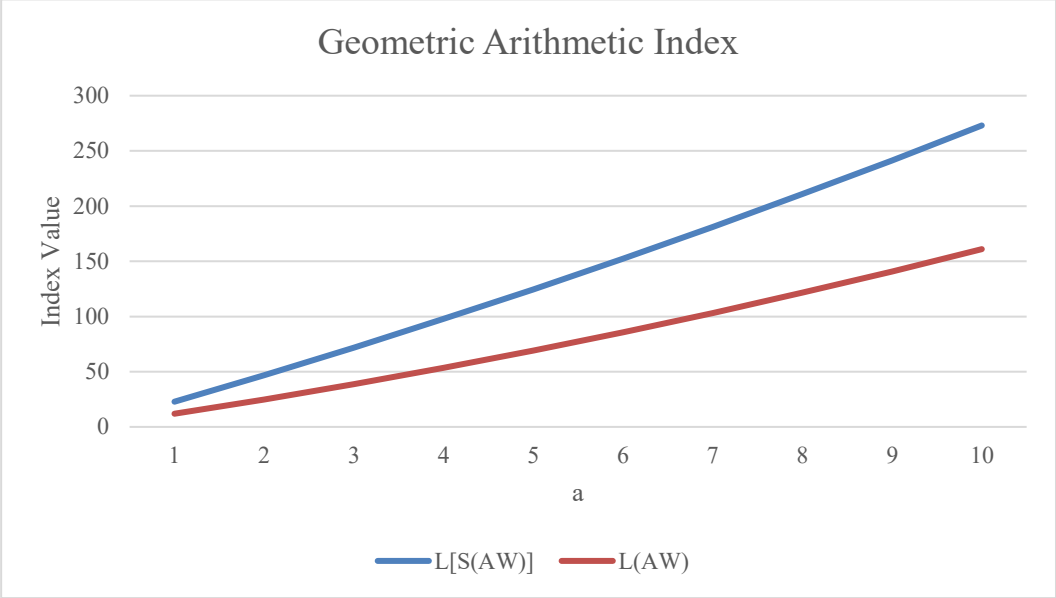


Figure 9. Graph of Geometric Arithmetic Index Against a for $L(AW)_a^b$ and $L[S(AW)_a^b]$ when $b = 10$

From Fig. 9, it can be deduced that the increase of $L(AW)_a^b$ is more significant compared to $L[S(AW)_a^b]$. Therefore, it can be concluded that $L(AW)_a^b < L[S(AW)_a^b]$ for all a. Furthermore, Fig. 10 shows the comparison of Atom-Bond Connectivity Index for $L(AW)_a^b$ and $L[S(AW)_a^b]$.

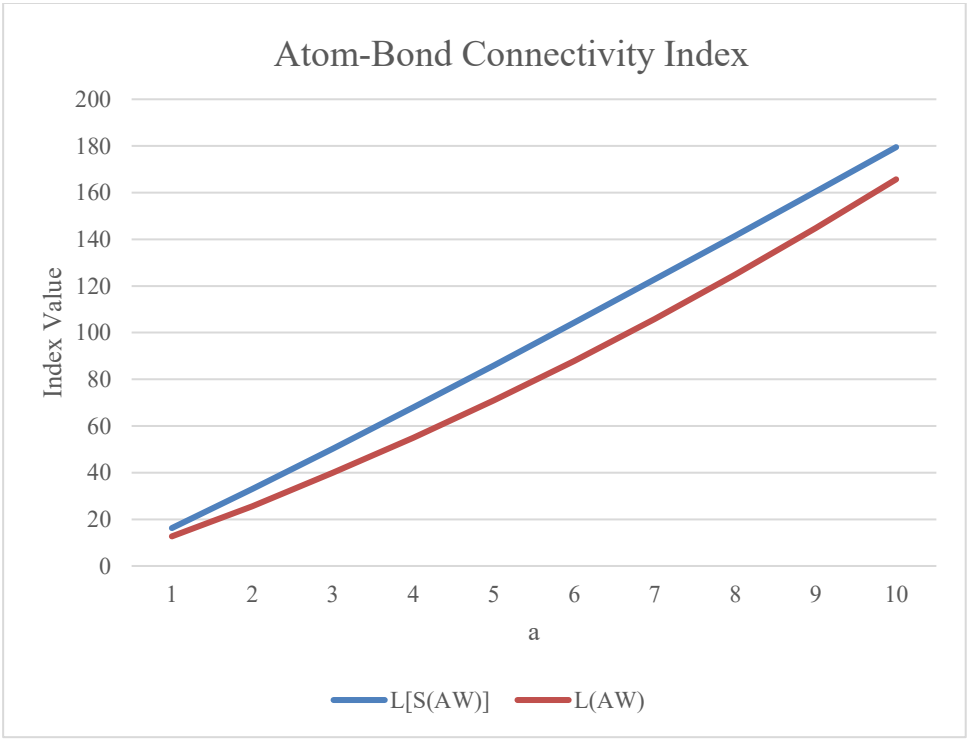


Figure 10. Graph of Atom-Bond Connectivity Index Against a for $L(AW)_a^b$ and $L[S(AW)_a^b]$ when $b = 10$

From Fig. 10, the difference between $L(AW)_a^b$ and $L[S(AW)_a^b]$ increases but then gradually decrease. Thus, most likely for a sufficiently large a, $L(AW)_a^b > L[S(AW)_a^b]$. In addition, Fig. 11 shows the comparison of First Zagreb Index for $L(AW)_a^b$ and $L[S(AW)_a^b]$.

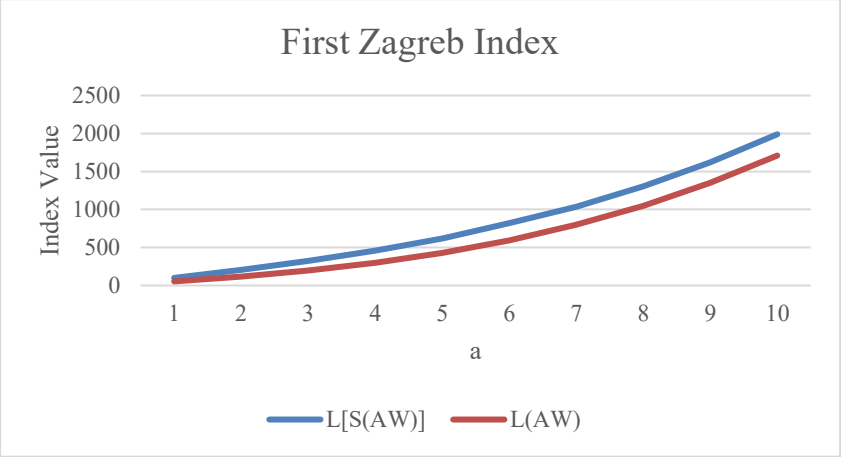


Figure 11. Graph of First Zagreb Index Against a for $L(AW)_a^b$ and $L[S(AW)_a^b]$ when $b = 10$

From Fig. 11, the difference between the values of $L(AW)_a^b$ and $L[S(AW)_a^b]$ is increasing. Therefore, we can conclude that for all a, $L(AW)_a^b < L[S(AW)_a^b]$. Following that, the comparison of Second Zagreb Index for $L(AW)_a^b$ and $L[S(AW)_a^b]$ is shown in Fig. 12.

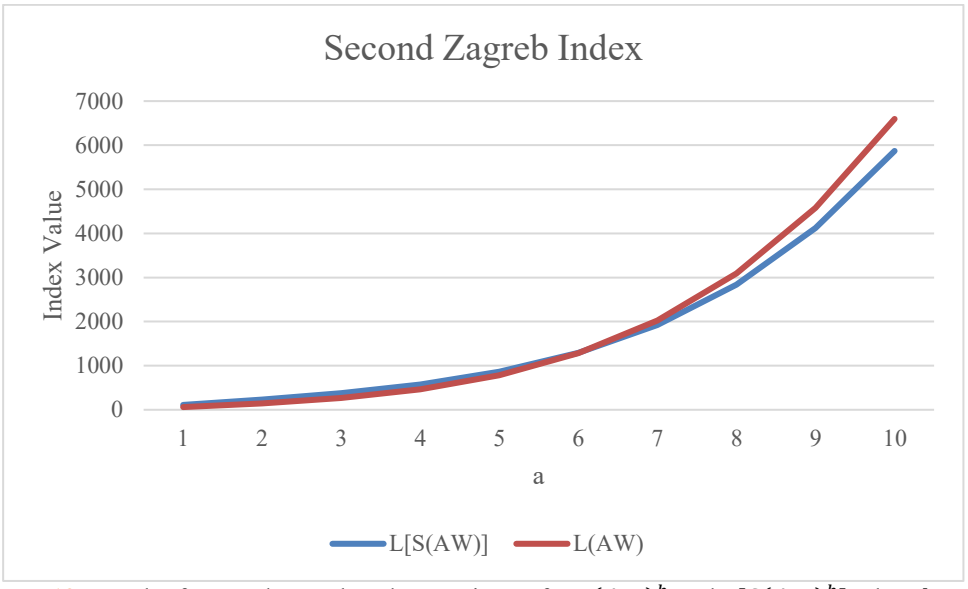


Figure 12. Graph of Second Zagreb Index Against a for $L(AW)_a^b$ and $L[S(AW)_a^b]$ when $b = 10$

From Fig. 12, it is obvious that for $a > 6$, the value of the Second Zagreb Index for $L(AW)_a^b > L[S(AW)_a^b]$.

4. CONCLUSION

This study successfully generalized and compared five key degree-based topological indices—Randić, Geometric-Arithmetic, Atom-Bond Connectivity, and the First and Second Zagreb indices—for the line graph and the line graph of the subdivision of the Abid-Waheed graph. By employing edge partitioning and method of induction, the research established general formulas for these indices, revealing that the line graph of the subdivision graph, $L[S(AW)_a^b]$ generally yields higher values for the Geometric-Arithmetic and First Zagreb indices compared to the standard line graph, $L[(AW)_a^b]$. Furthermore, comparative analysis showed that while $L[S(AW)_a^b]$values are initially higher for the Randić, Atom-Bond Connectivity, and Second Zagreb indices, the standard line graph tends to exceed these values as the number of branches a increases. Ultimately, these generalized numerical descriptors provide a foundational framework for predicting the physico-chemical properties of molecules modeled by these complex graph structures within QSPR and QSAR studies.

Author Contributions

Mohamad Nazri Husin: Conceptualization, Formal Analysis, Funding Acquisition, Investigation, Project Administration, Resources, Validation, Supervision, Writing - Original Draft and Writing - Review and Editing. Kee Yeong Chua: Data Curation, Investigation, Methodology, Resources, Software, Visualization, Writing - Original Draft. All authors discussed the results and contributed to the final manuscript.

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Declarations

The authors declare that there is no conflict of interest.

Declaration of Generative AI and AI-assisted technologies

The authors declare that no generative AI or AI-assisted technologies were used in the preparation of this manuscript, including for writing, editing, data analysis, or the creation of tables and figures.

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