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Exploring Topological Indices of Special Graphs through Computational Techniques

B.K. Keerthiga Priyatharsini[1], S. Balasundar[2]

[1]Assistant Professor, Department of Mathematics, University College of Engineering, Ramanathapuram, Tamilnadu, India.

Email ID: keerthi.priyatharsini@yahoo.com

[2]Assistant Professor, Department of Mathematics, Alagappa Chettiar Government College of Engineering and Technology, Karaikudi, Tamilnadu, India.

Email ID: balasundaraccet@gmail.com

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Abstract

By make use of the vertex degree of the graphs, the M −polynomials of the special graphs like Bull graphs, H −graphs, Butterfly graphs, and Cricket graphs were acquired and scrutinized in this paper. Also, with the help of M −polynomials of the abovesaid special graphs, the several vertex degree-dependent topological indices of the special graphs were also determined. Additionally, we computed the comparison table and provided a graphical representation of the determined topological indices.

Keywords: *M −Polynomial, Bull graphs, H −graphs, Butterfly graphs, Cricket graphs, Topological Indices.*

2020 Mathematics Subject Classification: *05C78.*

1. Introduction

The study of graphs, which are mathematical structures used to represent pairwise interactions between things, is the focus of graph theory, a foundational field of mathematics. A set of vertices, also known as nodes, and a set of edges joining these vertices make up a graph. Graph theory has developed into an essential tool in a variety of fields, including computer science, engineering, social sciences, and biology, since its formal inception in the 18th century, especially with Euler's solution to the Königsberg bridge problem.

Graphs can be used in graph theory to depict a variety of related structures, including social interactions, communication networks, and transportation routes. The area encompasses a broad range of graph forms, each with unique characteristics and uses, including directed or undirected graphs, weighted graphs, trees, and hypergraphs.

Chemical graph theory is a specialized field that emerged from the intriguing application of graph theory in the world of chemistry. This branch models and analyzes molecular structures using ideas from graph theory. Chemical graph theory allows for the study of complicated molecules through their corresponding molecular graphs, where atoms are represented by vertices and chemical bonds by edges.

Chemical graph theory serves as a bridge between mathematics and chemistry, enabling researchers to predict molecular properties, assess isomerism, and design new compounds. It plays a significant role in cheminformatics, drug discovery, and theoretical chemistry, offering computational techniques for solving chemical problems that are otherwise difficult to tackle experimentally.

Together, graph theory and chemical graph theory offer powerful frameworks for modeling, analysis, and problem-solving across both abstract mathematical domains and practical scientific applications.

The structural (topological) representation of molecules, usually represented as molecular graphs, is the source of topological indices, which are numerical descriptors. Atoms are shown as vertices and bonds as edges in these kinds of graphs. Without the need for intricate geometric or electronic data, these indices offer a straightforward but useful method of quantifying molecular attributes by capturing key aspects of a molecule's connection and structure.

Chemical graph theory gave rise to the idea of topological indices, which are now fundamental to research on quantitative structure–activity relationships (QSAR) and quantitative structure–property relationships (QSPR). These indices let researchers predict the chemical, physical, and biological properties of molecules and are essential tools in cheminformatics, computational chemistry, and drug discovery.

2.Topological indices

By converting a chemical molecule structure into a mathematical number, the topological index is calculated. It correlates to certain physical-chemical characteristics, such as the stability, stain energy, and boiling temperature of a chemical molecule with a subatomic structure. It is an invariant over formation planning and a positive integer associated with molecular structure that represents its topology. Wiener developed the theory of the topological index in 1947 by working on the boiling temperature of paraffin. He assigned the term path number to this index. The topological index hypothesis was developed, and the path number was dubbed the Weiner index. Because this type of research focuses on the topological inter-connectivity of chemical structure and their description, countless studies and papers have been published over the decades to investigate the connections between chemical properties and graph-theoretical dependent topological indices.A topological index is a quantitatively calculated number derived from the molecular graph. It is linked to chemical constitution, showing that numerous physical, chemical, and biological processes are correlated with chemical structure. The following defines a few of the degree-based topological indices that we employ in this work.

Topological indices are broadly classified based on the type of graph parameters they depend on—such as degree, distance, or eigenvalues—and include well-known indices like the Wiener index, Zagreb indices, and Randić index. Their ability to correlate molecular structure with activity or properties has made them invaluable for molecular modeling, screening of chemical libraries, and designing new compounds with desired characteristics.

Definition 2.1: ABC Index

The Atom–Bond Connectivity (ABC) index, originally introduced by Estrada and co-authors, is defined for a graph Gas

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$$

where each term corresponds to an edge $uv$and d_u, d_vdenote the degrees of the incident vertices.

Definition 2.2: First Zagreb Index

The first Zagreb index, attributed to Gutman and Trinajestić, is expressed as

$$M_1(G) = \sum_{uv\in E(G)} (d_u + d_v),$$

which sums the degree totals of all vertex pairs forming the edges of G.

Definition 2.3: Second Zagreb Index

The second Zagreb index, also introduced by Gutman and Trinajestić, is given by

$$M_2(G) = \sum_{uv\in E(G)} (d_u d_v),$$

representing the cumulative product of degrees over all edges.

Definition 2.4: Harmonic Index

The harmonic index, formulated by Fajtlowicz and collaborators, is defined as

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d_u + d_v},$$

which incorporates harmonic contributions of degree sums for each edge.

Definition 2.5: Hyper Zagreb Index

The hyper Zagreb index, introduced by Shirdel and colleagues, takes the form

$$HM(G) = \sum_{uv\in E(G)} (d_u + d_v)^2,$$

reflecting the squared degree sum for every edge in the graph.

Definition 2.6: Third Zagreb Index

The third Zagreb index, proposed by Fath-Tabar and co-authors, is defined as

$$ZG_3(G) = \sum_{uv\in E(G)} | d_u - d_v |,$$

which measures the degree difference across each edge.

Definition 2.7: Forgotten Index

The forgotten (or F-index), introduced by Furtula et al., is described as

$$F(G) = \sum_{uv\in E(G)} (d_u^2 + d_v^2),$$

capturing the sum of squared degrees associated with the endpoints of each edge.

Definition 2.8: Symmetric Division Index

The symmetric division index is defined as

$$SSD(G) = \sum_{uv\in E(G)} (\frac{P}{Q} + \frac{Q}{P}),$$

where $P = \min(d_u, d_v)$and $Q = \max(d_u, d_v)$for every edge uv.

Definition 2.9: Randić Index

The Randić index, formulated by Milan Randić, is expressed as

$$R(G) = \sum_{uv\in E(G)} \sqrt{\frac{1}{d_u d_v}},$$

reflecting inverse contributions of vertex degrees along the edges.

Definition 2.10: Sum Connectivity Index

The sum connectivity index, introduced by Zhou and Trinajstić, is defined as

$$S(G) = \sum_{uv\in E(G)} \sqrt{\frac{1}{d_u + d_v}},$$

which incorporates the reciprocal of vertex-degree sums.

Definition 2.11: GA Index

The geometric–arithmetic (GA) index, proposed by Vukićević and colleagues, is described as

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

derived from geometric and arithmetic means of degrees.

Graph polynomials develop a number of algebraic methods for encoding information already existing in a graph and obtaining hidden information from it. The M, Tutte, Forgotten, Hosoya, Pi, Schultz, and Modified Schultz polynomials are among the more important graph algebraic polynomials that were first described in graph theory.

The topological indices' values are often computed using their definitions. Nevertheless, we also have an alternative approach that obtains the topological index scores using the derivatives, fundamental, or any one of the graph polynomials at a given place. Thus, we can compute several topological indices using simply the graph polynomial. One such example that produces decent results for identifying different degree-dependent topological indices is the M-polynomial.

E. Deutsch and S. Klavžar introduced the M-polynomial for graph G in 2015 . This polynomial is illustrated as:

$$[G;\lambda,\mu] = \sum_{\delta\le i\le j\le A} m_{ij}(G)\lambda^i\mu^j$$

The $\{d_V,\ d_U\} = \{i,j\}$ equality holds in this case $m_{ij}(G)$ is the total count of edges vu when uv depending on the edge set $E(G)$, δ indicates the lowest degree of vertex, Δ indicates the highest degree of vertex depending on the vertex set $V(G)$.

Let G be a graph such that $V(G)$ denotes the vertex set and $E(G)$ denotes the edge set of G. For any vertex v, the degree $d(v)$ is defined as the number of edges in G that are incident to this particular vertex. The length of shortest path between two vertices u and v in a graph G is referred to as distance $d(u,v)$. If G is a graph having p vertices and q edges then we say order of G is p and size of G is q. A graph having order p and size q will be referred to as $(p,q)-$ graph.

4. Topological Indices of Butterfly graph:

The butterfly graph, also known as the knot graph and the hourglass graph, is a planar, undirected graph with five vertices and six edges in the mathematical discipline of graph theory. It is isomorphic to the friendship graph F_2 and can be created by combining two copies of the cycle graph C_3 with a shared vertex.

The butterfly graph is both Eulerian and a penny graph (which suggests that it is unit distance and planar), with diameter 2 and girth 3, radius 1, chromatic number 3, and chromatic index 4. Additionally, it is a graph with one vertex and two edges connected.

Only three simple graphs with five vertices are not elegant. The butterfly graph is one of them. The complete graph K_5 and cycle graph C_5 are the other two.

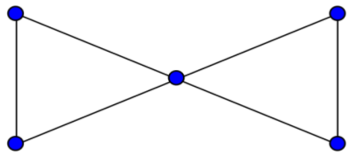


Figure 1: Butterfly Graph

Observation: 4.1 Edge Partition of Butterfly Graph:

$E(2,2) = 2, \mathrm{E}(2,4) = 4$

1. **ABC Index:**

   For the graph G, the Atom–Bond Connectivity index

$$ABC(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{d_\alpha + d_\beta - 2}{d_\alpha d_\beta}}$$

   evaluates to **4.2426**.

2. **Randić Index:**

   The Randić index of G, computed through

$$R(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{1}{d_\alpha d_\beta}},$$

   has a value of **2.4142**.

3. **Sum Connectivity Index:**

   Using

$$S(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{1}{d_\alpha + d_\beta}},$$

   the sum connectivity index for the graph is **2.6330**.

4. **GA Index:**

   The geometric–arithmetic (GA) index is determined by

$$GA(G) = \sum_{\alpha\beta \in E(G)} \frac{2\sqrt{d_\alpha d_\beta}}{d_\alpha + d_\beta},$$

   and its calculated value is **5.7712**.

5. **First Zagreb Index:**

   The first Zagreb index, defined as

$$M_1(G) = \sum_{\alpha\beta\in E(G)} (d_\alpha + d_\beta),$$

   yields a total of **32** for the given graph.

6. **Second Zagreb Index:**

   The second Zagreb index, given by

$$M_2(G) = \sum_{\alpha\beta\in E(G)} (d_\alpha d_\beta),$$

   is evaluated to be **40**.

5. Topological Indices of H −graph

Definition: The" H graph is the tree on 6 vertices illustrated above.

Observation:5.1 Edge partition of H −graph:$\mathrm{E}(1,3) = 4, \mathrm{E}(3,3) = 1$

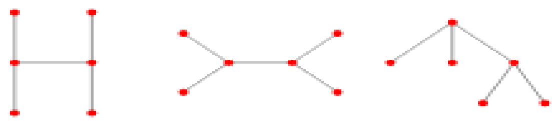


Figure 2: H-graph

1. **ABC Index:**

   For the graph G, the Atom–Bond Connectivity index

$$ABC(G) = \sum_{\alpha\beta\in E(G)} \sqrt{\frac{d_\alpha + d_\beta - 2}{d_\alpha d_\beta}}$$

   evaluates to **3.9327**.

2. **Randić Index:**

   The Randić index of G, computed through

$$R(G) = \sum_{\alpha\beta\in E(G)} \sqrt{\frac{1}{d_\alpha d_\beta}},$$

   has a value of **2.8868**.

3. **Sum Connectivity Index:**

   Using

$$S(G) = \sum_{\alpha\beta\in E(G)} \sqrt{\frac{1}{d_\alpha + d_\beta}},$$

the sum connectivity index for the graph is **2.4083**.

4. **GA Index:**

   The geometric–arithmetic (GA) index is determined by

$$GA(G) = \sum_{\alpha\beta\in E(G)} \frac{2\sqrt{d_\alpha d_\beta}}{d_\alpha + d_\beta},$$

   and its calculated value is **1.8660**.

5. **First Zagreb Index:**

   The first Zagreb index, defined as

$$M_1(G) = \sum_{\alpha\beta\in E(G)} (d_\alpha + d_\beta),$$

   yields a total of **22** for the given graph.

6. **Second Zagreb Index:**

   The second Zagreb index, given by

$$M_2(G) = \sum_{\alpha\beta\in E(G)} (d_\alpha d_\beta),$$

   is evaluated to be **21**.

6.Topological Indices of Cricket graph

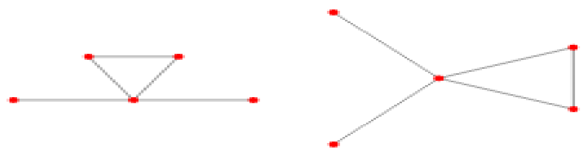


Figure 3: Cricket graph

Observation: 6.1 Edge Partition of Cricket Graph:

$\boldsymbol{E(1,4) = 2, E(2,4) = 2, E(2,2) = 1.}$

1. **ABC Index:**

   For the graph G, the Atom–Bond Connectivity index

$$ABC(G) = \sum_{\alpha\beta\in E(G)} \sqrt{\frac{d_\alpha + d_\beta - 2}{d_\alpha d_\beta}}$$

   evaluates to **3.8534**.

2. **Randić Index:**

   The Randić index of G, computed through

$$R(G) = \sum_{\alpha\beta\in E(G)} \sqrt{\frac{1}{d_\alpha d_\beta}},$$

   has a value of **2.2071**.

3. **Sum Connectivity Index:**

   Using

$$S(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{1}{d_\alpha + d_\beta}},$$

   the sum connectivity index for the graph is **2.2109**.

4. **GA Index:**

   The geometric–arithmetic (GA) index is determined by

$$GA(G) = \sum_{\alpha\beta \in E(G)} \frac{2\sqrt{d_\alpha d_\beta}}{d_\alpha + d_\beta},$$

   and its calculated value is **4.4856**.

5. **First Zagreb Index:**

   The first Zagreb index, defined as

$$M_1(G) = \sum_{\alpha\beta \in E(G)} (d_\alpha + d_\beta),$$

   yields a total of **26** for the given graph.

6. **Second Zagreb Index:**

   The second Zagreb index, given by

$$M_2(G) = \sum_{\alpha\beta \in E(G)} (d_\alpha d_\beta),$$

   is evaluated to be **28**.

7. Topological Indices of Bull graph:

In graph theory, a triangle with two disjoint pendant edges forms the bull graph, a planar, undirected graph with five vertices and five edges. The graph has a chromatic number of 3, a chromatic index of 3, a radius of 2, a diameter of 3, and a girth of 3, among other significant structural characteristics. Furthermore, because the bull graph is self-complementary, a block graph, a split graph, an interval graph, and claw-free, it is a member of several well-known graph classes. It has both 1-edge and 1-vertex connection.

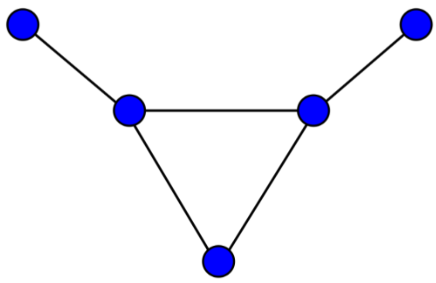


Figure:4 Bull Graph

Observation: 7.1 Edge Partition of Bull Graph:

$E(1,3) = 2, E(2,3) = 2, E(3,3) = 1.$

1. **ABC Index:**

   For the graph G, the Atom–Bond Connectivity index

$$ABC(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{d_\alpha + d_\beta - 2}{d_\alpha d_\beta}}$$

   evaluates to **3.7139**.

2. **Randić Index:**

   The Randić index of G, computed through

$$R(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{1}{d_\alpha d_\beta}},$$

   has a value of **2.3045**.

3. **Sum Connectivity Index:**

   Using

$$S(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{1}{d_\alpha + d_\beta}},$$

   the sum connectivity index for the graph is **2.3026**.

4. **GA Index:**

   The geometric–arithmetic (GA) index is determined by

$$GA(G) = \sum_{\alpha\beta \in E(G)} \frac{2\sqrt{d_\alpha d_\beta}}{d_\alpha + d_\beta},$$

   and its calculated value is **4.692**.

5. **First Zagreb Index:**

   The first Zagreb index, defined as

$$M_1(G) = \sum_{\alpha\beta \in E(G)} (d_\alpha + d_\beta),$$

   yields a total of **24** for the given graph.

6. **Second Zagreb Index:**

   The second Zagreb index, given by

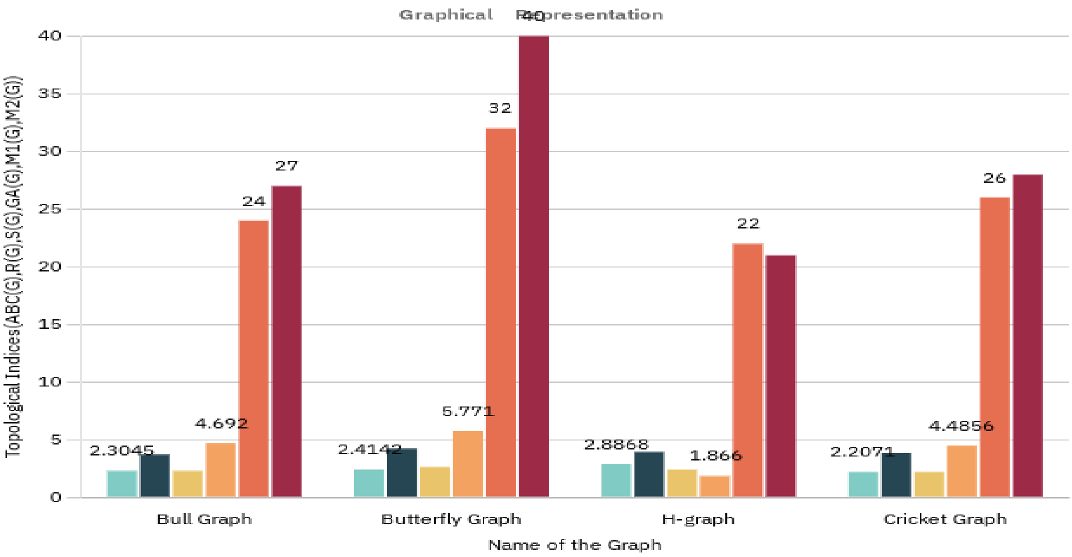
$$M_2(G) = \sum_{\alpha\beta \in E(G)} (d_\alpha d_\beta),$$

   is evaluated to be **27**.

8. Comparison Table:

Name of the Graph	$ABC(G)$	$R(G)$	$S(G)$	$GA(G)$	$M_1(G)$	$M_2(G)$
Bull Graph	3.7139	2.3045	2.3026	4.692	24	27
Butterfly Graph	4.2426	2.4142	2.6330	5.771	32	40
H-graph	3.9327	2.8868	2.4083	1.8660	22	21
Cricket Graph	3.8534	2.2071	2.2109	4.4856	26	28

9.Graphical IIustration:



10. Conclusion

The Bull graph, Butterfly graph, H-graph, and Cricket graph are some of the particular types of graphs for which we have conducted a thorough investigation of topological indices in this work. These indices are useful tools for describing and contrasting various graph architectures since they are mathematical descriptors that are derived from the structural characteristics of graphs. We were able to draw attention to both the commonalities and the clear differences that emerge across the graphs under consideration by methodically calculating and evaluating these indices.

To further comprehend the relative behavior of these graphs with respect to their topological descriptors, a comparison analysis of the acquired values was carried out. This comparison sheds light on how structural modifications in graphs affect the topological measurements that go along with them. We also used bar charts to graphically show the results in order to improve clarity and visualization, which made the differences in the indexes easier to understand.

The study's findings highlight the importance of topological indices in graph theory and show how they might be used in fields where graph structures are commonly used, like chemistry, computer networks, and biological modeling. This work establishes the framework for expanding comparable analysis to additional graph families, allowing researchers to find more extensive patterns and uses of topological indices in a variety of fields.

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