The Nepali Mathematical Sciences Report
Regd No.: 53/033-034, ISSN: 2392–411X
http://www.journal.cdmathtu.edu.np
Year: 2025, Volume: 42, No. 2
Pages: 162–177
https://doi.org/10.3126/nmsr.v42i2.88560
Research Article

Revan Topological Indices of Quadrilateral Snake Graphs: Polynomial Formulations, Python Implementation, and Applications

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Received: 26 September, 2025 Accepted: 10 November, 2025 Published Online: 30 December, 2025

Abstract

This study presents a detailed exploration of the Revan family of topological indices and their polynomial representations for diverse classes of quadrilateral snake graphs. Originating from the concept introduced by V. R. Kulli, Revan indices integrate both the minimum and maximum vertex degrees, which provide a refined measure of graph connectivity and structure. The research systematically derives explicit analytical expressions for Revan indices and their corresponding polynomials for four principal graph variants standard, alternate, double, and cyclic quadrilateral snake graphs highlighting their distinctive structural characteristics and degree-based relationships. To complement the theoretical formulations, a Python-based computational framework was developed to automate the calculation and symbolic representation of these indices. This implementation enables efficient validation of analytical results and facilitates the extension of Revan-based metrics to larger and more complex graph families. The findings underscore the potential of Revan indices as powerful structural descriptors in mathematical chemistry and network theory, with promising applications in quantitative modeling, cheminformatics, and the broader field of graph-based molecular design.

Keywords: Revan index, Quadrilateral snake graph, and Python Program.
AMS(MOS) Subject Classification: 05C05,05C12,05C35.

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1 Introduction

Graph theory is a fundamental branch of mathematics that provides valuable tools for analyzing complex structures, particularly in network science and mathematical chemistry. Among various graph-based metrics, Revan indices, introduced by V. R. Kulli, have emerged as significant indicators of structural properties. These indices, along with their polynomial representations, offer a systematic approach to studying the connectivity and characteristics of different graph families [1]-[4].

The present study focuses on computing the Revan indices and their polynomial counterparts for various forms of quadrilateral snake graphs, including standard, alternate, double, and cycle variations. By deriving explicit mathematical formulations for each graph type, we identify distinct structural patterns and relationships. The results enhance the understanding of topological indices in graph theory, with potential applications in network analysis, molecular modeling, and optimization problems.

A Python-based tool was developed to automate the calculation of Revan indices and associated polynomials in support of this investigation. This implementation enables symbolic manipulation, rapid index generation for any graph size, and efficient pattern recognition in large graph families. It ensures computational accuracy, significantly reduces manual effort, and can be easily adapted to other topological index frameworks.

Furthermore, this study compares the Revan indices with several classical topological indices such as the Wiener, Zagreb, Randic, and ABC indices, highlighting their differences and advantages. The effectiveness of each index is evaluated in applications including drug design, chemical stability prediction, and QSPR/QSAR modeling, emphasizing their sensitivity to variations in vertex and edge degrees. By including this comparative analysis, the Revan indices are positioned as a flexible and analytically robust alternative for both theoretical and applied research.

In recent years, researchers have developed various types of indices that can be categorized as degree-based, eigenvalue-based, eccentricity-based, temperature-based, distance-based, matching and mixed based topological indices. The Zagreb indices of square snake graphs were analyzed by Mahalank et al. [5] to investigate structural features relevant to mathematical chemistry. This approach was later extended by kulli et al. [6], who introduced and computed the Revan indices and their polynomial forms for the same class of graphs. Expanding upon these foundational works, the current study investigates a new family of graphs, namely quadrilateral snake graphs, and examines their Revan indices in standard, alternate, double, and cyclic forms. In addition to obtaining explicit expressions for Revan indices and their polynomials, this work presents a Python-based implementation to automate and validate the computations.

2 Basic Notions and Revan Indices

Graph theory provides the mathematical language used to describe and analyze the structure of complex systems. A simple connected graph $G = (V, E)$ is composed of a finite non-empty set of vertices $V(G)$ and a set of edges $E(G)$. For a vertex $x \in V(G)$, the degree $d_G(x)$ is the number of edges incident to x. The minimum and maximum vertex degrees of G are denoted by $\delta(G)$ and $\Delta(G)$, respectively. All graphs considered in this study are finite, undirected and connected. The Revan vertex degree for each vertex $x \in V(G)$ is defined as

$$r_G(x) = \Delta(G) + \delta(G) - d_G(x). \tag{1}$$

The edge xy denotes the Revan edge connecting the Revan vertices x and y. Various Revan indices, including first, second and third-order indices and their polynomials are computed to assess the quadrilateral snake graph. Two topological indices based on degrees were presented and examined in 1972 [1].
V. R. Kulli[7],[8] introduced first, second and third revan indices as:

$$R_1(G) = \sum_{xy \in E(G)} [r_G(x) + r_G(y)] \tag{2}$$

$$R_2(G) = \sum_{xy \in E(G)} r_G(x) r_G(y) \tag{3}$$

$$R_3(G) = \sum_{xy \in E(G)} |r_G(x) - r_G(y)| \tag{4}$$

In 2018, V. R. Kulli[7],[8] introduced first Revan polynomial, second Revan polynomial and third Revan polynomial of a simple connected graph G as:

$$R_1(G, X) = \sum_{xy \in E(G)} X^{[r_G(x) + r_G(y)]} \tag{5}$$

$$R_2(G, X) = \sum_{xy \in E(G)} X^{[r_G(x) . r_G(y)]} \tag{6}$$

$$R_3(G, X) = \sum_{xy \in E(G)} X^{|r_G(x) - r_G(y)|} \tag{7}$$

where X is a variable, x and y are vertices.
The Revan vertex index and polynomial [7],[8] of a graph G is defined as

$$R_{01}(G) = \sum_{x \in V(G)} r_G(x)^2 \tag{8}$$

$$R_{01}(G, X) = \sum_{x \in V(G)} X^{r_G(x)^2} \tag{9}$$

3 Results and Discussion

3.1 Quadrilateral Snake Graph

A Quadrilateral snake graph (QS_n) is derived from a path $v_1, v_2, v_3, v_4, ..., v_n$ by connecting new vertices u_i and w_i to v_i and v_{i+1} respectively, and then connecting u_i and w_i see Chitra Ramaprakash [9]. let n denote the number of quadrilateral units in the graph. Hence, the Quadrilateral Snake Graph (QS_n) has $|V| = 3n + 1$ vertices and $|E| = 4n$ edges.

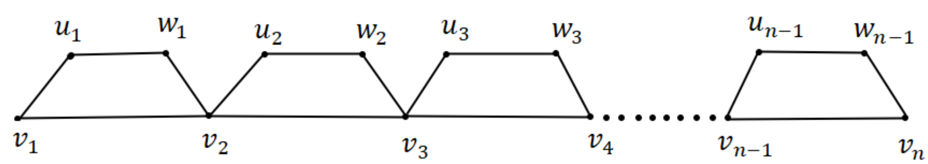

Figure 1: Quadrilateral Snake Graph

Table 1: Vertex partition of QS_n

$d_G(x)$	$\|V\|$
2	2n + 2
4	n - 1

Table 2: Edge partition of QS_n

$(d_G(x), d_G(y))$	$\|E\|$
(2,2)	n + 2
(2,4)	2n
(4,4)	n - 2

Theorem 3.1. *Let G be the Quadrilateral snake graph (QS_n). Then*

$$R_{01}(G) = 36n + 28$$
$$R_{01}(G, X) = (2n + 2)X^{16} + (n - 1)X^4.$$

Proof. Let G be the quadrilateral snake graph (QS_n) and $|V(G)| = 3n + 1$. Thus, we have $\Delta(G) = 4,\ \delta(G) = 2$. The vertex set can be partitioned as,

$$V_1 = \{x \in V(G)|d_G(x) = 2\}, |V_1| = 2n + 2,$$
$$V_2 = \{x \in V(G)|d_G(x) = 4\}, |V_2| = n - 1,$$

Clearly, we find $\Delta(G)+\delta(G)=6$. Thus, $r_G(x)=6-d_G(x)$. There are two types of Revan vertices are found in the quadrilateral snake graph (QS_n):

$$\begin{aligned} RV_1 &= \{x\in V(G)|r_G(x)=4\}, |RV_1|=2n+2,\\ RV_2 &= \{x\in V(G)|r_G(x)=2\}, |RV_2|=n-1, \end{aligned}$$

To find $R_{01}(G)$ and $R_{01}(G,X)$,

$$\begin{aligned} R_{01}(G) &= \sum_{x\in V(G)} r_G(x)^2\\ &= (2n+2)4^2+(n-1)2^2\\ R_{01}(G) &= 36n+28.\\ R_{01}(G,X) &= \sum_{x\in V(G)} X^{r_G(x)^2}\\ &= (2n+2)X^{4^2}+(n-1)X^{2^2}\\ R_{01}(G,X) &= (2n+2)X^{16}+(n-1)X^4. \end{aligned}$$

□

Theorem 3.2. *Let G be the Quadrilateral snake graph (QS_n). Then*

$$\begin{aligned} R_1(G) &= 24n+8\\ R_2(G) &= 36n+24\\ R_3(G) &= 4n\\ R_1(G,X) &= (n+2)X^8+(2n)X^6+(n-2)X^4\\ R_2(G,X) &= (n+2)X^{16}+(2n)X^8+(n-2)X^4\\ R_3(G,X) &= 2n(1+X^2). \end{aligned}$$

Proof. Let G be the quadrilateral snake graph QS_n and $|E(G)|=4n$. Then, we have the following results,

$$\begin{aligned} E_1 &= \{xy\in E(G)|d_G(x)=d_G(y)=2\}, |E_1|=n+2\\ E_2 &= \{xy\in E(G)|d_G(x)=2, d_G(y)=4\}, |E_2|=2n\\ E_3 &= \{xy\in E(G)|d_G(x)=d_G(y)=4\}, |E_3|=n-2 \end{aligned}$$

we have $r_G(x)=\Delta(G)+\delta(G)-d_G(x)$, where $\Delta(G)=4$ and $\delta(G)=2$. Then $r_G(x)=6-d_G(x)$

$$\begin{aligned} RE_1 &= \{xy\in E(G)|r_G(x)=r_G(y)=4\}, |RE_1|=n+2\\ RE_2 &= \{xy\in E(G)|r_G(x)=4, r_G(y)=2\}, |RE_2|=2n\\ RE_3 &= \{xy\in E(G)|r_G(x)=r_G(y)=2\}, |RE_3|=n-2 \end{aligned}$$

Using the revan edge partition of graph QS_n and indices formula, we get

$$\begin{aligned}
R_1(G) &= \sum_{xy\in E(G)} [r_G(x)+r_G(y)] \\
&= (n+2)(4+4)+2n(4+2)+(n-2)(2+2) \\
R_1(G) &= 24n+8. \\
R_2(G) &= \sum_{xy\in E(G)} r_G(x)r_G(y) \\
&= (n+2)16+2n(8)+(n-2)(4) \\
R_2(G) &= 36n+24. \\
R_3(G) &= \sum_{xy\in E(G)} |r_G(x)-r_G(y)| \\
&= (n+2)(0)+2n(2)+(n-2)(0) \\
R_3(G) &= 4n. \\
R_1(G,X) &= \sum_{xy\in E(G)} X^{[r_G(x)+r_G(y)]} \\
&= (n+2)X^{(4+4)}+(2n)X^{(4+2)}+(n-2)X^{(2+2)} \\
R_1(G,X) &= (n+2)X^8+(2n)X^6+(n-2)X^4. \\
R_2(G,X) &= \sum_{xy\in E(G)} X^{[r_G(x).r_G(y)]} \\
&= (n+2)X^{(4\times4)}+(2n)X^{(4\times2)}+(n-2)X^{(2\times2)} \\
R_2(G,X) &= (n+2)X^{16}+(2n)X^8+(n-2)X^4. \\
R_3(G,X) &= \sum_{xy\in E(G)} X^{|r_G(x)-r_G(y)|} \\
&= (n+2)X^0+2n(X^2)+(n-2)X^0 \\
R_3(G,X) &= 2n(1+X^2).
\end{aligned}$$

□

Example: For $n = 2$ in the Quadrilateral Snake Graph (QS_n), we have $|V| = 7$ vertices and $|E| = 8$ edges. Substituting $n = 2$ in Theorems 3.1 and 3.2.

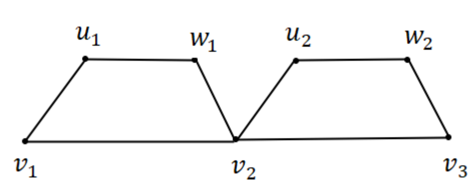

Figure 2: Quadrilateral snake graph (QS_2)

The Revan indices for the snake graph are computed in detail in Theorem 3.1 and

Theorem 3.2. For all other graphs, only their Revan vertex and edge partitions and corresponding diagrams are provided, as the derivations follow in a similar manner.

3.2 Alternating Quadrilateral Snake Graph

An Alternate Quadrilateral snake graph is derived from a path $v_1, v_2, v_3, v_4, ..., v_n$ by connecting new vertices u_i and w_i to v_i and v_{i+1}(alternatively) respectively, and then connecting u_i and w_i. It is denoted by AQS_n see Chitra Ramaprakash [9]. let n denote the number of alternating quadrilateral units in the graph. Hence, the Alternating Quadrilateral Snake Graph (AQS_n) has $|V| = 4n + 4$ vertices and $|E| = 5n + 4$ edges.

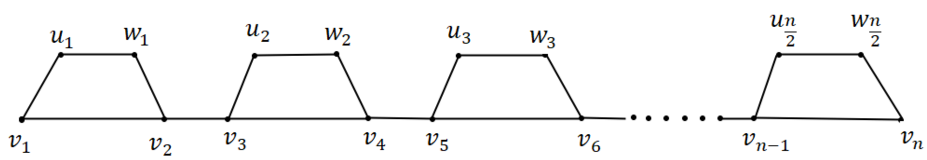

Figure 3: Alternating Quadrilateral Snake Graph

Table 3: Vertex partition of AQS_n

$d_G(x)$	$\|V\|$
2	2n + 4
3	2n

Table 4: Edge partition of AQS_n

$(d_G(x), d_G(y))$	$\|E\|$
(2,2)	n + 3
(2,3)	2n + 2
(3,3)	2n - 1

Theorem 3.3. *Let G be the alternating quadrilateral snake graph (AQS_n). Then*

$$R_{01}(G) = 26n + 36$$
$$R_{01}(G, X) = (2n + 4)X^9 + (2n)X^4.$$

Theorem 3.4. *Let G be the alternating quadrilateral snake graph (AQS_n). Then*

$$\begin{aligned}
R_1(G) &= 24(n+1)\\
R_2(G) &= 29n+35\\
R_3(G) &= 2n+2\\
R_1(G,X) &= (n+3)X^6+(2n+2)X^5+(2n-1)X^4\\
R_2(G,X) &= (n+3)X^9+(2n+2)X^6+(2n-1)X^4\\
R_3(G,X) &= 3n+2+(2n+2)X.
\end{aligned}$$

Example: For $n=1$ in the Alternating Quadrilateral Snake Graph (AQS_n), we have $|V|=8$ vertices and $|E|=9$ edges. Substituting $n=1$ in Theorems 3.3 and 3.4.

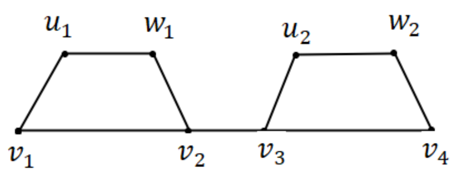

Figure 4: Alternate Quadrilateral snake graph (AQS_1)

3.3 Double Quadrilateral Snake Graph

A Double Quadrilateral snake graph consists of two quadrilateral snakes that have a common path and is denoted by DQS_n see Chitra Ramaprakash [9]. let n denote the number of double quadrilateral units in the graph. Hence, the Double Quadrilateral Snake Graph (DQS_n) has $|V|=5n+1$ vertices and $|E|=7n$ edges.

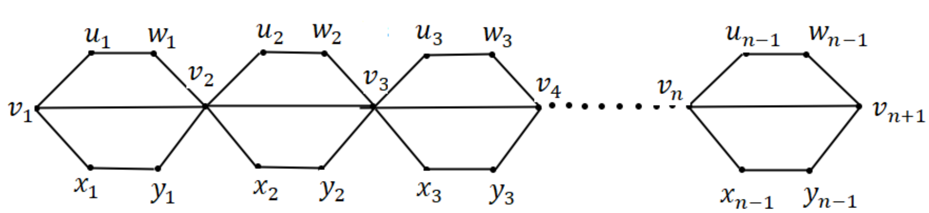

Figure 5: Double Quadrilateral Snake Graph

Theorem 3.5. *Let G be the double quadrilateral snake graph (DQS_n). Then*

$$\begin{aligned}
R_{01}(G) &= 148n+46\\
R_{01}(G,X) &= (4n)X^{36}+2X^{25}+(n-1)X^4.
\end{aligned}$$

Table 5: Vertex partition of DQS_n

$d_G(x)$	$\|V\|$
2	4n
3	2
6	n - 1

Table 6: Edge partition of DQS_n

$(d_G(x), d_G(y))$	$\|E\|$
(2,2)	2n
(2,3)	4
(2,6)	4n - 4
(3,6)	2
(6,6)	n - 2

Theorem 3.6. *Let G be the double quadrilateral snake graph (DQS_n). Then*

$$\begin{aligned} R_1(G) &= 60n + 18 \\ R_2(G) &= 124n + 84 \\ R_3(G) &= 16n - 6 \\ R_1(G, X) &= (2n)X^{12} + 4X^{11} + (4n-4)X^8 + 2X^7 + (n-2)X^4 \\ R_2(G, X) &= (2n)X^{36} + 4X^{30} + (4n-4)X^{12} + 2X^{10} + (n-2)X^4 \\ R_3(G, X) &= 3n + 4X + (4n-4)X^4 + 2X^3 - 2. \end{aligned}$$

Example: For $n = 3$ in the Double Quadrilateral Snake Graph (DQS_n), we have $|V| = 16$ vertices and $|E| = 21$ edges. Substituting $n = 3$ in Theorems 3.5 and 3.6.

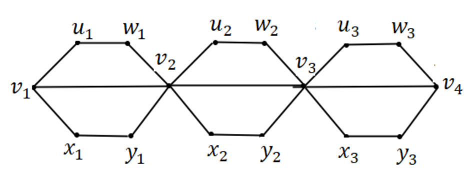

Figure 6: Double Quadrilateral snake graph (DQS_3)

3.4 Alternating Double Quadrilateral Snake Graph

An Alternate Double Quadrilateral snake graph consists of two alternate quadrilateral snakes that have a common path and is denoted by $ADQS_n$ see Chitra Ramaprakash [9].

let n denote the number of alternating double quadrilateral units in the graph. Hence, the Alternating Double Quadrilateral Snake Graph ($ADQS_n$) has $|V| = 6n + 6$ vertices and $|E| = 8n + 7$ edges.

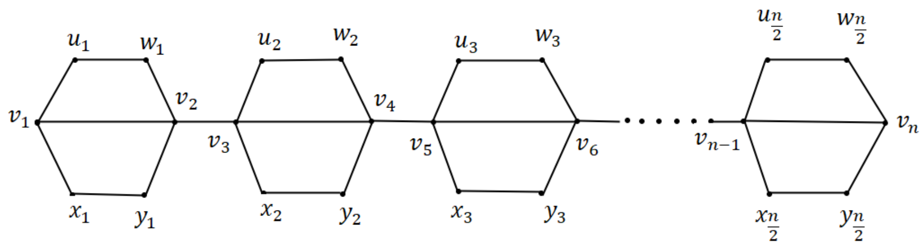

Figure 7: Alternating Double Quadrilateral Snake Graph

Table 7: Vertex partition of $ADQS_n$

$d_G(x)$	$\|V\|$
2	4n + 4
3	2
4	2n

Table 8: Edge partition of $ADQS_n$

$(d_G(x), d_G(y))$	$\|E\|$
(2,2)	2n + 2
(2,3)	4
(2,4)	4n
(3,4)	2
(4,4)	2n - 1

Theorem 3.7. *Let G be the alternating double quadrilateral snake graph ($ADQS_n$). Then*

$$\begin{aligned} R_{01}(G) &= 72n + 82 \\ R_{01}(G, X) &= (4n + 4)X^{16} + 2X^9 + 2nX^4. \end{aligned}$$

Theorem 3.8. *Let G be the alternating double quadrilateral snake graph $(ADQS_n)$. Then*

$$\begin{aligned}
R_1(G) &= 48n + 50\\
R_2(G) &= 72n + 88\\
R_3(G) &= 8n + 6\\
R_1(G, X) &= (2n + 2)X^8 + 4X^7 + (4n)X^6 + 2X^5 + (2n - 1)X^4\\
R_2(G, X) &= (2n + 2)X^{16} + 4X^{12} + (4n)X^8 + 2X^6 + (2n - 1)X^4\\
R_3(G, X) &= 4n + 1 + 6X + (4n)X^2.
\end{aligned}$$

Example: For $n = 1$ in the Alternating Double Quadrilateral Snake Graph $(ADQS_n)$, we have $|V| = 12$ vertices and $|E| = 15$ edges. Substituting $n = 1$ in Theorems 3.7 and 3.8.

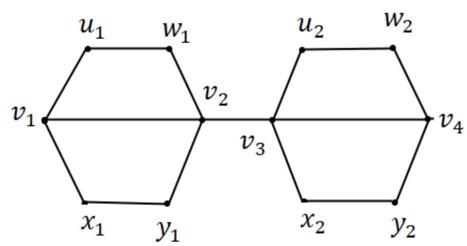

Figure 8: Alternate Double Quadrilateral snake graph $(ADQS_1)$

3.5 Cycle Quadrilateral Snake Graph

A Cycle Quadrilateral snake graph is derived from a cycle $v_1, v_2, v_3, v_4, ..., v_n$ by connecting new vertices u_i and w_i to v_i and v_{i+1} respectively and then connecting u_i and w_i. It is denoted by CQS_n. let n denote the number of cycle quadrilateral units in the graph. Hence, the Cycle Quadrilateral Snake Graph (CQS_n) has $|V| = 3n$ vertices and $|E| = 4n$ edges.

Table 9: Vertex partition of CQS_n

$d_G(x)$	$\|V\|$
2	2n
4	n

Theorem 3.9. *Let G be the cycle quadrilateral snake graph (CQS_n). Then*

$$\begin{aligned}
R_{01}(G) &= 36n\\
R_{01}(G, X) &= (2n)X^{16} + nX^4.
\end{aligned}$$

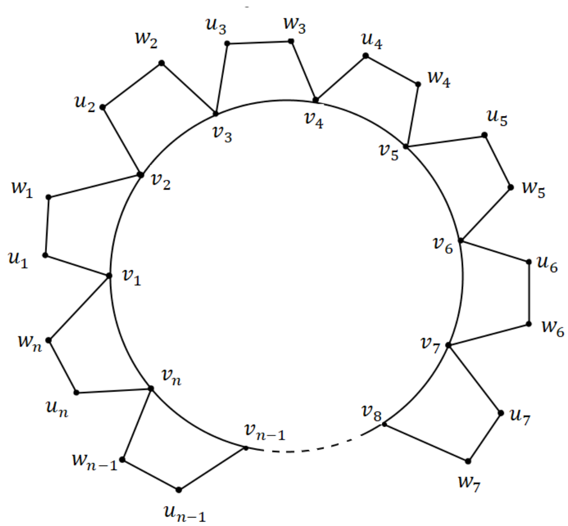

Figure 9: Cycle Quadrilateral Snake Graph

Table 10: Edge partition of CQS_n

$(d_G(x), d_G(y))$	$\|E\|$
(2,2)	n
(2,4)	2n
(4,4)	n

Theorem 3.10. *Let G be the cycle quadrilateral snake graph (CQS_n). Then*

$$\begin{aligned} R_1(G) &= 24n \\ R_2(G) &= 36n \\ R_3(G) &= 4n \\ R_1(G,X) &= nX^8 + (2n)X^6 + nX^4 \\ R_2(G,X) &= nX^{16} + (2n)X^8 + nX^4 \\ R_3(G,X) &= 2n(1+X^2). \end{aligned}$$

4 Python-Based Implementation

Graph theory and mathematical chemistry have rapidly advanced in recent years, and the integration of computational techniques has become essential for analyzing large and complex molecular structures. In this study, a Python-based implementation was developed to automate the computation of Revan indices and their corresponding polynomial expressions for different families of quadrilateral snake graphs. Using this implementation, users can automatically generate standard, alternate, double, and cycle quadrilateral snake graphs and compute the first, second, and third Revan indices along with their associated polynomial forms.The script is modular, scalable, and capable of efficiently processing graphs with a high level of structural complexity. To evaluate its computational performance, the program records the runtime for each graph size and compares the computed results with analytical formulas derived in the theoretical sections. The runtime results show an almost linear increase with respect to the number of quadrilateral units n, demonstrating that the algorithm is computationally efficient and well optimized. The analytical and computed values show complete agreement, confirming the accuracy and reliability of the developed implementation.The output data, including vertex and edge counts, computed Revan indices, polynomial coefficients, analytical comparisons, and runtime information, are automatically saved in an Excel file, which has been provided as supplementary material for reference and verification. This computational automation significantly reduces manual effort, eliminates calculation errors, and improves reproducibility and precision of graph-theoretical research.

5 Application of Revan Topological Indices and Quadrilateral Snake Graphs

Topological indices are effective numerical descriptors that convert a compound's molecular structure into a measurable mathematical form. These indices are widely used in Quantitative Structure–Property Relationship (QSPR) and Quantitative Structure–Activity Relationship (QSAR) studies to establish relationships between molecular structure and experimentally observed physicochemical or biological properties. They play an essential role in the early stages of virtual screening and compound prioritization in modern drug design. When a drug molecule is represented as a molecular graph, with atoms as vertices and bonds as edges, topological indices such as the Revan and Hyper-Revan indices capture key structural characteristics including connectivity, branching, and atomic irregularity. These structural features often correlate with important pharmacological properties such as solubility, stability, bioavailability, and binding affinity. The process of building QSPR/QSAR models typically begins with the computation of these topological indices for a dataset of molecules, followed by regression or machine-learning analysis to identify statistical correlations or predictive equations. In comparison with many classical indices, the Revan family of indices provides a higher-resolution representation of molecular topology because of its degree-dependent and polynomial formulations. This makes Revan indices particularly suitable for QSPR/QSAR modeling, as they can sensitively reflect minor structural variations that influence molecular behavior. Topological indices are generally applied after the structural data of a molecule are known but before experimental synthesis or biological testing, enabling researchers to computationally filter large compound libraries and prioritize molecules with desirable predicted characteristics.

The present study extends this concept by deriving analytical expressions of revan indices for quadrilateral snake graphs (QS_n) and their variants. These graph structures effectively model the chain-like and cyclic frameworks commonly found in organic and drug-like molecules. The computed Revan indices and their polynomial forms from QSn graphs can be directly used as molecular descriptors in QSPR/QSAR models to quantify structural parameters such as connectivity, branching, and irregularity. Because the derived equations express index values as a function of graph size (n), they simulate the behavior of molecules with varying chain lengths or repeating structural units, providing scalable descriptors for complex molecular systems. In practical applications, these QSn-based Revan indices can serve as input variables for regression and machine-learning models predicting molecular properties such as solubility, lipophilicity ($logP$), or binding affinity. The results from these theoretical computations can also be integrated with Multi-Criteria Decision-Making (MCDM) techniques such as TOPSIS or AHP to rank or prioritize compounds according to multiple predicted properties. This combined strategy links the mathematical findings of the present study with real-world computational drug design, thereby enhancing the accuracy, interpretability, and efficiency of QSPR/QSAR-based decision-making processes. Beyond pharmaceutical research, quadrilateral snake graphs also find applications in nanotechnology, materials science, and communication network analysis. Their repetitive, grid like topology serves as a useful model for nanostructures, polymeric backbones, and lattice-based carbon frameworks such as graphene derivatives. In computer and electrical engineering, similar graph architectures are employed for routing optimization, circuit design, and parallel processing interconnection networks, where the quadrilateral pattern supports efficient data flow and fault tolerance. Consequently, the mathematical formulations and revan index relations established in this work provide a versatile foundation applicable not only to molecular modeling but also to broader fields involving complex network structures and nanoscale materials.

6 Conclusion

This research comprehensively investigated the revan indices and their polynomial representations across various types of quadrilateral snake graphs. The study systematically analyzed the structural characteristics of the standard, alternate, double, and cycle forms, deriving explicit mathematical formulations for their corresponding revan indices and polynomials. The results demonstrate that these indices effectively capture subtle topological variations within graph families, particularly in differentiating vertex degrees and edge interactions. Through the derivation of analytical equations, the degree-based connectivity and structural relationships of each graph type were clearly established. In addition, a python-based computational framework was implemented for the automated calculation of revan indices, enhancing the scalability, accuracy, and reproducibility of the analysis. Furthermore, the study emphasizes the applicability of revan-based topological measures in molecular property prediction and QSPR/QSAR modeling. By comparing these indices with classical descriptors such as the Wiener and Zagreb indices, the work demonstrates the superior structural sensitivity and descriptive power of the Revan family. The overall findings highlight both the theoretical depth and the practical relevance of revan indices, offering a robust foundation for their future application in cheminformatics, drug design, and molecular modeling.

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