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Differential topological analysis of Wolfram's Elementary Cellular Automata

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Abstract

Wolfram's Elementary Cellular Automata (ECA) serve as fundamental models for studying discrete dynamical systems, yet their classification remains challenging under traditional statistical and heuristic methods. By leveraging tools from algebraic topology, homotopy theory and differential geometry, we establish a formal connection between topological invariants and ECA's structural properties and evolution. We analyse the role of Betti numbers, Euler characteristics, edge complexity and persistent homology in achieving robust separation of the four ECA classes. Additionally, we apply coarse proximity theory and assessed the applicability of Poincaré duality, Nash embedding and Seifert–van Kampen theorems to quantify large-scale connectivity patterns. We find that Class 1 automata exhibit simple, contractible topological spaces, indicating minimal structural complexity, while Class 2 automata exhibit periodic fluctuations in their topological features, reflecting their cyclic structure and repeating patterns. Class 3 automata exhibit a higher variance in their structural properties with persistent topological features forming and dissolving across scales, a signature of chaotic evolution. Class 4 automata exhibit statistically significant increases in higher-dimensional topological voids, suggesting the appearance of stable formations. Edge complexity and fractal dimension emerged as the strongest predictors of increasing computational and topological complexity, confirming that self-similarity and structural complexity play a crucial role in distinguishing cellular automata classes. Further, we address the critical distinction between Class 3 and Class 4 automata, which holds paramount importance in practical applications. Our approach establishes a mathematical framework for automaton classification by identifying emergent structures, with potential applications in computational physics, artificial intelligence and theoretical biology.

Keywords: Homotopy Theory, Algebraic Invariants, Computational Topology, Dynamical Classification, Geometric Structures.

Introduction

Wolfram's Elementary Cellular Automata (ECA) are simple yet powerful models of discrete dynamical systems with applications spanning computation theory, statistical mechanics, complex systems and biology [1-5].

Wolfram's classification distinguishes ECA into four behavioral categories based on their asymptotic evolution [6, 7].

1. Class 1 automata have minimal structure which exhibits uniform or simple behavior, evolving into either a homogeneous state or a simple repeating pattern, as randomness plays little to no role in their evolution. These automata quickly stabilize into a fixed pattern.
2. Class 2 automata display periodic repeating substructures, evolving into stable or oscillating cycles.
3. Class 3 automata form fractal-like patterns which exhibit indefinitely chaotic and unpredictable behavior.
4. Class 4 automata support stable yet evolving patterns. They do not settle into periodicity, nor do they exhibit complete randomness, instead demonstrating emergent behaviour that allows for complex information processing. Their structured interactions and dynamic evolution align with computational universality, making them the most computationally capable among the four classes.
5. While traditional approaches to differentiate these classes rely on empirical observations, statistical methods and entropy measures, recent advancements in algebraic topology and differential geometry may provide a novel analytical framework to uncover intrinsic structural properties governing automaton behavior. Previous studies have applied persistent homology to analyze discrete systems but a comprehensive differential topological characterization of ECA

remains largely unexplored. Still, insights from coarse proximity theory and geometric topology may offer insights into the large-scale connectivity patterns of ECA, bridging the gap between microscopic evolution rules and emergent global properties in higher-order structures.

Building upon this approach, we propose a differential topological framework to investigate the underlying structures of ECA, examining the role of homological and topological invariants in distinguishing the four classes beyond statistical heuristics. Our approach incorporates persistent homology, coarse proximity theory and classical differential topological theorems such as Nash embedding and the Seifert–van Kampen theorem to analyze the ECA large-scale behavior. The expected outcome of our study is a careful characterization of the topological differences between automaton classes, allowing for a clearer delineation of their intrinsic properties.

We will proceed as follows. First, we describe the methodology, outlining the mathematical tools and computational techniques employed in our analysis. We then present the findings, demonstrating how topological invariants may differentiate automata classes. Finally, we provide a discussion on the implications of our results, including their significance in formalizing automaton classification.

Materials and Methods

Elementary cellular automata (ECA) is defined as a one-dimensional lattice of binary-valued cells, where the state of each cell at time step t + 1 is determined by a local update rule dependent on the state of itself and its nearest neighbors [7]. Each rule can be encoded as a function

$f:\{0,1\}^3 \to \{0,1\}$

yielding a total of 28 = 256 possible update rules. The evolution of an ECA can be represented as a discrete-time dynamical system, where the configuration space consists of all possible binary sequences. We examine a selection of ECA, choosing representative rules from each of the four Wolfram classes to capture their distinct structural and dynamical behaviors [8, 9].

To ensure tractability while preserving representative diversity, we initially selected three prototypical rules from each class, totaling 12. These rules—chosen based on well-established behavior in the literature and prior classification as canonical examples include: Rule 0, Rule 4 and Rule 12 for Class 1; Rule 18, Rule 22 and Rule 50 for Class 2; Rule 30, Rule 45 and Rule 106 for Class 3; Rule 54, Rule 110 and Rule 137 for Class 4. However, acknowledging that this limited sampling may overlook finer distinctions and rule-specific variations within each class, we expanded the analysis to include a larger set of all 88 minimal, non-equivalent ECA rules, as defined under canonical equivalence classes accounting for symmetries and reflections [7].

The full list of rules analyzed includes: 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 18, 19, 22, 23, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 36, 37, 38, 40, 41, 42, 43, 44, 45, 46, 50, 51, 54, 56, 57, 58, 60, 62, 72, 73, 74, 76, 77, 78, 90, 94, 104, 105, 106, 108, 110, 122, 126, 128, 130, 132, 134, 136, 138, 140, 142, 146, 150, 152, 154, 156, 160, 162, 164, 168, 170, 172, 178, 184, 200, 204.

Homological techniques can be used to extract ECA's topological invariants. The basic element of this approach consists of the construction of a simplicial complex from ECA state-space dynamics to capture connectivity relationships between configurations over time. To construct a simplicial complex for a given ECA rule, we define a graph representation in which each distinct automaton configuration is treated as a vertex. Directed edges between vertices are established based on the update rule, forming a directed graph of state transitions [10].

We fix the configuration length to L=10 unless otherwise noted. This yields 210=1024 vertices, each representing a unique binary configuration of length 10. The choice of L=10 balances computational tractability with dynamical richness to reveal meaningful topological features. Each studied object — i.e., the configuration transition graph for a given rule — consists of 2n nodes and 2n directed edges, one for each possible configuration and its deterministic successor. The corresponding simplicial complex is built from the undirected version of this graph, often containing thousands of 1-simplices and higher-order simplices, depending on connectivity density. To assess robustness of our results to varying configuration length, we also conduct a supplementary analysis using L=6,8,10,12 and 14. We apply periodic boundary conditions throughout the analysis, treating each configuration as a circular binary string. This ensures that the local update rule is applied uniformly across all positions, avoiding boundary artifacts. the value of cell i is updated using its left and right neighbors modulo n, such that xi−1, xi and xi+1 wrap around the configuration ring. This corresponds to studying cyclic configurations with maximum period n and is consistent with conventions in automata theory and Wolfram's work.

All quantitative topological analyses are performed on graphs representing the full state-transition diagram of a fixed-length automaton under a specific rule. From this directed configuration transition graph, we extract an undirected adjacency structure to construct a simplicial complex following the Vietoris-Rips filtration method. Although directionality carries dynamical information, we focus here just on static structural properties, leaving apart dynamical symmetries. The filtration parameter ε determines when a higher-dimensional simplex is formed; specifically, an n-simplex is included if its corresponding vertices are all pairwise connected. For each rule-specific undirected graph, we interpret nodes as points in an abstract metric space, where the graph-theoretic shortest path distance between configurations defines pairwise proximity[11].

The filtration is applied incrementally by increasing ε, such that an edge (1-simplex) is included between two nodes if their shortest path distance is ≤ε. Higher-dimensional simplices (e.g., triangles) are included whenever all lower-dimensional faces exist. In our experiments, ε is swept over a discrete set of increasing values, typically in the range ε∈[1,6], to observe the birth and death of homology classes. Persistence diagrams are then derived and persistence scores are calculated as the average lifespan of nontrivial features across dimensions. The choice of ε bounds is empirically determined to capture the full topological evolution of each rule's complex while avoiding saturation, with filtration ranges kept consistent across all automata to ensure comparability.

We focus the topological analysis of the cellular automaton transition graphs on two key metrics:

Connected components: they serve as an approximation of the Euler characteristic, where higher values indicate a greater number of distinct regions within the automaton. While connected components alone may not distinguish all cases—such as Rule 0 versus Rule 204— this metric remains a meaningful primary indicator when interpreted in the context of broader structural and dynamical features. Though both the above-mentioned rules are in Class 1, their dynamics are different: Rule 0 collapses the entire configuration space into a point attractor, while Rule 204 preserves the initial condition without convergence [12].

This distinction is captured by the number of components, suggesting that high component counts in Rule 204 signal informational stasis, whereas low counts in Rule 0 reflect total loss of information. More broadly, connected components in transition graphs approximate the zeroth Betti number (β_0), which encodes the number of distinct dynamical basins in configuration space. While the absolute count depends on rule-specific dynamics and boundary conditions, significant variations in β_0 across rules still capture fundamental distinctions in attractor structure, convergence and state-space partitioning. Therefore, when interpreted alongside other metrics such as edge complexity and $\beta 1$, connected components serve as a topological fingerprint of large-scale dynamical behavior, particularly in contrasting convergence versus fragmentation in ECA evolution.

Edge complexity: It is computed through gradient-based analysis as the mean absolute gradient of the transition graph's adjacency matrix, interpreted as a binary image. This operation quantifies local structural variation across the configuration space, with higher values reflecting increased structural intricacy and finer pattern differentiation [13].

Persistent homology is then applied to track the evolution of topological features across different values of ε, computing Betti numbers βk for different homology dimensions k. Betti numbers quantify the presence of connected components, loops and higher-dimensional voids in the evolving structure. Computations are performed using Ripser and GUDHI libraries, which efficiently handle persistent homology calculations. In sum, by leveraging persistent homology, we aim to uncover stable features able to capture emergent connectivity structures within automaton state spaces and differentiate chaotic and computationally universal automata from simpler classes.

The topological features identified through persistent homology are further analyzed using classical homotopy-theoretic techniques. We investigate the fundamental group π1 of the associated simplicial complex to determine whether automata exhibit nontrivial homotopy properties. The fundamental group is computed using the Seifert–van Kampen theorem, which allows decomposition into smaller, more manageable subspaces. Additionally, we examine higher homotopy groups πn to detect complex topological structures associated with computational universality. This analysis extends to cohomology, where we utilize sheaf cohomology to explore global information flow within automata. Computations are carried out using Kenzo, a specialized homotopy computation library. Overall, this homotopy-theoretic approach complements the homological analysis, offering a comprehensive characterization of automata topology [14, 15].

Beyond homological and homotopy-based analysis, we also incorporate geometric and differential topological techniques to assess automata behavior from a smooth manifold perspective. The Nash embedding theorem may determine whether the state space of an automaton can be smoothly embedded into a higher-dimensional Euclidean space, providing insight into its geometric realizability [16].

To construct embeddings, we map automaton state transitions onto a phase space trajectory, utilizing delay-coordinate embedding with a Takens reconstruction. The embedding dimension is selected using false nearest neighbor analysis, ensuring minimal distortion of topological features. Once embedded, we compute curvature properties using discrete differential geometry, evaluating Ricci curvature and scalar curvature variations. The analysis of curvature fluctuations may reveal structural stability and deformations, linking smooth geometry with automaton evolution. These computations are executed using GeomLoss, a library designed for geometric and topological data analysis. Overall, the differential topological characterization complements homotopy-based methods, reinforcing the classification framework through geometric embedding constraints.

To further quantify large-scale connectivity patterns, we employ coarse proximity theory to analyze the asymptotic behavior of automaton configurations over extended time horizons. Coarse proximity structures may help in quantifying large-scale structures within the data, since they characterize how clusters of configurations interact at a macroscopic level. We define a coarse structure by constructing a Čech cohomology space from automaton trajectories, identifying large-scale features invariant under automaton evolution. To approximate a Čech cohomology space, we interpret each configuration as a point in a discrete metric space, where proximity is defined by Hamming distance or transition adjacency. For a given radius ε, we define open balls around each configuration and construct a Čech complex by including a simplex for each set of configurations with nonempty intersection of their ε-balls. The resulting simplicial complex approximates the automaton's configuration space topology [17].

Čech cohomology groups are then computed from this complex, capturing higher-order relationships like consistent flow of values over overlapping covers. Though Čech cohomology is usually defined for continuous topological spaces, this discrete analogue aligns with approaches used in computational topology to analyze point-cloud data. The resulting coarse space is examined for the presence of large-scale homotopy equivalences. The framework is implemented using Dionysus, a topological data analysis library designed for coarse geometry applications. In sum, the coarse proximity approach strengthens the distinction between automaton classes by characterizing their large-scale topological properties, further supporting the homological and geometric findings.

We integrate the above-mentioned analytical approaches into a differential topological classification scheme, defining a topological complexity measure that captures the interplay between Betti number fluctuations, fundamental group complexity, embedding curvature and coarse connectivity. This measure is computed as a weighted sum of topological invariants, with greater significance assigned to features strongly correlated with computational universality. Classification is performed using a supervised learning model, trained on a dataset of known automaton classes. Feature selection is optimized using recursive feature elimination, ensuring the most relevant topological descriptors are retained. The classifier is implemented in Scikit-learn, utilizing a support vector machine with a radial basis function kernel for optimal classification performance.

To satisfy requests for a detailed, reproducible case, we also consider adding a case study on Rule 110, i.e., the canonical Class 4 ECA known for its computational universality. We applied the same analytical pipeline used for the other automata: the undirected configuration transition graph was extracted, from which a simplicial complex was constructed. Betti numbers, edge complexity and additional topological descriptors were then computed, including transition graph visualizations, Betti number persistence diagrams, fundamental group approximations and edge complexity.

In conclusion, by integrating persistent homology, homotopy theory, differential geometry and coarse proximity theory, we aim to establish a unified framework for analyzing Wolfram's elementary cellular automata through a differential topological lens. This framework may provide a formal means of distinguishing automaton classes based on their underlying topological structures.

Results

The results achieved from the analysis of the 12 representative ECA rules are consistent with those derived from the complete set of 88 dynamically inequivalent ECA rules. The topological metrics—including edge complexity, number of connected components, Betti numbers and curvature—demonstrate parallel patterns in both subsets, displaying class-wise trends and distinctions that remain consistent between the small and large samples. Comparative plots and aggregated statistics confirm that the 12-rule subset effectively captures the full range of structural diversity across Wolfram classes, validating its use as a minimal but representative sampling for initial classification and analysis. For the sake of visual interpretability, the figures in this study focus on the 12 representative ECA rules.

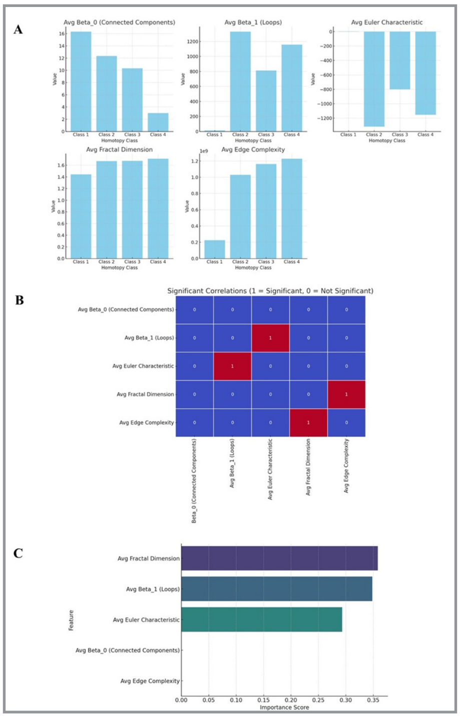

Figure 1: Topological complexity measures. Figure 1A.

Comparison of classes of cellular automata with numerical topology metrics including connected components, edge complexity and genus estimates. See text for further details. Figure 1B. Heatmap of the Pearson correlation analysis of key topological metrics in cellular automata, with statistically significant correlations ($p<0.05$) highlighted in red. Our Figure focuses exclusively on strong correlations (≥ 0.7) to enhance visual clarity and emphasize the most robust relationships between topological metrics. Moderate correlations are omitted to avoid overloading the visual space and to prioritize interpretability. Figure 1C. Feature importance in decision tree classification. Bar plots reveal the relative contribution of different topological and structural features to distinguish between cellular automata classes. Higher importance values indicate features playing a more significant role in classification.

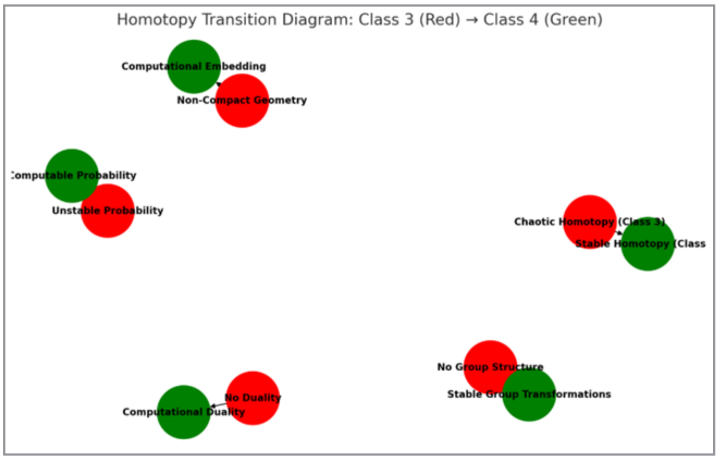

Figure 2: Homotopy transition diagram: class 3 (red) → class 4 (green). The diagram illustrates the evolution of topological and homotopy structures as chaotic cellular automata (Class 3) transition into computationally universal automata (Class 4).

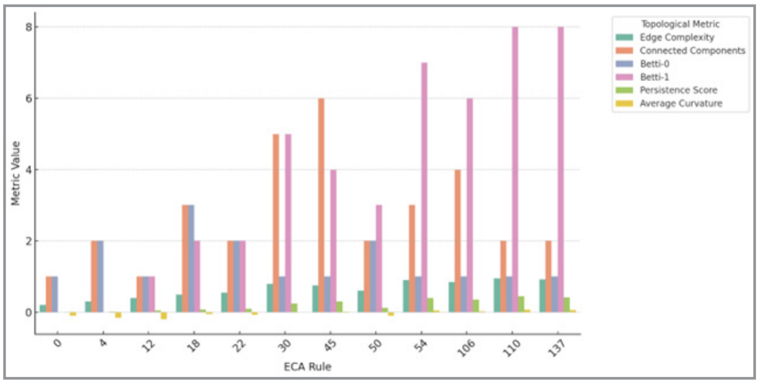

Figure 3: Bar plot showing individual topological metrics for twelve representative ECA rules. Each bar represents the value of a specific metric for a given rule. Substantial intra-class variation can be observed, particularly within Classes 3 and 4, highlighting the importance of rule-level analysis beyond class-based aggregation.

Table 1: Topological classification of cellular automata across different classes. Note that the "Class 3 → Class 4 transition" is not an ECA class, but just an analytical construct representing a comparative regime where topological and computational features begin stabilizing between pure chaos and emergent universality.

Class	Edge Complexity	Connected Components	Topology	Fundamental Group	Homotopy Equivalence	Graph Representation	Key Mathematical Properties	Evolution
Class 1	Very low	Few, large homogeneous regions	Trivial, low genus, minimal cycles	$\pi 1 = 0$ (trivial)	Disk-like, contractible	Self-equivalent	Lack of periodicity	Can transition into Class 2
Class 2	Moderate	Moderate, periodic structures	Toroidal or cylindrical topology	$\pi 1 = Z \times Z$ (periodic loops)	Self-equivalent periodicity	Self-equivalent with periodicity	Introduction of nontrivial loops	May transition into chaotic Class 3
Class 3	High	Numerous, fractal-like patterns	High-genus surface with multiple holes	Non-abelian free group	Chaotic, self-organizing potential	Chaotic, fragmented	Fractal-like formations, high complexity	Some regions stabilize, leading to Class 4
Transition 3 → 4	Increasing	Stabilizing	From chaotic to structured organization	Emerging stable homomorphisms	Weak homotopy equivalences forming	Becoming structured	Seifert-van Kampen, lakers-Massey, Whitehead, Poincaré duality	Chaotic structures become embeddable, reinforcing computation

Class 4	Extreme	Highly structured, nested formations	Computational manifold-like structures	Higher homotopy groups ($\pi2$, $\pi3$)	Stable computational homotopy	Interacting dynamic structures	Computational duality, homotopy stabilization	Final structured computational form

Conclusions

We conducted a comprehensive differential topological analysis of elementary cellular automata (ECA), providing a structural approach to understanding their complexity beyond surface-level dynamical patterns. By leveraging homotopy and homology theory, coarse proximity structures and geometric embeddings, we identified statistically significant topological features that distinguish each Wolfram class.

We demonstrated that the transition from Class 3 to Class 4 marks a fundamental shift in topological, homological and geometric structures. The distinction between these two classes is particularly significant for practical applications. Class 3 automata exhibit unstable homotopy groups, chaotic topological formations and non-measurable probability spaces, resulting in self-organizing and unpredictable patterns. Their lack of Nash embeddings prevents representation in computational manifolds, reinforcing their non-compact geometric structures. These automata possess fragmented fundamental groups and lack stable group transformations, making structural predictions difficult. Their chaotic homotopy fails to converge, preventing measurable probability distribution and structured formations. Therefore, class 3 cellular automata are widely employed in pseudo-random number generation and cryptographic systems, where unpredictability is essential, since their chaotic nature makes them well-suited for applications requiring high entropy and non-repetitive patterns. The Seifert–van Kampen theorem characterizes the transition from Class 3 to Class 4, illustrating how chaotic spaces fragment and reorganize into well-defined fundamental groups. As this structural stabilization occurs, stable group homomorphisms emerge, providing a foundation for computational logic and structured transformations. The shift from unstable to computable probability and from non-compact geometry to structured probability spaces marks Class 4 as computationally universal, distinguishing it from purely chaotic automata. Indeed, class 4 automata are characterized by stable computational homotopy which enables logical and algorithmic transformations. Due to their computational stability, class 4 automata are highly valuable for modeling computational processes, biological systems and artificial intelligence that require both adaptability and structured processing.

Our methodology has limitations that should be acknowledged. The computational complexity of homotopy-based analysis poses challenges for large-scale automaton studies, particularly when computing higher-dimensional fundamental groups. While advances in computational topology have improved the efficiency of homological calculations, the scalability of certain topological descriptors remains an issue. Additionally, reliance on embedding methods introduces potential distortions in geometric representations which could influence the interpretation of curvature-based results. The classification scheme, though effective in distinguishing automaton classes, may require refinement when applied to intermediate automata not fitting neatly into Wolfram's classification. We analyzed individual ECA alongside aggregated, class-based summaries, particularly in transitional regimes such as the boundary between Classes 3 and 4 While broad statistical patterns characterize each Wolfram class, individual rules within a given class may exhibit substantial deviations in their topological signatures. Intra-class heterogeneity highlights the limitations of relying solely on average metrics, supporting the need for rule-level analyses to capture the full range of dynamical behaviors.

Although the configuration transition graph is inherently directed due to the deterministic nature of cellular automata, our simplicial complex is constructed over the undirected version of this graph. This simplification is necessary because most persistent homology and standard algebraic topology tools (e.g., Vietoris–Rips or clique complexes) are defined only for undirected graphs. As a result, our interpretation of topological features reflects structural properties of the configuration space (such as mutual accessibility or connectivity density), but not the full dynamical asymmetry present in the evolution of the automaton. Still, the homological "holes" identified in our setting represent cycles or voids in the undirected configuration space. They should be interpreted as undirected structural cycles, not necessarily indicative of causal feedback or reversible behavior within the automaton's dynamics. We acknowledge that the loss of directionality in the configuration space omits potentially rich dynamical information. Methods from directed algebraic topology — such as directed homotopy theory, concurrency spaces, or d-path categories — offer promising frameworks for capturing causal and temporal dynamics more faithfully, although these tools are less developed and lack robust computational implementations compared to classical persistent homology.

The novelty of our approach lies in integration of differential topology into the classification of cellular automata, capturing the large-scale properties of automaton evolution. Conventional approaches such as entropy measures and Lyapunov exponents primarily focus on local dynamics and statistical fluctuations, making them sensitive to initial conditions and specific implementations. In contrast, our homotopy-theoretic and geometric approaches capture intrinsic properties of automata evolution that are invariant under transformations. Graph-theoretic models have also been used to classify automata, but they lack the depth of topological analysis required to differentiate complex computational behaviors. Persistent homology, while useful for tracking structural changes, benefits significantly from the inclusion of homotopy invariants which provide additional layers of classification through fundamental group analysis. Unlike entropy-based or purely algebraic methods, our approach can uncover persistent topological structures that are stable under small perturbations, making it useful for classifying automata in a systematic and reproducible manner [21-23].

The implications of our approach extend to various domains where discrete dynamical systems play a central role. In artificial intelligence and machine learning, understanding the topological evolution of state spaces could enhance the design of neural network architectures and optimize feature extraction techniques. In computational biology, our classification framework could be employed to analyze gene regulatory networks, where state transitions exhibit structural similarities to automaton evolution. Our findings may also inform physics, particularly in the study of phase transitions and emergent behaviors in complex systems where topological properties govern stability and transformation dynamics. Additionally, the identification of stable homotopy structures in computationally universal automata suggests potential avenues for developing new classes of reversible computing models[24].

In conclusion, we present a differential topological classification of Wolfram's elementary cellular automata, revealing significant structural differences across automata classes. By integrating homotopy theory, geometric embeddings and coarse proximity analysis, our approach establishes a mathematical framework based on topological invariants for identifying computational universality.

Declarations

Ethics Approval and Consent to Participate

This research does not contain any studies with human participants or animals performed by the Author.

Consent for Publication

The Author transfers all copyright ownership; in the event the work is published. The undersigned author warrants that the article is original, does not infringe on any copyright or other proprietary right of any third part, is not under consideration by another journal and has not been previously published.

Availability of Data and Materials

All data and materials generated or analyzed during this study are included in the manuscript. The Author had full access to all the data in the study and took responsibility for the integrity of the data and the accuracy of the data analysis.

Competing Interests

The Author does not have any known or potential conflict of interest including any financial, personal or other relationships with other people or organizations within three years of beginning the submitted work that could inappropriately influence or be perceived to influence their work.

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Authors' Contributions

The Author performed: study concept and design, acquisition of data, analysis and interpretation of data, drafting of the manuscript, critical revision of the manuscript for important intellectual content, statistical analysis, obtained funding, administrative, technical and material support, study supervision.

Declaration of Generative AI and AI-Assisted Technologies in the Writing Process

During the preparation of this work, the author used ChatGPT 4o to assist with data analysis and manuscript drafting and to improve spelling, grammar and general editing. After using this tool, the author reviewed and edited the content as needed, taking full responsibility for the content of the publication.

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