



INTERNATIONAL JOURNAL OF TRENDS IN EMERGING RESEARCH AND DEVELOPMENT

INTERNATIONAL JOURNAL OF TRENDS IN EMERGING RESEARCH AND DEVELOPMENT

Volume 4; Issue 1; 2026; Page No. 178-182

Received: 08-10-2025

Accepted: 18-12-2025

Published: 22-01-2026

Graph-Theoretic and Persistent Homology Methods for Multiscale Topological Data Analysis

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DOI: <https://doi.org/10.5281/zenodo.22658763>

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Abstract

Graph theory and topological data analysis provide complementary mathematical approaches for studying the structural organization of complex data. Graph theory represents relationships through vertices and edges, whereas topological data analysis extends this representation to higher-dimensional structures capable of identifying connected components, cycles, cavities, and persistent geometric patterns. The present paper examines the integration of graph-theoretic methods with persistent homology for multiscale topological data analysis. Particular attention is given to graph construction, simplicial complexes, Vietoris–Rips complexes, filtrations, homology groups, Betti numbers, persistence diagrams, barcodes, and the birth and death of topological features. The paper adopts a theoretical, descriptive, and analytical methodology based on mathematical concepts and developments reported up to 2025. It explains how graph structures form the one-dimensional foundation of simplicial complexes and how persistent homology extends conventional graph connectivity by investigating topological features across multiple spatial or functional scales. Applications in image analysis, biological networks, medical imaging, brain connectivity, point-cloud analysis, and machine learning are discussed. The analysis indicates that persistent homology provides a robust framework for distinguishing significant structural patterns from short-lived fluctuations or noise. The study concludes that combining graph theory with persistent homology provides an effective mathematical framework for multiscale analysis of complex data and offers substantial potential for computational topology, artificial intelligence, and scientific data analysis.

Keywords: Graph Theory, Persistent Homology, Topological Data Analysis, Simplicial Complex, Vietoris–Rips Complex, Filtration, Betti Numbers, Persistence Diagram, Multiscale Analysis

1. Introduction

Graph theory is a fundamental branch of discrete mathematics concerned with the representation of objects and relationships. A graph is generally expressed as

$$G = (V, E),$$

where V represents a set of vertices and E represents edges connecting selected pairs of vertices. Graph-based representations are useful because they simplify complex systems into discrete structures that can be analyzed using connectivity, paths, cycles, components, centrality, clustering, spanning trees, cut vertices, and other mathematical properties.

Topology, on the other hand, investigates structural properties that remain meaningful under continuous transformations. Important topological concepts include connectedness, compactness, continuity, holes, cavities, homology, and higher-dimensional relationships. Previous graph-theoretic work shows that graphs can effectively model selected topological relationships, but an ordinary graph mainly records pairwise relationships and may fail to preserve higher-order topological information.

Topological Data Analysis, commonly known as TDA, provides a modern mathematical framework for studying the shape and organization of data. Rather than relying only on averages, correlations, distances, or local features, TDA investigates global structural patterns. A central technique in

TDA is persistent homology, which examines the appearance and disappearance of topological features across multiple scales.

The transition from graph theory to persistent homology is natural. Data points may first be represented as vertices in a graph, with edges introduced according to a similarity or distance condition. Higher-order relationships can then be incorporated through simplicial complexes. As the distance threshold changes, new edges and simplices appear, producing a filtration. Persistent homology tracks connected components, loops, and higher-dimensional cavities through this filtration.

Earlier work on simplicial complexes already establishes graphs as the one-dimensional foundation of richer topological structures and identifies persistent homology as a method for tracking topological features across scales. The present paper develops this relationship as its central theme.

2. Objectives of the study

The major objectives of the study are:

1. To examine the relationship between graph theory and topological data analysis.
2. To explain the construction of simplicial complexes from graph-based data.
3. To analyze filtrations and Vietoris–Rips complexes in multiscale data analysis.
4. To examine homology groups and Betti numbers as measures of topological structure.
5. To explain persistent homology through birth, death, persistence diagrams, and barcodes.
6. To study applications of persistent homology in image, biological, medical, and network data.
7. To examine the integration of persistent homology with machine learning developments reported up to 2025.

3. Research Methodology

The present study adopts a theoretical, descriptive, and analytical research methodology. It is based on established mathematical concepts from graph theory, algebraic topology, computational topology, simplicial topology, and topological data analysis.

The study does not use fabricated experimental datasets or artificial performance values. Instead, mathematical definitions, constructions, relationships, and contemporary applications are examined conceptually. This approach follows the pattern of the attached studies, which use theoretical analysis rather than artificial empirical results.

The literature and developments considered in this paper are restricted to material available up to 2025.

4. Graph Representation of Complex Data

Many forms of data can be represented naturally as graphs. Suppose a dataset consists of points.

$$X = \{x_1, x_2, \dots, x_n\}.$$

Each point may be represented as a vertex. An edge between x_i and x_j may be introduced when the distance between the two points is below a selected threshold ϵ :

$$d(x_i, x_j) \leq \epsilon.$$

4.1 This produces a proximity graph

At small values of ϵ , the graph may contain many isolated vertices or disconnected components. As ϵ increases, more edges appear and separate components begin to merge. This changing connectivity structure provides the foundation for multiscale topological analysis.

Graphs therefore provide an initial discrete representation, but they remain limited to pairwise relations. To study higher-order structure, a richer object is required.

5. Simplicial Complexes

A simplicial complex extends graph theory by incorporating interactions involving more than two vertices.

A vertex is a 0-simplex, an edge is a 1-simplex, a filled triangle is a 2-simplex, and a tetrahedron is a 3-simplex.

Thus, a graph may be viewed as the one-dimensional skeleton of a simplicial complex. This distinction is important because a triangle in a graph may represent only three pairwise edges, whereas a filled 2-simplex represents a genuine higher-order relation. The attached work on topological networks emphasizes precisely this difference between pairwise and higher-order structures.

Simplicial complexes allow mathematical analysis of structures that ordinary graphs cannot fully represent, especially holes, cavities, and multi-way interactions.

6. Vietoris–Rips Complex

The Vietoris–Rips complex is one of the most widely used constructions in TDA.

Given a set of points and a scale parameter ϵ , vertices are connected whenever the distance between them is at most ϵ . Whenever a set of vertices forms a complete clique in the resulting graph, the clique is filled with the corresponding simplex.

The Vietoris–Rips complex at scale ϵ may be denoted by

$$VR_\epsilon(X).$$

As ϵ increases, the complex becomes progressively richer:

$$VR_{\epsilon_1}(X) \subseteq VR_{\epsilon_2}(X) \subseteq \dots$$

for

$$\epsilon_1 < \epsilon_2 < \dots.$$

This nested sequence forms a filtration. The attached work identifies Vietoris–Rips construction as an important bridge from graphs to persistent topology.

7. Filtration and Multiscale Analysis

A filtration is a sequence of nested topological structures:

$$K_0 \subseteq K_1 \subseteq K_2 \subseteq \dots \subseteq K_m.$$

At early stages, the structure may contain isolated points. Later, edges form, components merge, loops appear, and eventually holes may be filled.

This scale-dependent behavior is important because structural features may exist only temporarily. Some

features may appear because of noise, while others may persist across a wide range of parameter values. Persistent homology is designed to distinguish these behaviors.

8. Homology and Betti Numbers

Homology is an algebraic method for identifying topological holes.

The k -th homology group is generally denoted by H_k .

Its dimension is represented by the k -th Betti number:

$$\beta_k = \dim H_k.$$

The principal interpretations are

β_0 = number of connected components,

β_1 = number of independent one-dimensional loops,

and

β_2 = number of independent one-dimensional loops

Graph theory is especially effective for analyzing connected components and cycles, but simplicial homology is more precise because a graph cycle may be filled by a higher-dimensional simplex and therefore may not represent a genuine topological hole. This distinction is emphasized in the attached simplicial-complex study.

9. Persistent Homology

Persistent homology studies how homological features change through a filtration.

A topological feature has a birth time, representing the scale at which it first appears, and a death time, representing the scale at which it disappears or merges into another structure.

The persistence of a feature is

$$P = d - b,$$

where b denotes birth and d denotes death.

Features with short persistence may represent noise or small-scale irregularities. Features with long persistence are often interpreted as more stable structural characteristics.

This does not mean that every long-lived feature is automatically scientifically meaningful, but persistence provides a principled method for distinguishing relatively stable topological patterns from transient ones.

10. Persistence Barcodes

A barcode represents each topological feature as an interval

$$[b_i, d_i).$$

Each interval begins when a feature appears and ends when it disappears.

Long bars indicate persistent structures, whereas short bars correspond to short-lived structures.

Separate barcodes may be produced for different homological dimensions, such as H_0 , H_1 , and H_2 .

Barcodes therefore provide an intuitive visual representation of multiscale topology.

11. Persistence Diagrams

A persistence diagram represents topological features as points.

$$(b_i, d_i)$$

in a two-dimensional plane.

The horizontal coordinate denotes birth and the vertical coordinate denotes death. Features close to the diagonal

$$b = d$$

have short persistence. Features far from the diagonal persist over a wider range of scales.

Persistence diagrams are useful because they convert complex topological information into a compact geometric representation that can be compared across datasets.

12. Zero-Dimensional Persistent Homology

Zero-dimensional persistent homology focuses on connected components.

At the beginning of a filtration, each vertex may form its own connected component. As edges appear, components merge.

Thus, H_0 provides a direct connection between graph theory and persistent homology.

Classical graph algorithms determine connected components at one selected threshold. Persistent homology extends this by examining how connectivity changes across an entire range of thresholds.

This makes persistent H_0 particularly useful for clustering and hierarchical structural analysis.

13. One-Dimensional Persistent Homology

One-dimensional persistent homology identifies loop-like structures.

As edges and triangles appear, loops may be created and later filled.

A loop born at one threshold may persist for several filtration levels before disappearing.

This allows TDA to distinguish persistent cyclic structures from local graph cycles. Previous work in the attached papers notes that graph cycles and genuine topological holes are not necessarily identical.

14. Applications in Digital and Medical Imaging

Persistent homology has significant applications in digital image analysis.

Images can be converted into graphs or cubical complexes. Connected components, loops, cavities, and shape characteristics may then be studied across intensity or spatial thresholds.

Medical imaging is particularly suitable for this approach because anatomical structures often possess complex connectivity and shape. Blood vessels, neurons, airways, tumors, retinal networks, and cellular structures can contain diagnostically relevant topological information.

The attached digital-topology paper identifies medical imaging, vascular networks, neuronal structures, tumors, retinal systems, and tissue organization as important application areas.

Persistent homology provides information that may

complement conventional intensity, texture, or local feature analysis.

15. Applications in Biological and Network Data

Biological systems frequently contain both pairwise and higher-order relationships.

Brain connectivity, protein interactions, metabolic networks, cellular systems, and neural structures can be represented using graphs and simplicial complexes.

Persistent homology can examine how network structure changes when edge thresholds are varied. This is particularly useful when network connections are weighted by correlation, similarity, distance, or interaction strength.

Instead of selecting only one arbitrary network threshold, persistent methods examine the entire range.

16. Persistent Homology and Machine Learning

Recent developments up to 2025 increasingly combine topological information with machine learning.

Persistence diagrams and barcodes can be transformed into numerical feature representations and incorporated into classification or prediction models.

Persistent-homology-based information has also been combined with graph convolutional networks and deep-learning architectures, particularly in medical and biological applications. The attached paper on digital topology explicitly notes integration of persistent homology with graph neural networks and topology-aware learning as a major contemporary direction.

Topology-aware models are particularly useful when conventional prediction accuracy does not guarantee structural correctness. For example, a segmentation may achieve high pixel-level accuracy while incorrectly breaking one connected vessel into two pieces.

17. Advantages

The integrated graph-theoretic and persistent-homology approach provides several advantages.

First, graph theory offers simple and computationally manageable representations of complex relationships.

Second, simplicial complexes extend these models to higher-order structures.

Third, persistent homology avoids dependence on a single threshold by studying structures across multiple scales.

Fourth, persistence can distinguish stable features from short-lived structural variations.

Fifth, the framework can be applied to networks, images, point clouds, biological data, and scientific datasets.

Finally, it provides a mathematical link between pure topology and modern computational data analysis.

18. Limitations

Persistent homology also has limitations.

Large datasets can generate extremely large simplicial complexes. A dense graph may contain a very large number of cliques, increasing computational cost.

The selection of filtration function can influence results.

Noise may create artificial components or loops.

Interpretation of persistence diagrams is not always straightforward.

Furthermore, topological information alone may not capture all statistically or scientifically relevant characteristics.

Therefore, persistent homology should complement rather than automatically replace conventional analytical methods.

19. Major Findings

The theoretical analysis produces several major findings.

Graph theory provides the basic discrete representation for many TDA procedures. Simplicial complexes extend pairwise graph relationships into higher-dimensional structures. Vietoris–Rips complexes provide a systematic method for building multiscale simplicial representations from proximity graphs.

Persistent homology extends static graph analysis by examining connected components, cycles, and cavities across filtration scales. Betti numbers provide algebraic measures of these structures, while persistence diagrams and barcodes summarize their duration.

The analysis also shows that graph cycles should not automatically be equated with topological holes. Higher-dimensional simplices must be considered.

Finally, research directions reported through 2025 indicate increasing integration of persistent homology with medical imaging, biological network analysis, graph neural networks, and topology-aware artificial intelligence.

20. Future Scope

Future research may focus on efficient persistent-homology algorithms for large graphs and three-dimensional datasets. Multiparameter persistent homology represents another important direction because real datasets often depend on more than one filtration variable.

Dynamic persistent homology may be useful for temporal networks whose vertices, edges, and higher-dimensional interactions change over time.

The integration of persistent homology with explainable artificial intelligence, graph neural networks, Transformer architectures, medical imaging, neuroscience, remote sensing, and biological morphology also offers considerable future potential.

21. Conclusion

Graph theory and persistent homology together provide a powerful mathematical framework for multiscale topological data analysis. Graphs offer a natural way to represent pairwise relationships, connectivity, paths, and components, while simplicial complexes extend these representations to higher-order interactions.

Persistent homology provides an additional level of analysis by examining how topological features appear, persist, merge, and disappear as the scale parameter changes. Through Betti numbers, barcodes, and persistence diagrams, it becomes possible to quantify connected components, loops, and cavities over multiple levels of resolution.

The framework is particularly important because complex data rarely possesses meaningful structure at only one scale. A feature that appears at one threshold may disappear immediately, while another may remain stable over a large range. Persistent homology provides a rigorous means of distinguishing these patterns.

The study therefore concludes that graph-theoretic representations serve as the computational foundation of multiscale topology, while persistent homology provides the mathematical mechanism for evaluating structural stability

across scales. Their integration offers significant applications in image analysis, network science, biological systems, medical imaging, computational topology, and machine learning.

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