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Emerging Trends in Graph-Based Network Science: A Critical Review of Algorithms, Artificial Intelligence and Complex Network Applications

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ABSTRACT
Graph-based network science has evolved from its traditional foundations in discrete mathematics into an interdisciplinary field that integrates graph algorithms, network analysis, machine learning, artificial intelligence, knowledge representation, and temporal modelling. This study critically reviews this evolution, with particular emphasis on the transition from classical graph structures and algorithms to Graph Neural Networks (GNNs), knowledge graphs, dynamic graphs, and spatiotemporal graph learning. The study adopts a critical literature review approach, examining relevant academic research primarily published during 2020–2026 while incorporating foundational studies to establish the theoretical development of graph theory. The review focuses on five interconnected areas: graph-theoretical foundations and network structures, graph algorithms and network analytics, graph machine learning and GNNs, knowledge graphs and semantic reasoning, and dynamic and spatiotemporal graph learning. The findings indicate that traditional graph theory continues to provide the structural and mathematical foundation for contemporary network analysis, while GNNs enable data-driven learning from complex relational structures. Knowledge graphs further enhance graph intelligence by integrating semantic relationships and reasoning, whereas dynamic and spatiotemporal models provide more realistic representations of continuously evolving networks. However, the review identifies significant theoretical, computational and practical challenges, including scalability, interpretability, data quality, computational complexity, temporal evolution, heterogeneous network structures, privacy and reproducibility. A major gap identified is the fragmented treatment of classical graph theory, graph algorithms, graph learning, knowledge representation and dynamic network analysis. To address this gap, the study proposes an integrated graph-intelligence framework connecting mathematical graph foundations with algorithms, GNNs, knowledge graphs, dynamic and spatiotemporal learning, and intelligent decision support. The study concludes that future graph-based network science should emphasise scalable, explainable, adaptive and semantically informed graph-learning systems capable of transforming complex and continuously evolving relational data into reliable and actionable decision support.....

Keywords: Graph Theory, Network Science, Graph Neural Networks, Graph Machine Learning, Knowledge Graphs, Dynamic Graphs, Network Analytics, Artificial Intelligence..

INTRODUCTION

Graph theory has traditionally been regarded as an important area of discrete mathematics concerned with the representation of relationships between objects. A graph generally consists of vertices and edges, where vertices represent entities and edges describe relationships, interactions or connections among those entities. The origins of graph theory are commonly associated with Euler's solution to the Seven Bridges of Königsberg problem. Since then, the field has developed from a relatively specialized mathematical discipline into a foundation for analysing complex systems in science, engineering, computing and social research. The increasing availability of interconnected and high-dimensional data has substantially expanded the importance of graph-based modelling. Modern datasets rarely consist only of independent observations. Instead, information is frequently connected through social relationships, transportation routes, financial transactions, communication links, biological interactions, supply chains and digital platforms. Consequently, analysing individual observations independently can overlook the structural relationships that determine how information, resources, behaviour and risks move through a system.

Earlier literature has extensively documented classical graph structures, algorithms, colouring, labelling, domination, connectivity and network applications. The uploaded review similarly demonstrates that graph theory has been applied across computer science, transportation, communication, environmental science, biology and other disciplines. However, the contemporary research environment is increasingly shaped by artificial intelligence and data-intensive computational methods. This development has transformed the role of graphs from being primarily mathematical representations to becoming learnable structures.

One of the most important developments in this transition is Graph Neural Networks. GNNs are designed to learn functions from graph-structured data and have become an important approach for predictive modelling involving relationships among entities. Corso et al. (2024) describe GNNs as mathematical models capable of learning functions over graphs, with applications across different domains. Similarly, recent reviews identify GNN architectures, graph convolution, attention mechanisms, message passing and representation learning as major developments in graph-based artificial intelligence. The evolution of graph analytics has also created increasing interest in knowledge graphs. Knowledge graphs represent entities and relationships in a structured graph format and have become an important component of knowledge representation and artificial intelligence. Ji et al. examined knowledge graph representation learning, knowledge acquisition, graph completion, temporal knowledge graphs and knowledge-aware applications. More recent research has extended this area by combining GNNs with knowledge graph reasoning to improve the ability of systems to infer missing information and support intelligent applications.

Therefore, the contemporary study of graph-based systems requires a broader perspective than conventional graph theory alone. It requires integration among mathematical graph structures, network measures, algorithms, machine learning, artificial intelligence, knowledge representation and temporal modelling. Against this background, the present paper critically reviews the transition from traditional graph theory to graph-based network science, focusing particularly on emerging computational and artificial intelligence-based approaches. Rather than simply cataloguing graph types and applications, the study examines how graph research has evolved, what new methodological developments have emerged, what limitations remain and where future research should concentrate.

2. Conceptual Foundation of Graph-Based Network Science

2.1 Graphs as representations of relationships

A graph can be represented as:

G= (V, E)

where represents a set of vertices and represents a set of edges connecting pairs of vertices.

In a social network, individuals may represent vertices and relationships between individuals may represent edges. In transportation, locations can represent vertices while roads or railway connections represent edges. In biological networks, proteins or genes can represent vertices and biological interactions can represent edges.

The principal advantage of graph representation is therefore its ability to model relationships rather than merely individual entities.

2.2 Structural characteristics

Graph structures can differ according to direction, weight, connectivity and complexity. Important structures include directed, undirected, weighted, bipartite, complete, connected, disconnected, planar and tree-based graphs.

The uploaded source identifies a broad range of classical graph structures, including simple graphs, directed graphs, weighted graphs, multigraphs, complete graphs, bipartite graphs, regular graphs, connected graphs, planar graphs, trees, Eulerian graphs and Hamiltonian graphs.

These structures provide the mathematical foundation for modern network modelling.

2.3 Connectivity

Connectivity measures describe how strongly different parts of a network are connected. A highly connected network may facilitate the rapid movement of information, resources or individuals, whereas weak connectivity can create isolated components.

Connectivity has particular importance in transportation, communication, ecological networks and infrastructure planning. Earlier research has also used graph-theoretical approaches to understand landscape connectivity and the movement of organisms through fragmented environments.

2.4 Centrality

Centrality identifies structurally important vertices within a network. Common measures include:

Degree centrality

Betweenness centrality

Closeness centrality

Eigenvector centrality

Centrality is useful because not all nodes contribute equally to network functioning. A highly connected individual in a social network, for example, may influence information diffusion more strongly than a peripheral participant.

2.5 Graph algorithms

Classical graph algorithms include breadth-first search, depth-first search, shortest-path algorithms and minimum spanning tree approaches. These algorithms support routing, scheduling, network design, resource allocation and optimisation. The literature reviewed in the uploaded source repeatedly identifies these algorithms as important applications of graph theory in computer science and engineering.

3. From Graph Theory to Network Science

The historical development of graph theory demonstrates a movement from mathematical abstraction toward applied network analysis.

Traditional graph theory was primarily concerned with proving mathematical properties. Research on graph colouring, labelling, domination, distinguishing indices and structural properties illustrates this theoretical orientation. For example, the source review discusses probabilistic approaches, graph labelling and distinguishing indices as examples of mathematically focused research. This shift is significant because it changes the role of the graph from a mathematical object to an analytical representation of a real-world system.

4. Evolution of Graph Algorithms

Graph algorithms remain fundamental to network analysis. Their development can broadly be understood in four stages.

Stage 1: Classical algorithmic analysis

Early graph algorithms focused on traversal, paths, connectivity and optimisation. These methods remain important because they provide deterministic and interpretable solutions.

Stage 2: Large-scale network computation

The growth of digital networks created demand for algorithms capable of processing millions or billions of relationships. Scalability therefore became an important research issue.

Stage 3: Probabilistic and statistical network analysis

Researchers increasingly began analysing patterns of network formation, community structures, clustering and structural properties statistically.

Stage 4: Learning-based graph analytics

The latest stage integrates machine learning with graph structures. Instead of manually defining all network rules, models learn representations from the observed graph.

This transition is particularly important because conventional algorithms generally solve explicitly defined problems, whereas machine-learning models can identify complex patterns from data.

5. Graph Neural Networks and Graph Machine Learning

Graph Neural Networks represent one of the most important developments in contemporary graph research.

A conventional neural network assumes that observations can be represented as vectors, matrices or sequences. Graphs, however, are non-Euclidean structures in which relationships between observations are central. GNNs address this problem by allowing information to propagate between connected nodes.

A simplified message-passing process can be represented as:

$hv^{(l+1)}=\sigma(W^{(l)}.AGG(\{h_u^{(l)}:u\in N(v)\}))$

where represents the representation of node , represents its neighbouring nodes, represents an aggregation function, represents learnable parameters and represents an activation function.

Recent literature identifies graph convolutional networks, Graph SAGE, graph attention networks and message-passing architectures as important approaches in GNN research.

6. Knowledge Graphs and Intelligent Information Systems

Knowledge graphs provide a structured framework for representing entities, relationships and information.

A simple knowledge graph can represent:

Person → works for → Organisation

The relational structure allows systems to move beyond isolated records and reason over connected information. Ji et al. identify knowledge graph representation learning, knowledge acquisition, knowledge graph completion, temporal knowledge graphs and knowledge-aware applications as major research themes.

7. Dynamic and Temporal Graphs

One limitation of traditional graph modelling is the assumption that the network is static.

Consider a financial transaction network. The relationship between two entities may exist today but disappear tomorrow. Similarly, social interactions change continuously, traffic conditions vary by time and communication networks experience changing loads.

Dynamic graph research therefore incorporates temporal information.

A dynamic graph can be represented as:

Gt= (Vt, Et)

where the network structure at time may differ from the structure at time.

Recent reviews of dynamic GNNs emphasise that real-world graph structures and node attributes frequently evolve over time. Research therefore increasingly focuses on temporal dependencies, memory mechanisms, adaptive learning and large-scale dynamic networks.

Future graph research should therefore move beyond static snapshots toward continuous and adaptive network modelling.

8. Applications of Graph-Based Network Science

8.1 Social networks

Graph models can represent relationships between individuals, organisations and communities. Applications include:

Community detection

Influence analysis

Information diffusion

Fake-account detection

Recommendation systems

Social influence prediction

8.2 Transportation

Transportation systems can be represented through nodes representing locations and edges representing roads, railway routes or flight connections.

The development of spatiotemporal GNNs provides opportunities to combine network structure with changing traffic conditions.

8.3 Biological systems

Molecular structures, protein interactions and gene networks can naturally be represented as graphs.

The literature has historically demonstrated the usefulness of graph theory in chemistry and biological systems, while contemporary research increasingly integrates graph representation learning and GNNs.

9. Literature Review

Corso et al. (2024) provide a comprehensive examination of Graph Neural Networks (GNNs) and their growing importance in learning from graph-structured data. Their work highlights the ability of GNNs to capture relationships between interconnected entities and generate useful representations for prediction and classification tasks. Unlike conventional machine-learning approaches that generally treat observations independently, GNNs incorporate neighbourhood and relational information into the learning process. The study demonstrates the relevance of GNNs across several scientific and technological domains, including molecular modelling, physical systems and network analysis. However, challenges related to generalisation, computational requirements, data quality and interpretation of model outputs remain important areas for further investigation.

Ji et al. (2022) examined the development of knowledge graphs as a framework for representing entities and their relationships in a structured manner. Their review covers major areas including knowledge representation, knowledge acquisition, knowledge graph completion, representation learning, temporal knowledge graphs and knowledge-aware applications. The study demonstrates that knowledge graphs can support intelligent systems by allowing relationships among entities to be explicitly represented and subsequently used for reasoning and inference. However, knowledge incompleteness, knowledge acquisition and the representation of evolving information remain important challenges. These limitations indicate the need for approaches capable of combining structured knowledge with advanced learning techniques such as GNNs.

Zheng et al. (2025) focus specifically on Dynamic Graph Neural Networks, highlighting an important limitation of conventional graph-learning models: the assumption that graph structures remain static. In many real-world environments, relationships among entities continuously change. Social networks, financial transactions, communication systems and transportation networks are therefore better represented as dynamic structures. Dynamic GNNs attempt to incorporate temporal dependencies, changing topology and evolving node attributes into the learning process. The study indicates that temporal graph learning can provide a more realistic representation of continuously changing systems. However, scalability, heterogeneous information, limited datasets and the computational complexity of modelling evolving networks remain significant challenges.

Recent research on spatiotemporal Graph Neural Networks extends dynamic graph learning by integrating both spatial relationships and temporal dependencies. Such approaches are particularly relevant to transportation, environmental monitoring, healthcare, energy systems and smart-city applications, where network behaviour changes according to both location and time. Spatiotemporal graph models provide an opportunity to capture both the structural dependencies among entities and their changing characteristics over time. However, existing research continues to face challenges related to scalability, model complexity, explainability, data availability, uncertainty and the lack of standardised evaluation procedures. The literature therefore indicates a progressive movement from static graph representations toward dynamic, adaptive and context-sensitive graph intelligence. Collectively, the reviewed studies demonstrate that GNNs, knowledge graphs and dynamic graph models have developed rapidly, but these approaches are frequently examined independently. This fragmentation provides a strong basis for developing an integrated framework connecting graph theory, graph algorithms, graph machine learning, semantic reasoning and temporal network analysis.

10. Methodology

This study adopts a critical literature review approach to examine the evolution of graph theory into contemporary graph-based network science, with particular emphasis on graph algorithms, Graph Neural Networks (GNNs), knowledge graphs, dynamic graphs and spatiotemporal graph learning. Relevant literature was reviewed from peer-reviewed academic sources covering classical graph theory as well as recent developments in graph-based artificial intelligence. The review focused primarily on recent research published during 2020–2026, while foundational studies were considered where necessary to establish the theoretical development of graph theory. The literature was organised thematically around five major areas: graph-theoretical foundations, graph algorithms, graph machine learning, knowledge integration, and temporal/spatiotemporal graph analytics. Studies were examined according to their research focus, methodological approach, major findings and identified limitations. The synthesis was subsequently used to identify recurring research gaps relating to scalability, interpretability, data availability, temporal complexity, heterogeneous networks and the fragmented integration of classical and AI-based graph approaches. Based on this critical synthesis, an integrated conceptual framework was developed to demonstrate how graph structures can progress from basic representation and structural analysis toward intelligent, adaptive and decision-oriented graph analytics. This methodology is consistent with the review-oriented nature of the present study and does not involve primary data collection or empirical hypothesis testing.

11. Research Gap

The review of existing literature indicates that graph-based research has progressed substantially, but important conceptual and methodological gaps remain. First, traditional graph theory and contemporary graph-based artificial intelligence are frequently examined as separate areas, with limited integration between mathematical graph structures and machine-learning approaches. Second, many graph-learning studies continue to rely on static network representations, despite the fact that real-world social, financial, transportation and communication networks continuously evolve over time. The increasing attention to dynamic GNNs demonstrates the need to incorporate temporal changes into graph analysis. Third, although GNNs provide powerful learning capabilities, issues relating to scalability, computational complexity, interpretability and data availability continue to constrain their practical application. Fourth, knowledge graphs, graph learning and temporal modelling are often developed independently, creating a need for greater integration of structural, semantic and temporal information. Finally, spatiotemporal graph research is developing rapidly, but challenges remain concerning representation, scalability, methodological comparison and application across complex real-world systems. Therefore, the major research gap identified in this study is the absence of a unified conceptual framework connecting classical graph theory, graph algorithms, graph machine learning, knowledge graphs, dynamic graph analysis and spatiotemporal learning for intelligent decision support.

11. Research Objectives

To examine the evolution of graph theory from a mathematical foundation to contemporary graph-based network science.

To critically review the development of graph algorithms and graph machine-learning approaches, particularly Graph Neural Networks.

To examine the role of knowledge graphs in integrating semantic relationships and reasoning with graph-based learning.

To analyse the emerging importance of dynamic and spatiotemporal graph models for representing continuously evolving real-world networks.

To identify the major theoretical, computational and practical gaps in existing graph-based research.

12. Findings and Discussion

The review establishes that graph theory has evolved from a mathematical framework concerned primarily with vertices, edges, connectivity, paths, colouring, labelling and other structural properties into a broader interdisciplinary field of graph-based network science. Traditional graph theory provided the fundamental concepts and algorithms required to represent relationships among entities. Over time, these mathematical structures were applied to computer science, transportation, communication systems, biological networks, environmental systems and social networks. The major transformation has occurred with the growth of digital data and interconnected systems, where graphs are increasingly used not merely to describe network structures but also to analyse, predict and optimise complex behaviour. Thus, contemporary network science extends traditional graph theory by combining structural analysis with computational algorithms, statistical techniques, machine learning and artificial intelligence. The evolution can therefore be summarised as mathematical graph theory → applied network analysis → data-driven graph analytics → graph-based artificial intelligence.

The review shows that graph algorithms remain the fundamental computational foundation of graph analysis. Classical methods such as breadth-first search, depth-first search, shortest-path algorithms, clustering and optimisation are useful for solving well-defined network problems. However, the increasing complexity and scale of modern networks have encouraged a transition toward graph machine learning and Graph Neural Networks (GNNs). GNNs are particularly significant because they learn representations by incorporating information from connected neighbouring nodes rather than treating observations as independent. Recent literature demonstrates applications of GNNs in node classification, link prediction, graph classification, recommendation, fraud detection, molecular analysis, transportation and cybersecurity. The major finding is that GNNs represent a shift from rule-based graph analysis toward data-driven relational learning. Nevertheless, scalability, computational cost, interpretability, data requirements and model generalisation remain important limitations. Therefore, future graph algorithms are likely to involve a combination of classical algorithms and learning-based approaches rather than completely replacing traditional methods.

Study demonstrates that knowledge graphs extend graph analysis beyond structural relationships by incorporating semantic information. While conventional graphs primarily identify connections between entities, knowledge graphs can describe the meaning and type of those relationships. For example, relationships such as Customer–purchases–Product, Employee–works for–Organisation and Drug–interacts with–Protein provide structured semantic information. Knowledge graphs therefore support knowledge representation, information integration, graph completion and reasoning. Their integration with GNNs creates an opportunity to combine structured domain knowledge with data-driven representation learning. The major finding is that knowledge graphs can improve the contextual and semantic capabilities of graph-based artificial intelligence, particularly in complex decision environments. However, incomplete knowledge, knowledge acquisition, noisy information, temporal changes and reasoning complexity remain important challenges. Consequently, future graph research should increasingly integrate **graph structure + semantic knowledge + machine learning** rather than considering these components independently.

It finds that static graph models are insufficient for many contemporary applications because real-world networks frequently change over time. Social relationships, financial transactions, traffic networks, communication systems, cybersecurity networks and supply chains can continuously gain or lose nodes and relationships. These models are particularly relevant to transportation, environmental monitoring, healthcare, energy systems and smart-city applications. The major finding is that dynamic and spatiotemporal modelling provides a more realistic representation of evolving network systems than static graph approaches. However, temporal complexity, computational requirements, scalability, heterogeneous information and limited benchmark datasets remain important challenges. The research therefore indicates a clear movement from static graph analysis toward adaptive, dynamic and spatiotemporal graph intelligence.

Study identifies several important gaps. Theoretically, there is still a separation between classical mathematical graph theory and modern graph-based artificial intelligence, with limited integration of structural graph theory, machine learning, semantic reasoning and temporal modelling. Computationally, large-scale graphs create significant challenges related to processing speed, memory requirements, scalability and model complexity. GNNs also face issues such as over-smoothing and limited interpretability. Practically, many studies rely on benchmark datasets and controlled experimental environments rather than continuously changing real-world networks. Data sparsity, missing relationships, heterogeneous graphs, privacy concerns and reproducibility further restrict practical deployment. Another important gap is the limited integration of graph algorithms, GNNs, knowledge graphs and dynamic/spatiotemporal learning within one comprehensive framework. Therefore, the central gap identified by this study is the need for an integrated and scalable graph-intelligence framework that connects mathematical foundations, computational algorithms, artificial intelligence, semantic knowledge and temporal network analysis to produce explainable and actionable decision support.

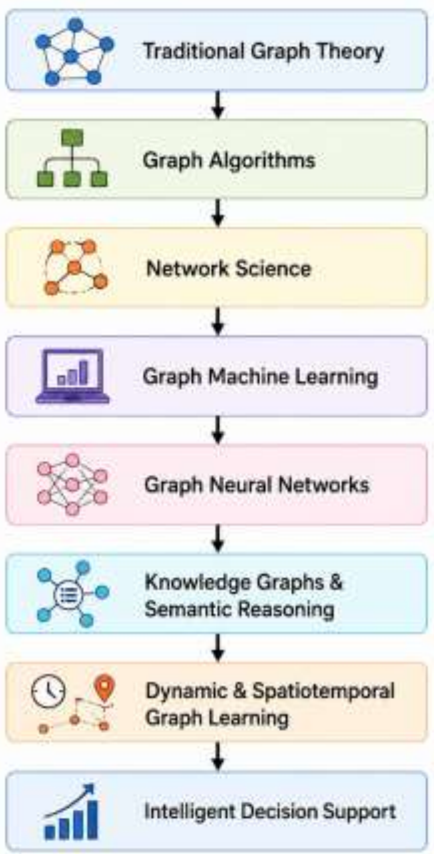

Figure 1: Evolutionary Framework of Graph-Based Network Science and Artificial Intelligence

13. Theoretical Implications

The study contributes theoretically by establishing a conceptual bridge between classical graph theory and contemporary graph-based artificial intelligence. The review demonstrates that traditional graph concepts such as vertices, edges, connectivity, centrality, paths and graph structures continue to provide the mathematical foundation for contemporary network analysis. At the same time, graph machine learning, Graph Neural Networks, knowledge graphs and dynamic graph models extend this foundation by enabling data-driven learning, semantic reasoning and temporal analysis. The proposed framework therefore provides an integrated perspective in which mathematical graph structures, computational algorithms and artificial intelligence are viewed as interconnected stages in the development of graph-based network science. The study further highlights the importance of combining structural, semantic, spatial and temporal information when analysing complex interconnected systems. This integrated perspective can provide a conceptual foundation for future interdisciplinary research connecting mathematics, computer science, artificial intelligence, network science and application-specific domains.

14. Future Research Directions

Future research in graph-based network science should focus on developing explainable, scalable and adaptive Graph Neural Networks (GNNs) capable of processing increasingly large and continuously evolving networks. Greater attention is required toward explainable GNNs that can identify the contribution of important nodes, edges and neighbourhood structures to model predictions, particularly in sensitive domains such as healthcare, finance and cybersecurity. Researchers should also develop large-scale GNN architectures using efficient neighbourhood sampling, graph partitioning, distributed processing and model-compression techniques. Another important direction is dynamic and continuous-time graph learning, which can capture changing relationships in financial transactions, social networks, transportation and communication systems more effectively than static graph models. The integration of knowledge graphs with GNNs and Large Language Models (LLMs) also provides opportunities to combine semantic knowledge, relational learning and natural-language reasoning. Future studies should further investigate multimodal graph learning by integrating text, images, sensor data, geographical information and transactional data to provide richer representations of complex systems. At the same time, privacy-preserving and federated graph learning should be explored to enable collaborative analysis of sensitive and distributed network data while maintaining privacy and security.

Another important research direction is the development of graph-based digital twins and spatiotemporal graph intelligence for real-time modelling and monitoring of complex physical, industrial and urban systems. Future studies can integrate GNNs, knowledge graphs and dynamic graph models with digital-twin environments to support predictive maintenance, infrastructure monitoring, industrial optimisation and real-time decision-making. Spatiotemporal graph models should also be strengthened to capture simultaneous spatial relationships and temporal changes in transportation, environmental, energy and smart-city systems, with greater attention to uncertainty, adaptive relationships and computational efficiency. Graph AI for smart cities represents a particularly promising area because transportation, energy, communication, healthcare and public-service systems are highly interconnected and can benefit from integrated graph-based decision support. Similarly, graph AI can strengthen cybersecurity and fraud detection by identifying suspicious relationships, evolving attack patterns, fraudulent transactions and coordinated activities. Future research in these areas should emphasise real-time anomaly detection, explainability, adversarial robustness, privacy, fairness and highly imbalanced datasets. Overall, future graph research should move toward integrated, intelligent and domain-sensitive frameworks capable of transforming complex and continuously evolving network relationships into reliable and actionable decision support.

15. Practical Implications

From a practical perspective, the proposed framework can guide researchers, organisations and technology developers in selecting appropriate graph-based techniques according to the characteristics of their networks. Classical graph algorithms can be used for routing, traversal, shortest-path analysis and optimisation, while GNNs can support prediction, classification, recommendation and representation learning. Knowledge graphs can enhance semantic representation and reasoning, whereas dynamic and spatiotemporal graph models can be applied to continuously evolving systems. The framework can therefore support practical applications in healthcare, finance, transportation, cybersecurity, biological systems, environmental management, manufacturing and smart cities. Organisations can also use the framework as a roadmap for progressing from basic network representation toward advanced graph-based decision support. However, practical implementation should consider scalability, explainability, data quality, privacy, computational cost and domain-specific requirements.

Conclusion

Graph-based network science has evolved from the mathematical foundations of traditional graph theory into a multidisciplinary field integrating graph algorithms, machine learning, Graph Neural Networks, knowledge graphs, and dynamic and spatiotemporal graph learning. The review demonstrates that these developments have expanded the ability of graph-based approaches to represent, analyse and learn from complex interconnected systems across diverse domains. However, challenges related to scalability, interpretability, data quality, computational complexity, temporal evolution and heterogeneous network structures remain significant. The study therefore proposes an integrated perspective connecting classical graph theory with contemporary graph-based artificial intelligence, providing a pathway from structural representation to intelligent decision support. Future graph research should focus on developing scalable, explainable, adaptive and semantically informed graph-learning frameworks capable of handling continuously evolving real-world networks and transforming complex relational data into reliable and actionable intelligence...

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