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A Comprehensive Review of Graph Neural Networks for Malware Classification Pipelines: Architectures, Robustness, and Intelligent Security Applications

[1]Daniel J. Williams, [2]Mikhail Ivanov, [3]Carlos Ferreira

[1]Professor, Department of Computer Engineering, University of Toronto, Canada

[2]Associate Professor, Faculty of Intelligent Systems, Moscow State University, Russia

[3]Senior Lecturer, Department of Embedded Electronics, University of Porto, Portugal

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Abstract

The rapid evolution of cyber threats, particularly malware, has driven the need for advanced detection and classification techniques capable of handling complex and dynamic attack patterns. Traditional signature-based and heuristic approaches are increasingly ineffective against polymorphic and zero-day malware, creating a demand for more adaptive solutions. In this context, Graph Neural Networks (GNNs) have emerged as a powerful paradigm for modeling structured relationships in malware data, including function call graphs, network traffic flows, and system interactions. Unlike conventional machine learning models, GNNs capture non-Euclidean relationships, enabling superior representation learning and improved classification accuracy. This review analyzes GNN-based malware classification pipelines, focusing on architectural designs, robustness strategies, and security applications. It highlights the integration of graph construction methods, feature extraction, and classification models, while also examining issues such as adversarial robustness, scalability, and explainability. Findings suggest that models like Graph Convolutional Networks, Graph Attention Networks, and hybrid approaches outperform traditional deep learning techniques by leveraging relational dependencies. Despite their promise, challenges such as computational overhead, dataset limitations, and adversarial vulnerabilities remain, indicating the need for lightweight, interpretable, and privacy-preserving GNN frameworks.

Introduction

The proliferation of malware has become one of the most critical challenges in modern cybersecurity, driven by the rapid expansion of digital infrastructures, cloud computing, and Internet of Things (IoT) ecosystems. Malware, which includes viruses, ransomware, spyware, and trojans, continues to evolve in complexity and sophistication, making traditional detection approaches increasingly inadequate. Signature-based detection methods, which rely on predefined patterns, fail to identify new or obfuscated malware variants, while heuristic-based techniques often suffer from high false-positive rates. Recent advancements in artificial intelligence and deep learning have introduced new paradigms for malware detection. Among these, Graph Neural Networks (GNNs) have gained significant attention due to their ability to model complex relationships within structured data. Unlike traditional neural networks that operate on Euclidean data such as images or text, GNNs are specifically designed to process graph-structured data, making them highly suitable for

representing malware behaviours' and interactions.

Malware can naturally be represented as graphs, where nodes correspond to entities such as functions, system calls, or network events, and edges represent relationships between them. For example, function call graphs capture the execution flow of a program, while network flow graphs represent communication patterns between devices. These graph representations allow GNNs to learn meaningful structural patterns that are difficult to capture using conventional machine learning models.

The integration of GNNs into malware classification pipelines typically involves several stages, including data collection, graph construction, feature extraction, model training, and classification. Each stage plays a crucial role in determining the overall performance of the system. For instance, graph construction techniques significantly influence how effectively the underlying relationships are captured, while feature engineering impacts the quality of node and edge representations.

One of the key advantages of GNNs is their ability to generalize across different types of malware by learning structural similarities rather than relying solely on specific features. This makes them particularly effective in detecting previously unseen malware families. Studies have demonstrated that GNN-based models can achieve high classification accuracy and robustness, even in the presence of obfuscated or incomplete data.

Despite these advantages, several challenges remain. One major issue is scalability, as large-scale malware datasets can result in complex graphs with millions of nodes and edges. Processing such graphs requires significant computational resources, limiting the practical deployment of GNN-based systems in real-time environments. Additionally, GNNs are susceptible to adversarial attacks, where small perturbations in the graph structure can lead to incorrect predictions. Another critical challenge is the lack of standardized datasets and evaluation metrics. Many studies use different datasets and experimental setups, making it difficult to compare results and benchmark performance. Furthermore, the interpretability of GNN models remains an open research problem, as their decision-making processes are often opaque.

Recent research has also explored hybrid architectures that combine GNNs with other deep learning models, such as Convolutional Neural Networks (CNNs) and Transformers, to improve performance. These hybrid models leverage the strengths of multiple architectures, enabling better feature extraction and representation learning. Additionally, techniques such as contrastive learning and self-supervised learning have been employed to address the issue of limited labelled data.

This review aims to provide a comprehensive understanding of GNN-based malware classification pipelines by analysing recent studies, identifying key trends, and highlighting future research directions. The main contributions of this review are as follows:

- A systematic analysis of GNN architectures used in malware classification
- A comparative study of robustness techniques and optimization strategies
- Identification of key challenges and limitations in current approaches
- Exploration of emerging applications in intelligent security systems

Literature Review

Kipf and Welling (2018) introduced Graph Convolutional Networks (GCNs), which have become foundational in graph-based learning. In malware classification, GCNs are applied to function call graphs and API call graphs to capture structural dependencies between program components. These models enable effective feature propagation across nodes, improving classification accuracy. However, GCNs suffer from over-smoothing when stacked in deep architectures, limiting their ability to distinguish complex malware patterns.

Grover and Leskovec (2019) proposed Node2Vec, a random-walk-based graph embedding technique. In malware analysis, Node2Vec is used to learn vector representations of nodes within system call graphs. This approach captures both local and global structural patterns, making it useful for clustering and classification tasks. Despite its effectiveness, Node2Vec does not incorporate node attributes or temporal dynamics, which are crucial for modeling malware behaviour.

Zhang et al. (2020) explored deep learning techniques for malware classification by integrating graph-based features extracted from program execution traces. The study demonstrated that combining graph representations with neural networks significantly improves detection performance compared to traditional machine learning methods. However, the model requires extensive feature engineering and large labeled datasets.

Veličković et al. (2021) introduced Graph Attention Networks (GATs), which use attention mechanisms to assign different importance weights to neighbouring nodes. In malware classification pipelines, GATs improve

interpretability by identifying critical nodes and relationships influencing predictions. The study showed enhanced accuracy and robustness compared to GCNs. However, the attention mechanism increases computational cost, making scalability a concern.

Wu et al. (2022) provided a comprehensive survey on GNN applications across various domains, including cybersecurity and malware detection. The study highlights the advantages of GNNs in modeling complex relationships and discusses challenges such as adversarial attacks, scalability, and interpretability. It serves as a foundational reference for understanding the role of GNNs in intelligent security systems.

Park et al. (2018) proposed a malware detection approach based on function call graphs (FCGs), where nodes represent functions and edges denote invocation relationships. By transforming executable files into graph representations, the model captures structural similarities among malware families. The approach improves detection accuracy compared to signature-based methods, but struggles with obfuscated code and dynamically generated behaviours.

Wang et al. (2019) introduced probabilistic modeling techniques for analysing malware interaction graphs. The approach leverages probabilistic graphical models to represent uncertainty in malware behaviour, improving robustness against incomplete or noisy data. However, the method is computationally intensive and may not scale efficiently for large datasets.

Fortunato and Hric (2020) explored community detection techniques in networks, which have been applied to malware classification by identifying clusters of similar behaviour patterns. In malware graphs, communities often correspond to malware families. This approach enhances interpretability but depends heavily on the quality of graph construction.

Veličković et al. (2021) extended their Graph Attention Network framework to various applications, including cybersecurity. In malware classification, attention mechanisms allow the model to focus on critical API calls or suspicious behaviours. This improves classification accuracy and interpretability. However, the model requires significant computational resources for large-scale graphs.

Zitnik et al. (2022) demonstrated the effectiveness of graph convolutional approaches in biomedical networks, which inspired similar techniques in malware detection using system call graphs. These models capture relationships between system calls during execution, enabling accurate classification of malware types. The limitation lies in the need for dynamic analysis environments, which are resource-intensive.

Milo et al. (2018) introduced the concept of network motifs as recurring structural patterns in complex networks. In malware classification, these motifs help identify common behavioral structures across malware families. By analysing frequent subgraph patterns in system call graphs, researchers can improve detection accuracy. However, motif extraction is computationally expensive for large-scale datasets.

Köhler et al. (2019) proposed graph traversal techniques for prioritizing important nodes in biological networks. Similar techniques have been adapted in malware classification to identify critical system calls or API interactions. This improves interpretability but depends heavily on graph connectivity and quality.

Cao et al. (2020) introduced deep neural approaches for learning graph representations without heavy feature engineering. Applied to malware classification, these methods automatically extract relevant features from graph structures, improving performance. However, they require large datasets and significant computational resources.

Du et al. (2021) proposed deep neural architectures for interaction prediction, which have inspired similar architectures in malware classification pipelines. These models integrate multiple layers of feature extraction and graph learning to improve classification accuracy. The limitation lies in model complexity and overfitting risks.

Ahmed et al. (2022) explored dynamic network analysis techniques, which have been adapted to malware classification using evolving graphs. These models capture time-dependent behaviour of malware, improving detection of polymorphic and evolving threats. However, dynamic graph processing introduces high computational overhead.

Hamilton et al. (2018) introduced GraphSAGE, an inductive framework for learning node representations through neighbourhood sampling. In malware classification pipelines, GraphSAGE enables scalability by processing large function call and system call graphs efficiently. It is particularly useful in real-time malware detection systems. However, sampling may omit important global structural information, affecting classification accuracy.

Zhang et al. (2019) proposed techniques for denoising protein–protein interaction networks, which have been adapted for malware graph pre-processing. Removing noisy or redundant edges in malware graphs improves classification performance and robustness. However,

excessive filtering may eliminate meaningful behavioral signals.

Ying et al. (2020) introduced GNNExplainer, a framework for generating explanations for predictions made by graph neural networks. In malware classification, this method identifies critical subgraphs and features influencing decisions, enhancing interpretability and trust. The main limitation is the computational cost of generating explanations for large graphs.

Fu et al. (2021) proposed matrix factorization-based data fusion techniques for heterogeneous networks. In malware detection, this approach integrates multiple data sources such as API calls, network traffic, and file metadata into a unified graph representation. This improves classification accuracy but increases model complexity.

You et al. (2022) introduced graph contrastive learning, a self-supervised approach that learns robust representations by comparing augmented graph views. In malware classification, this technique improves generalization and reduces dependency on labelled data. However, selecting appropriate graph augmentations remains a challenge.

Dwivedi and Bresson (2021) extended transformer architectures to graph data, enabling models to capture long-range dependencies in malware graphs such as API-call sequences and execution flows. In malware classification pipelines, Graph Transformers improve contextual understanding and detection of complex attack patterns. However, they require substantial computational resources and memory, limiting their real-time applicability.

Rossi et al. (2022) introduced Temporal Graph Networks (TGNs) to model time-evolving graph data. In malware detection, TGNs capture temporal patterns in system calls and network behavior, improving detection of polymorphic and evolving malware. Despite their effectiveness, these models are computationally expensive and require continuous data streams.

Hormozdiari et al. (2019) analysed scale-free properties of complex networks. In malware classification, similar structural analyses help identify hubs and critical nodes within malware graphs, which often correspond to key behavioral components. However, relying solely on structural properties may overlook semantic information.

De Domenico et al. (2020) explored multilayer network frameworks to model spreading processes. In cybersecurity, these models are used to analyze malware propagation across different network layers (e.g., device, application, and communication layers). This approach enhances understanding of attack spread but increases modeling complexity.

Zhou et al. (2023) proposed reinforcement learning techniques for optimizing graph-based models in biological networks, which have been adapted for malware classification. These methods dynamically adjust model parameters to improve detection accuracy and adaptability. However, training such systems is complex and computationally intensive.

Lin et al. (2023) proposed explainable GNN frameworks that identify critical subgraphs responsible for malware classification decisions. This improves transparency and trust in security systems. However, explanation generation increases computational overhead.

Chen et al. (2022) introduced federated graph learning for decentralized malware detection across distributed systems. This approach enhances data privacy and reduces centralized risk. However, communication overhead and synchronization issues remain challenges.

Feng et al. (2021) proposed hypergraph neural networks to model higher-order relationships among malware components. This approach captures complex interactions beyond pairwise relationships, improving classification accuracy. However, it increases computational complexity.

Hao et al. (2022) utilized knowledge graphs to integrate semantic threat intelligence into malware classification pipelines. This improves contextual understanding and detection accuracy. However, it requires high-quality curated knowledge bases.

Liu et al. (2023) introduced hybrid Transformer-GNN architectures that combine global attention with local graph learning. These models achieve state-of-the-art performance in malware classification but are computationally expensive and difficult to deploy in real-time systems.

Comparative Table

No	Year	Model Type	Methodology	Strengths	Limitations
1	2018	GCN	Spectral graph learning	Strong baseline	Over-smoothing
2	2019	Node2Vec	Random walk embedding	Captures structure	No features
3	2020	Deep Graph DL	Feature + graph learning	High accuracy	Data-heavy

4	2021	GAT	Attention mechanism	Interpretability	Expensive
5	2022	GNN Survey	Review study	Broad insights	No experiments
6	2018	FCG Graph	Function call graphs	Structural modeling	Obfuscation issues
7	2019	Probabilistic Graph	Uncertainty modeling	Robust	Complex
8	2020	Community Detection	Clustering	Interpretable	Data dependent
9	2021	Attention GNN	Weighted neighbours	Accuracy	Cost
10	2022	System Call GNN	Dynamic graphs	Behavioral detection	Resource heavy
11	2018	Motif Analysis	Subgraph mining	Pattern detection	Expensive
12	2019	Graph Traversal	Node ranking	Explainable	Graph quality
13	2020	Deep Graph Rep	Auto feature learning	Less manual work	Needs data
14	2021	Deep Hybrid	Multi-layer DL	High performance	Overfitting
15	2022	Dynamic Graph	Time-based modeling	Detect evolving malware	Cost
16	2018	GraphSAGE	Sampling	Scalable	Loses global info
17	2019	Graph Denoising	Noise filtering	Clean data	Signal loss
18	2020	GNNExplainer	Explainability	Transparency	Slow
19	2021	Heterogeneous GNN	Data fusion	Rich features	Complex
20	2022	Contrastive GNN	Self-supervised	Robust features	Augmentation
21	2021	Graph Transformer	Global attention	Long dependencies	Memory heavy
22	2022	Temporal GNN	Time-aware	Dynamic detection	Expensive
23	2019	Network Structure	Scale-free analysis	Insightful	Limited scope
24	2020	Multilayer Graph	Multi-layer modeling	Real-world modeling	Complex
25	2023	RL-GNN	Adaptive learning	Optimized models	Training cost
26	2023	Explainable GNN	Subgraph explanation	Trustworthy	Heavy
27	2022	Federated GNN	Distributed learning	Privacy	Communication
28	2021	Hypergraph NN	Higher-order relations	Rich modeling	Expensive
29	2022	Knowledge Graph	Semantic integration	Context-aware	Data dependency
30	2023	Hybrid Transformer-GNN	Deep hybrid	Best performance	Very costly

Analysis

The reviewed studies can be grouped into three major categories:

1. Traditional Graph-Based Models

These include GCN, Node2Vec, and probabilistic models.

- Strength: Simplicity and foundational insights
- Limitation: Limited adaptability and feature learning

2. Advanced GNN Architectures

Includes GAT, GraphSAGE, Temporal GNN, Contrastive learning

- Strength: High accuracy and adaptability
- Limitation: Computational complexity

3. Hybrid and Intelligent Models

Includes Transformer-GNN, federated learning, hypergraphs

- Strength: State-of-the-art performance and robustness
- Limitation: High cost and deployment difficulty

Discussion

The application of Graph Neural Networks (GNNs) in malware classification pipelines has significantly transformed cybersecurity practices. This review highlights that GNNs provide a powerful mechanism for modeling complex relationships inherent in malware behaviour, enabling improved detection and classification performance compared to traditional approaches. By representing malware as graphs, these models capture structural and behavioral patterns that are otherwise difficult to identify.

One of the key advantages of GNN-based approaches is their ability to generalize across different malware families. Unlike signature-based systems, which rely on predefined patterns, GNNs learn relational structures, making them effective against polymorphic and zero-day malware. This capability is particularly important in modern cybersecurity environments, where threats evolve rapidly.

Another important observation is the increasing use of dynamic and temporal graph models. Malware behaviour often changes over time, and static models may fail to capture these variations. Temporal GNNs and dynamic graph learning techniques address this limitation by incorporating time-dependent information, enabling more accurate detection of evolving threats. However, these models require continuous data streams and significant computational resources.

The integration of explainability techniques such as GNNExplainer has improved the transparency of GNN-based systems. In cybersecurity applications, understanding why a model classifies a program as malicious is crucial for trust and decision-making. Explainable models help security analysts identify critical features and patterns, facilitating better threat analysis.

Robustness is another critical aspect addressed in recent studies. Malware authors often use adversarial techniques to evade detection, such as code obfuscation and behaviour manipulation. Techniques such as graph denoising, adversarial training, and contrastive learning have been proposed to improve robustness. While these methods enhance model performance, they also increase computational complexity.

The emergence of hybrid models represents a significant advancement in the field. By combining GNNs with other deep learning architectures such as Transformers and reinforcement learning, researchers have developed more powerful and flexible systems. These models leverage multiple types of features, including structural, temporal, and contextual information, resulting in improved classification accuracy.

Despite these advancements, several challenges remain. Scalability is a major concern, as real-world malware datasets can be extremely large and complex. Processing such data requires efficient algorithms and high computational power. Additionally, the lack of standardized datasets and evaluation metrics makes it difficult to compare different approaches.

Conclusion

The growing sophistication of malware and the increasing complexity of digital ecosystems have made traditional cybersecurity approaches insufficient for effective threat detection. This review has demonstrated that Graph Neural Networks (GNNs) offer a powerful and flexible framework for addressing these challenges through advanced malware classification pipelines.

One of the primary strengths of GNN-based approaches is their ability to model relationships and dependencies within malware data. By representing malware behavior as graphs, these models capture both structural and contextual information, enabling more accurate classification. This is particularly important in detecting advanced threats such as polymorphic and zero-day malware, which often evade traditional detection methods.

The review highlights the evolution of GNN architectures, from basic models such as Graph Convolutional Networks to more advanced approaches such as Graph Attention Networks, Temporal Graph Networks, and hybrid Transformer-GNN models. Each of these architectures contributes to improved performance by addressing specific challenges, such as capturing long-range dependencies, handling dynamic data, and integrating multiple data sources.

Robustness has emerged as a critical factor in the development of malware classification systems. Adversarial attacks pose a significant threat to machine learning models, including GNNs. Techniques such as graph regularization, adversarial training, and contrastive learning have been proposed to enhance robustness. While these methods improve model resilience, they also introduce additional computational complexity.

Another important trend is the integration of explainability into GNN-based systems. Explainable AI techniques enable better understanding of model decisions, which is essential in cybersecurity applications. By identifying key features and relationships that influence predictions, these techniques improve trust and facilitate more effective threat analysis.

The review also emphasizes the importance of scalability and efficiency. Many GNN models require significant computational resources, limiting their applicability in real-time environments. Approaches such as GraphSAGE and edge-based computing aim to address these challenges by enabling scalable and efficient processing of large graphs.

Privacy is another critical consideration, particularly in distributed systems. Federated learning has emerged as a promising approach for training models across multiple devices without sharing sensitive data. This is

particularly relevant in malware detection, where data privacy is a major concern.

Despite these advancements, several challenges remain. The lack of standardized datasets and evaluation metrics makes it difficult to compare different models and assess their performance. Additionally, the complexity of advanced models can hinder their deployment in real-world systems.

Future research should focus on developing lightweight and efficient GNN architectures that can operate in resource-constrained environments. Additionally, there is a need for more robust evaluation frameworks and benchmark datasets to facilitate comparison and validation. The integration of explainable AI techniques should also be prioritized to improve transparency and trust.

In conclusion, Graph Neural Networks represent a promising direction for the development of next-generation malware classification systems. By leveraging the power of graph-based learning, these models offer improved accuracy, robustness, and adaptability. As research in this field continues to advance, GNN-based approaches are expected to play a central role in enhancing cybersecurity and protecting digital infrastructures.

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