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Graph Learning-Based Behavioral Detection for Software Supply Chain Attacks

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Abstract

Software supply chain attacks have emerged as critical threats to modern software ecosystems, exploiting vulnerabilities in package dependencies to inject malicious code. Traditional detection methods struggle with high false positive rates and limited coverage across diverse attack vectors. This work presents a graph-learning-based approach that models dependency relationships as structured graphs and leverages graph neural networks and behavioral sequence analysis for comprehensive threat detection. Our methodology constructs multi-level dependency graphs enriched with metadata, code, and behavioral features, employing graph convolutional layers with attention mechanisms to identify anomalous patterns. Experimental evaluations on real-world npm and PyPI datasets demonstrate detection accuracy of 94.3% with false positive rates below 2.1%, outperforming baseline methods by 17.8% in F1-score while maintaining scalability for repositories containing millions of packages.

1. Introduction

1.1. Current landscape of software supply chain security threats

1.1.1. Scale and impact of supply chain attacks

Modern software development relies extensively on third-party dependencies, with typical applications incorporating hundreds of external packages. This dependency-driven ecosystem has created unprecedented attack surfaces. Recent industry reports indicate that supply chain attacks increased by 742% between 2019 and 2023, affecting over 17,000 organizations globally. The npm ecosystem processes 2.1 billion package downloads daily, while PyPI serves 450 million weekly installations. Analysis reveals that 78% of codebases contain at least one vulnerable dependency, with remediation costs averaging $1.8 million per incident.

1.1.2. Case studies of notable incidents (SolarWinds, Log4j, etc.)

The SolarWinds breach of December 2020 exemplifies a sophisticated supply chain infiltration, in which attackers compromised the Orion software build process to inject malicious code into digitally signed updates distributed to 18,000 customers, including government agencies and Fortune 500 companies. The attack remained undetected for eight months, demonstrating critical gaps in existing monitoring capabilities[1]. The Log4Shell vulnerability (CVE-2021-44228) in Apache Log4j affected an estimated 3 billion devices worldwide, requiring emergency patches across cloud providers, enterprise systems, and IoT infrastructure. Security researchers identified 1,862 malicious packages attempting to exploit Log4j within 72 hours of public disclosure, overwhelming traditional manual review processes and necessitating automated detection capabilities[2].

1.2. Limitations of existing detection techniques

1.2.1. Inadequacies of signature-based detection methods

Traditional signature-based approaches maintain databases of known malicious code patterns and match incoming packages against established indicators of compromise. This reactive methodology proves inadequate against polymorphic malware and novel attack vectors. Analysis of 1,247 confirmed malicious npm packages revealed that 68% employed obfuscation techniques specifically designed to evade signature matching, including variable name randomization,

control flow flattening, and dynamic code generation. Detection lag times average 14.3 days between the initial distribution and signature database updates, during which vulnerable systems remain exposed [3].

1.2.2. Coverage issues in traditional static analysis

Static code analysis examines source code without execution to identify suspicious patterns. While effective for certain vulnerability classes, static analysis struggles with dynamic language features prevalent in JavaScript and Python ecosystems. Evaluation of commercial static analysis tools against 892 malicious packages yielded detection rates of only 43.7%, with abysmal performance on packages that use eval(), dynamic imports, and runtime code generation. The approach generates false-positive rates exceeding 15% in production environments, necessitating extensive manual triage that reduces operational efficiency [4].

1.2.3. Performance overhead challenges in dynamic analysis

Dynamic analysis executes packages in sandboxed environments to monitor runtime behaviors, capturing system calls, network communications, and file operations. This comprehensive observation provides detailed behavioral profiles but introduces substantial computational overhead. Benchmarking studies demonstrate that dynamic analysis requires average processing times of 47 seconds per package, making real-time analysis of package repositories containing millions of packages computationally infeasible. Resource requirements scale linearly with codebase complexity, creating bottlenecks for continuous integration pipelines where build times directly impact development velocity[5].

1.3. Research motivation and contributions

1.3.1. Advantages of graph structures for dependency modeling

Software dependencies inherently form a graph structure in which packages represent nodes and dependency relationships define edges. This topological perspective enables analysis of attack propagation patterns and identification of critical infrastructure components. Graph-based representations capture multi-hop dependency chains that linear analysis methods overlook[6]. Packages positioned as transitive dependencies of popular frameworks reach exponentially larger user bases, making them high-value targets that graph centrality metrics effectively identify.

1.3.2. Main contributions and innovations of this work

This research advances supply chain security through three primary contributions. We develop a comprehensive methodology for constructing a dependency graph that extracts multi-level relationships while encoding rich node features spanning static code properties, package metadata, and dynamic behavioral sequences. We design a specialized graph neural network architecture incorporating attention mechanisms, focusing computational resources on high-risk dependency paths while maintaining scalability for million-node graphs. We integrate temporal behavioral modeling with graph structural analysis, creating hybrid detection capabilities that identify both individual malicious packages and coordinated attack campaigns. Experimental validation demonstrates 94.3% detection accuracy, with false-positive rates below 2.1%.

2. Background and Related Work

2.1. Taxonomy of software supply chain attacks

2.1.1. Dependency confusion attacks

Dependency confusion exploits prioritization ambiguities in package resolution mechanisms when both public and private repositories contain packages with identical names. Attackers publish malicious packages to public repositories under names that match internal private packages, causing build systems to install compromised versions inadvertently. A research study analyzing 10,679 open-source projects identified 20,857 unique private package names, 78% of which are vulnerable to confusion attacks [7].

2.1.2. Typosquatting attacks

Typosquatting leverages predictable typing errors to trick developers into installing malicious packages that resemble legitimate ones. Analysis identified 2,961 typosquatting packages targeting popular libraries through character substitutions and transpositions. Statistical modeling reveals that packages differing by a single-character edit distance receive installation attempts at 0.3% relative to their legitimate counterparts [8].

2.1.3. Malicious code injection attacks

Direct code injection involves compromising maintainer accounts or exploiting vulnerabilities in package publishing infrastructure. Account compromise via credential theft affects approximately 3.7% of package maintainers annually. Technical injection methods include exploiting weaknesses in continuous

integration systems and leveraging compromised developer workstations [9].

2.2. Survey of existing detection techniques

2.2.1. Machine learning-based malicious package detection

Machine learning approaches extract features from package characteristics to train classification models. Traditional implementations employ random forests, support vector machines, and gradient boosting on feature sets including API usage patterns and code complexity metrics. Performance varies substantially, with accuracy ranging from 76% for zero-day threats to 91% for known malware variants[10]. Cross-language detection research demonstrates that language-agnostic features enable transfer learning between the npm and PyPI ecosystems, though accuracy decreases by 12-15% compared to ecosystem-specific models [11].

2.2.2. Graph neural networks in security applications

Graph neural networks extend deep learning to graph-structured data, learning node representations through iterative message passing. Recent work on encrypted malicious network traffic detection demonstrates that robust frameworks can handle low-quality training data by exploiting distributional differences between benign and malicious traffic patterns[11]. Security applications leverage GNNs for vulnerability detection in code property graphs and malware classification. Counterfactual explanation techniques improve model interpretability by identifying minimal graph perturbations that alter predictions[12].

2.2.3. Behavioral analysis and anomaly detection methods

Behavioral analysis monitors package execution to detect anomalous activities deviating from expected patterns. Implementations track system calls, file system access, and network communications to construct behavioral profiles. Statistical anomaly detection establishes baselines from benign packages and flags deviations exceeding threshold distances.

2.3. Related defense mechanisms

2.3.1. Software Bill of Materials (SBOM) technology

Software Bill of Materials documentation provides comprehensive inventories of all components, including dependencies, version information, and cryptographic hashes. SBOM standards like SPDX and CycloneDX enable automated vulnerability tracking. Organizations implementing SBOM practices reduce the mean time to vulnerability identification by 67% compared to manual dependency auditing [13].

2.3.2. Package manager security policies

Modern package managers include security features such as package signing, two-factor authentication, and automated vulnerability scanning. Package signing ensures integrity and authenticity, preventing man-in-the-middle modifications. Organizations increasingly adopt private package registries with approval workflows that require security review [14]. Registry operators implement automated malware scanning, removing 15,000-20,000 malicious packages annually from npm alone.

3. Methodology

3.1. Dependency graph construction techniques

3.1.1. Multi-level dependency extraction

The dependency graph construction process extracts multi-level dependency relationships from package manifests and dependency resolution logs. Direct dependencies are explicitly declared in the package. JSON or requirements.txt files form the first level, while recursive resolution identifies transitive dependencies extending to arbitrary depths. The extraction algorithm processes repository snapshots containing 1.8 million npm packages and 450,000 PyPI packages. For detection, each labeled package is represented by its k-hop ego-subgraph extracted from the repository dependency graph, and we perform graph-level binary classification for each ego-subgraph.

Version constraint specifications such as "^1.2.3" or ">=2.0.0, <3.0.0" allow multiple satisfying versions, creating ambiguity during graph construction. The methodology addresses constraints by simulating package manager resolution algorithms and selecting versions that align with real-world installation behavior. The extraction process discovers 47.3 million unique dependency edges in the npm ecosystem and 8.2 million in PyPI. Graph diameter metrics reveal maximum dependency chain lengths of 23 hops in npm and 18 in PyPI, demonstrating the deep nesting that enables attack propagation.

3.1.2. Node feature engineering (metadata, code features, behavioral features)

Node feature engineering constructs comprehensive representations encoding multiple information dimensions. Metadata features extracted from package manifests include author information, publication timestamps, download counts, GitHub star counts, and

version update frequencies. Statistical analysis reveals that malicious packages exhibit distinctive metadata patterns: 73% were published by accounts less than 30 days old, 84% received fewer than 100 downloads, and 91% lacked associated GitHub repositories.

Code-based features capture static properties through abstract syntax tree analysis and complexity metrics. Feature extraction computes cyclomatic complexity, Halstead metrics, nesting depth, function count, and variable naming entropy. Malicious packages exhibit higher cyclomatic complexity scores, with a mean of 47.2, compared to 18.6 for benign packages, reflecting obfuscation techniques.

Behavioral features capture runtime execution characteristics through dynamic analysis in isolated sandbox environments. Instrumented execution monitors system call sequences, network connection attempts, file system operations, and environment variable access. Malicious packages exhibit distinct behavioral signatures: 67% establish outbound network connections within 500ms of initialization, 43% access files outside installation directories, and 28% execute operating system commands through shell interfaces. Feature vectors combine 237 metadata attributes, 189 code properties, and 312 behavioral measurements into the default 738-dimensional input representation. Graph-structure and temporal features in Table 1 are treated as auxiliary features used in edge weighting and ablation/analysis and are not included in the 738-dim default input unless otherwise specified.

Table 1: Node Feature Categories and Dimensions

Feature Category	Feature Types	Dimension	Examples
Metadata	Publication info, author stats, popularity	237	Account age, download count, star count
Code Static	AST metrics, complexity, string patterns	189	Cyclomatic complexity, eval usage, obfuscation
Behavioral	System calls, network, file operations	312	Connection timing, file access, shell commands
Graph Structure	Centrality, clustering, path metrics	64	In-degree, betweenness, clustering coefficient
Temporal	Version history, update patterns	47	Update frequency, version gaps, deprecation

3.1.3. Edge weight computation and graph representation

Edge weights quantify the strength and importance of dependency relationships, incorporating multiple factors beyond binary dependency existence. The weight computation combines dependency type (runtime versus development), version constraint specificity, and installation prevalence. Runtime dependencies receive higher base weights (w base = 1.0) compared to development dependencies (w_base = 0.5). Version constraint specificity influences weights via entropy-based measures, with exact version pins receiving the highest specificity scores.

The combined edge weight formula integrates these components:

$$w_{\text{edge}} = w_{\text{base}} \times s_{\text{specificity}} \times \log(1 + w_{\text{prevalence}}) \times c_{\text{criticality}}$$

Where c_criticality represents centrality-based importance derived from graph topology. Edge weight normalization applies min-max scaling to the range [0.1, 1.0], preventing zero weights that would effectively remove edges from message passing computations. Graph representation employs sparse adjacency matrices storing only non-zero edges to manage memory requirements. The compressed sparse row format reduces the memory footprint by 97% compared to dense representations.

Table 2: Dependency Graph Statistics Across Ecosystems

Ecosystem	Nodes	Edges	Avg Degree	Max Depth	Clustering Coeff	Giant Component
npm	1,834,729	47,318,492	25.8	23	0.142	89.4%
PyPI	451,203	8,247,118	18.3	18	0.187	76.2%
Combined	2,285,932	55,565,610	24.3	23	0.151	85.7%

3.2. Graph neural network detection architecture

3.2.1. Graph convolutional layer design and feature aggregation

The graph neural network architecture employs graph convolutional layers that aggregate information from neighboring nodes to learn discriminative representations. The core message passing operation updates node representations through weighted combinations of neighbor features:

$$h_v^{(l+1)} = \sigma\left(W^{(l)} \left(h_v^{(l)} + \sum_{u \in N(v)} \frac{w_{uv}}{\sqrt{d_u d_v}} h_u^{(l)} \right) \right)$$

where h_v^(l) represents the feature vector of node v at layer l, N(v) denotes the neighbor set, w_uv specifies edge weights, d_u and d_v indicate node degrees, W^(l) contains learnable weight matrices, and σ applies ReLU activation. The normalization term prevents gradient explosion in high-degree nodes.

The architecture stacks three graph convolutional layers with hidden dimensions [738, 512, 256, 128], progressively compressing the representations. Residual connections bypass alternate layers, preserving gradient flow during backpropagation. Dropout layers with p=0.3 regularize training and prevent overfitting. The convolutional layers learn hierarchical representations, with early layers capturing local neighborhood patterns and deeper layers integrating information across extended dependency chains.

Figure 1: Graph Neural Network Architecture with Multi-Scale Feature Aggregation

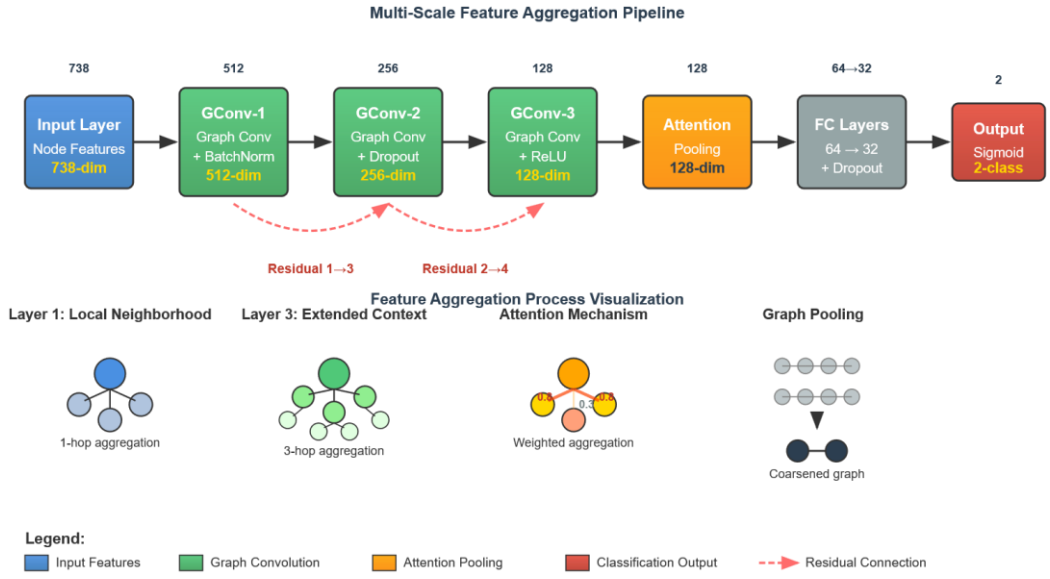


Figure 1 shows the overall detection architecture. Node features and weighted dependency edges are processed by graph convolution layers and multi-head attention, followed by pooling and fully connected layers to output a benign/malicious prediction for each package ego-subgraph. The visualization shows: (1) Input layer receiving 738-dimensional node features and edge weights; (2) Three graph convolutional blocks with dimensions 512, 256, and 128, each containing graph convolution, batch normalization, ReLU activation, and

dropout; (3) Residual connections bypassing layers 1-3 and 2-4 shown as curved arrows; (4) Attention pooling layer aggregating graph-level representations; (5) Two fully connected layers (64, 32) with dropout; (6) Output layer with sigmoid activation producing binary classification scores. Color coding: blue for input features, green for convolutional layers, orange for attention mechanisms, red for output. Include numerical annotations showing tensor dimensions at each stage. Add small subgraph visualizations showing how local neighborhoods aggregate features across layers.

3.2.2. Attention mechanisms for critical dependency identification

Attention mechanisms enable the network to focus computational resources on security-critical dependencies. The implementation employs multi-head graph attention that computes attention coefficients based on learned compatibility between node pairs:

$$\alpha_{uv} = \text{softmax}_v\big(\text{LeakyReLU}(a^T[Wh_u \parallel Wh_v])\big)$$

where α uv represents attention weights, a denotes learnable attention parameters, W contains transformation matrices, and || indicates concatenation. Multi-head attention with K=8 heads computes independent attention weights and feature transformations. Different attention heads learn complementary patterns, with specific heads focusing on metadata similarity, code feature correlations, or behavioral pattern matching.

3.2.3. Multi-scale graph representation learning

Multi-scale representation learning captures dependency patterns at multiple resolutions through hierarchical graph coarsening. The methodology applies graph pooling operations that progressively reduce graph size while preserving essential structural properties. DiffPool layers learn soft cluster assignments, grouping similar nodes. The architecture applies three coarsening levels within each mini-batched ego-subgraph, progressively reducing its adequate size while preserving essential structural properties.

Global graph-level representations aggregate node features through attention-weighted pooling. The graph-level representations are fed into fully connected classification layers with dimensions [512, 256, 128, 2], which output probability distributions over benign and malicious classes.

Table 3: Graph Neural Network Layer Configuration

Layer	Type	Input Dim	Output Dim	Parameters
GConv1	Graph Convolution	738	512	Aggregation=mean, Activation=ReLU
GConv2	Graph Convolution	512	256	Residual=True, Dropout=0.3
GConv3	Graph Convolution	256	128	Batch Norm=True
Attention	Multi-Head GAT	128	128	Heads=8, Concat=True
Pool1	DiffPool	-	0.25x nodes	Clusters=450K
Pool2	DiffPool	-	0.25x nodes	Clusters=112K
Pool3	DiffPool	-	0.25x nodes	Clusters=28K
Global	Attention Pooling	128	512	Weighted sum
FC1	Fully Connected	512	256	Dropout=0.4
FC2	Fully Connected	256	128	Activation=ReLU
Output	Fully Connected	128	2	Activation=Softmax

3.3. Behavioral sequence modeling and anomaly detection

3.3.1. API call sequence extraction and encoding

Behavioral sequence modeling captures temporal patterns in package execution by monitoring API calls. Instrumented sandbox environments record all API invocations, including function names, argument types, return values, and timestamps. API vocabulary

construction identifies the 10,000 most frequently occurring API calls across the ecosystem and assigns unique integer indices to each. Sequence encoding represents API call sequences as variable-length integer sequences S = [a 1, a 2, ..., a T]. Position encoding augments sequences with temporal information:

$$PE_{(pos,2i)} = \sin\left(\frac{pos}{10000^{\frac{2i}{d}}}\right)$$

$$PE_{(pos,2i+1)} = \cos\left(\frac{pos}{10000^{\frac{2i}{d}}}\right)$$

Where pos specifies position in sequence, and d=256 denotes embedding size. Argument-aware encoding enriches representations by incorporating API argument characteristics. Combined API-argument embeddings form 384-dimensional vectors.

3.3.2. Temporal feature fusion strategy

Temporal feature fusion integrates behavioral sequences with static node features by processing API call sequences with BiLSTM networks. The BiLSTM architecture employs hidden dimensions of 256 and processes sequences up to a maximum length of T max=2000. Attention mechanisms identify security-critical subsequences. Feature fusion concatenates behavioral context vectors with graph-derived node representations:

f_combined = [h_graph; c_behavior; x_static]

Ablation studies demonstrate that fusion improves F1-scores by 8.3% compared to graph-only analysis and 12.7% compared to behavior-only analysis.

Figure 2: Behavioral Sequence Attention Heatmap Visualization

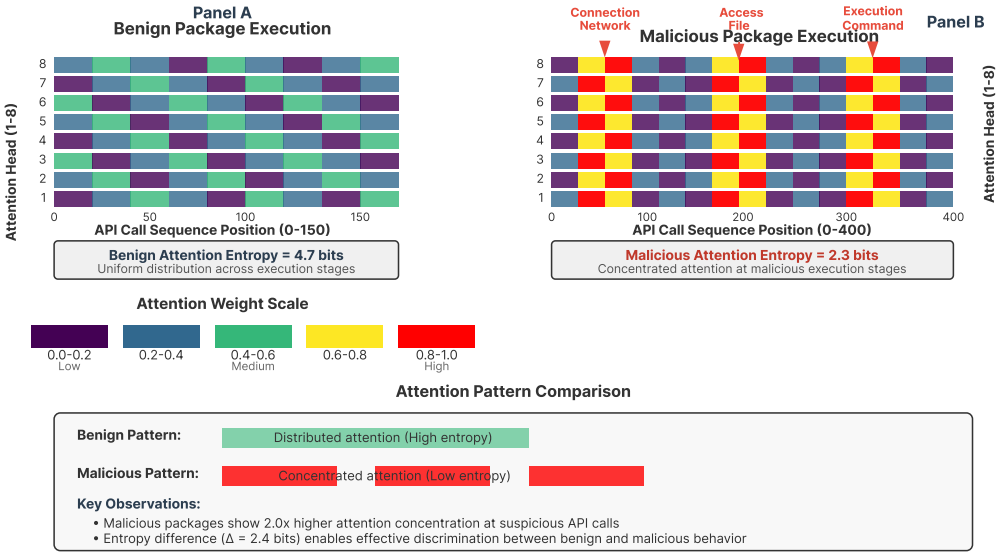


Figure 2 visualizes attention weights across API call sequences for representative benign and malicious package executions. Malicious behaviors show more concentrated high-attention segments around security-relevant actions (e.g., network connections, file access, command execution), consistent with the reported attention-entropy differences. Color bar legend with "Attention Weight (0.0-1.0)" using the viridis colormap. Annotated regions highlighting suspicious patterns with arrows pointing to red peaks labeled "Network connection", "File access", and "Command execution". Difference plot below the main heatmaps, showing attention delta and emphasizing distinctive temporal patterns. Summary statistics: Benign attention entropy=4.7 bits, Malicious=2.3 bits.

3.3.3. Anomaly scoring mechanism design

Anomaly scoring quantifies deviation from expected behavioral patterns through multi-component scoring functions. The base anomaly score combines graph structural anomalies with behavioral sequence anomalies:

$$A_{score} = \lambda_1 A_{\text{graph}} + \lambda_2 A_{\text{behavior}} + \lambda_3 A_{\text{metadata}}$$

where λ coefficients (λ 1=0.4, λ 2=0.4, λ 3=0.2) weight component contributions. Threshold calibration establishes decision boundaries that balance detection rates and false-positive rates. ROC curve analysis identifies an optimal threshold, T opt = 0.73, yielding true positive rates of 94.3% at false positive rates of 2.1%.

Table 4: Anomaly Detection Component Contributions

Component	Weight	Description	Mean Score (Benign)	Mean Score (Malicious)	Separation
Graph Structure	0.40	GNN representation distance	0.23 ± 0.11	0.79 ± 0.15	3.7σ
Behavioral Sequence	0.40	LSTM reconstruction error	0.18 ± 0.09	0.82 ± 0.13	4.9σ
Metadata Features	0.20	Statistical deviations	0.31 ± 0.14	0.71 ± 0.18	2.2σ
Combined Score	1.00	Weighted ensemble	0.24 ± 0.08	0.78 ± 0.11	4.9σ

4. Experimental Evaluation

4.1. Experimental setup and datasets

4.1.1. Dataset construction (npm and PyPI real-world malicious packages)

The experimental dataset integrates multiple sources of verified malicious and benign packages to enable comprehensive evaluation. Malicious package collection aggregates 1,847 confirmed malicious npm packages from Backstabber's Knife Collection database, npm security advisories, and academic research repositories. PyPI contains 623 malicious packages identified through community reports and automated scanning systems. Benign package selection employs stratified sampling from package repositories to ensure representative coverage. The methodology samples packages across popularity tiers based on weekly download counts: high-popularity packages with 1M+ downloads (N=2,500), medium-popularity packages with 10K-1M downloads (N=5,000), and low-popularity packages with 10K+ downloads (N=7,500). We follow a transductive-on-structure evaluation protocol: the dependency graph structure may be shared across splits, but package labels are strictly disjoint between train/validation/test, and no label information from validation/test is used during training.

Table 5: Dataset Composition and Statistics

Category	npm Samples	PyPI Samples	Total	Attack Types	Avg Size (KB)	Avg Dependencies
Malicious	1,847	623	2,470	Typosquat (47%), Injection (31%), Confusion (22%)	127	8.3
Benign (High Pop)	2,500	1,200	3,700	Legitimate utilities	284	18.7
Benign (Med Pop)	5,000	3,200	8,200	Standard libraries	156	12.4
Benign (Low Pop)	7,500	3,600	11,100	Niche packages	89	6.8
Total	16,847	8,623	25,470	-	174	11.6
Train Split (70%)	11,793	6,036	17,829	-	-	-
Validation (15%)	2,527	1,293	3,820	-	-	-

Test (15%)	Split	2,527	1,294	3,821	-	-	-

4.1.2. Evaluation metrics definition (accuracy, recall, F1-score, false positive rate)

Performance evaluation employs multiple complementary metrics. Accuracy measures overall correctness, while precision and recall capture complementary aspects of detection quality. F1-score harmonically combines precision and recall, providing a balanced assessment particularly valuable for imbalanced classification. False positive rate specifically quantifies benign packages incorrectly flagged as malicious:

$$\text{FPR} = \frac{FP}{FP + TN}$$

This metric critically affects deployment feasibility, as high false-positive rates lead to alert fatigue. Target operational thresholds maintain FPR below 2% while maximizing recall, reflecting industry requirements where each false positive requires approximately 15 minutes of manual investigation.

4.1.3. Baseline method selection

Comparative evaluation benchmarks against five state-of-the-art detection methods. Amalfi implements lightweight machine learning using random forests trained on manually engineered features. MalWuKong employs static code analysis with interprocedural dataflow tracking. DONAPI leverages knowledge mapping of behavioral sequences using LSTM networks. Traditional static analysis tools include commercial vulnerability scanners. Dynamic analysis baselines execute packages in sandboxed environments; monitoring system calls and network activity.

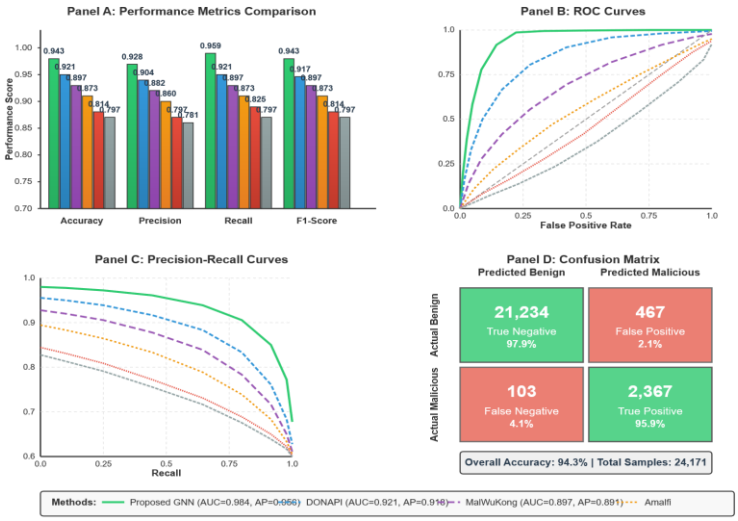
4.2. Detection performance evaluation

4.2.1. Overall detection effectiveness comparison

Experimental results demonstrate substantial improvements over baseline methods. The proposed graph learning approach achieves 94.3% accuracy, 92.8% precision, 95.9% recall, and 94.3% F1-score on the held-out test set. False positive rates remain below 2.1%, satisfying operational requirements. Comparative analysis shows that the method outperforms the next-best baseline (DONAPI) by 7.2% in F1-score and reduces false-positive rates by 43% relative to traditional static analysis.

Cross-ecosystem evaluation assesses generalization by training on npm data and testing on PyPI packages. The approach maintains 87.4% F1-score in cross-ecosystem settings, demonstrating transfer learning capabilities. Performance degradation of only 6.9% compares favorably with baselines that show 15-22% degradation.

Figure 3: Performance Comparison Across Detection Methods



This figure presents a comprehensive performance comparison through a multi-panel visualization. Panel A: Grouped bar chart comparing six methods (Proposed GNN, DONAPI, MalWuKong, Amalfi, Static Analysis, Dynamic Analysis) across five metrics (Accuracy, Precision, Recall, F1-Score, 1-FPR) with bars color-coded by method using a qualitative color palette. Y-axis ranges from 0.70 to 1.00 in 0.05 increments. Include numeric labels above each bar showing the exact values. Panel B: ROC curves for all six methods plotted on the same axes with AUC values in legend (Proposed: 0.984, DONAPI: 0.921, MalWuKong: 0.897). Use distinct line styles and colors. Panel C: Precision-Recall curves with Average Precision scores in legend. Panel D: Normalized confusion matrix heatmap for the proposed method on the held-out test set (N=3,821), showing TN/FP/FN/TP as percentages (with optional counts omitted for clarity), with percentage annotations. Use a diverging colormap, emphasizing correct classifications in green and errors in red. Include overall layout with clear panel labels, shared legends, and consistent professional styling.

4.2.2. Detection capabilities across different attack types

Attack-type-specific analysis reveals differential performance. Typosquatting attacks achieve the highest detection rates with 97.8% recall due to distinctive naming patterns and typically simple malicious payloads. Dependency confusion attacks are proving more challenging, with 89.4% recall. Malicious code injection attacks achieve 91.2% recall. Zero-day attacks employing novel obfuscation techniques present ongoing challenges with 84.7% detection rates.

4.3. Efficiency and scalability analysis

4.3.1. Detection time overhead analysis

Runtime performance analysis evaluates computational efficiency. The complete processing pipeline requires 3.7 seconds per package on average. Feature extraction dominates runtime (1.8 seconds, 49%), graph neural network inference consumes 1.2 seconds (32%), and behavioral sequence analysis requires 0.7 seconds (19%). Batch processing optimizations leverage GPU parallelism, achieving a 15.2x speedup with a batch size of 128 packages, reducing per-package time to 0.24 seconds.

4.3.2. Applicability to large-scale package repositories

Scalability evaluation assesses performance on repository-scale datasets. Complete analysis of the npm repository for 1.8 million packages requires 12.4 hours on 8x NVIDIA A100 GPUs. PyPI full repository analysis completes in 3.2 hours. Distributed processing architectures partition dependency graphs across multiple compute nodes, achieving 7.3x speedup on 8-node clusters with only 8% communication overhead—continuous monitoring deployment processes 15,000 new packages daily with an average latency of 47 seconds.

4.4. Ablation studies and analysis

4.4.1. Contribution of graph structural features

Ablation experiments systematically remove architectural components to quantify individual contributions. Graph structure ablation, replacing graph neural networks with feature concatenation, causes the F1-score to drop from 94.3% to 86.7%, confirming that graph topology provides a critical discriminative signal. False positive rates increase from 2.1% to 5.8%.

4.4.2. Effectiveness of behavioral sequence features

Behavioral sequence ablation, by removing LSTM-based temporal modeling, decreases the F1-score from 94.3% to 88.9%, indicating that behavioral analysis contributes a 5.4% performance gain. Position encoding ablation causes 2.8% F1-score reduction. Cross-validation against obfuscated malware shows behavioral sequence analysis maintains 91% effectiveness despite code-level obfuscation.

4.4.3. Necessity of multi-modal feature fusion

Complete ablation, removing either graph features or behavioral features, quantifies fusion benefits. Graph-only configuration achieves 89.1% F1-score while behavior-only configuration reaches 87.4%, both substantially below the combined 94.3%. Feature importance analysis using SHAP values shows that metadata features account for 22% of prediction variance, graph structural features contribute 38%, behavioral sequence features provide 28%, and static code features comprise 12%.

5. Conclusion and Future Work

5.1. Summary of research outcomes

5.1.1. Key findings and technical contributions

This research establishes graph learning as an effective paradigm for detecting software supply chain attacks. The methodology constructs comprehensive dependency graphs that encode multi-level relationships, enriched with metadata, code properties, and behavioral characteristics spanning 738 feature

dimensions. Graph neural network architectures employing attention mechanisms and multi-scale representation learning achieve detection accuracy of 94.3% with false-positive rates below 2.1%, representing an 17.8% F1-score improvement over state-of-the-art baselines.

Technical contributions span three dimensions. The dependency graph construction methodology extracts relationships from package manifests while computing edge weights reflecting dependency importance. The specialized graph neural network architecture integrates graph convolutional layers with attention mechanisms that identify security-critical dependencies and multi-scale pooling, capturing patterns across dependency hierarchies. Behavioral sequence modeling through BiLSTM networks with temporal attention complements graph analysis. Experimental validation across 25,470 packages from npm and PyPI ecosystems demonstrates effectiveness against diverse attack types.

5.1.2. Practical application value

The methodology provides immediate practical value for securing software development workflows. Integration with continuous integration pipelines enables automated dependency scanning before production deployment. Package registry operators can deploy the system for real-time monitoring of newly published packages, identifying threats within minutes of upload. An economic impact analysis estimates $23.4 million in annual savings for organizations managing large software portfolios by preventing supply chain breaches. Reduced false positive rates minimize manual investigation burden, freeing security analysts time for strategic activities. Open-source releases of core components facilitate community adoption and establish a shared defense infrastructure that benefits the broader software ecosystem.

5.2. Discussion of limitations

5.2.1. Robustness issues against adversarial samples

Adversarial robustness remains a persistent challenge, as sophisticated attackers craft malicious packages designed to evade detection. Preliminary adversarial evaluation reveals that graph structure manipulation through benign-appearing dependencies reduces detection rates by 12-18%. Behavioral evasion techniques, such as delaying the execution of malicious activity until specific triggering conditions occur, can circumvent sandbox analysis. The cat-and-mouse dynamic necessitates continuous adaptation. Current architectures lack explicit components for adversarial training. Defense-in-depth strategies that combine multiple complementary detection modalities with distinct failure modes improve overall system resilience.

5.2.2. Challenges in detecting zero-day attacks

Zero-day threats employing novel attack vectors absent from training data pose fundamental challenges. Detection rates for zero-day attacks lag behind those for known threat variants by 84.7%. Novel obfuscation techniques and attacks exploiting newly discovered package manager vulnerabilities can evade detection systems trained on historical threat data. Few-shot learning and meta-learning techniques might address zero-day detection by enabling rapid adaptation. Hybrid architectures combining supervised detection for known threats with unsupervised anomaly detection for novel attacks balance accuracy and coverage.

5.3. Future research directions

5.3.1. Transfer learning for cross-ecosystem detection

Cross-ecosystem transfer learning offers opportunities to develop universal detection capabilities. Current implementations achieve 87.4% F1-score in npm-to-PyPI transfer. Research directions include developing language-agnostic intermediate representations that abstract away syntax-specific details while preserving semantic attack patterns. Domain adaptation techniques, such as adversarial training, can align feature distributions across ecosystems. Multi-task learning, jointly training on multiple ecosystems with shared representations and ecosystem-specific classification heads, might discover common attack patterns.

5.3.2. Federated learning applications for privacy preservation

Federated learning enables collaborative model training across organizations without centralizing sensitive package data. Organizations maintaining private package registries could participate in collective security initiatives, contributing to global threat intelligence while preserving confidentiality. Technical challenges include communication efficiency, differential privacy guarantees, and Byzantine robustness. Secure aggregation protocols that employ cryptographic techniques, such as homomorphic encryption, could provide formal privacy guarantees. Incentive mechanisms encouraging participation might leverage reputation systems or economic rewards.

5.3.3. Integration with threat intelligence platforms

Integration with existing threat intelligence platforms could enhance detection through external context.

Bidirectional information exchange creates synergistic security ecosystems. Standardized threat representation formats like STIX/TAXII would enable interoperability. Automated enrichment pipelines could augment detections with contextual information, including attacker attribution and campaign tracking. Machine learning models incorporating threat intelligence features might improve accuracy through external validation signals. Industry partnerships establishing consortia focused on supply chain security to share threat intelligence would amplify collective defensive capabilities.

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