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Tri-Modal Contrastive Binary Analysis via Opcode Transformers, Control Flow Graph Isomorphism Networks, and System Call Embeddings: A Systematic Review of Zero-Day Malware Detection Frameworks

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Abstract

Identifying zero-day malware variants and reverse-engineering compiled binaries requires robust code similarity analysis. Legacy inspection pipelines evaluate software through isolated feature streams—such as disassembly byte flows, control-flow graphs, or dynamic execution logs. Unimodal analysis fails when attackers apply UPX packing, instruction substitution, control-flow flattening, or sandbox-stalling logic. To overcome single-perspective blind spots, recent security systems adopt Multi-Modal Binary Similarity Analysis (MMBSA), embedding static syntax, structural graphs, and runtime behavior into unified neural latent spaces. Guided by the PRISMA 2020 framework, this systematic review synthesizes 15 primary benchmark frameworks and over 50 core papers published from 2020 through 2026. We construct a three-axis taxonomy organizing existing systems by feature ingestion streams, neural fusion strategies, and downstream tasks. In addition, we detail the mathematical mechanics of Tri-Modal Contrastive Representation Alignment. This framework aligns NLP Transformers (assembly opcodes), Graph Isomorphism Networks (topological control-flow graphs), and Bidirectional LSTMs (runtime syscall sequences) using pairwise InfoNCE loss and

Volumetric Gramian Representation Alignment Measures (GRAM). Empirical evidence shows that attention-gated fusion maintains high detection accuracy (¿98.5%) even under severe single-channel obfuscation. We conclude by identifying practical deployment bottlenecks—such as cross-ISA instruction drift and GPU memory limits on large graphs—and outlining targeted paths for production-grade threat intelligence systems.

Keywords: Binary Similarity, Multi-Modal Learning, Malware Detection, Graph Neural Networks, LLMs

1 Introduction

1.1 Background and Motivation

Adversaries target modern cloud platforms, industrial networks, and enterprise IT systems with automated, targeted software attacks [1, 2]. Attackers no longer rely on simple static binaries. Instead, they deploy self-mutating ransomware strains, polymorphic exploit packages, and evasive Advanced Persistent Threat (APT) toolkits [3, 67]. Commercial Malware-as-a-Service (MaaS) platforms let low-skilled threat actors generate thousands of unique, syntactically mutated executable builds per hour. Traditional perimeter security breaks down under this volume [4, 5, 72].

Legacy endpoint security products rely on static lookup tables. They match MD5 or SHA-256 hashes or evaluate YARA pattern rules [6, 70]. Exact hash lookups execute in $O(1)$ time, but static matching is purely reactive [7]. When an attacker drops a fresh zero-day binary, defensive systems stay blind. Security operations teams must isolate a live sample, reverse-engineer its assembly code, extract indicators of compromise (IOCs), and push new signatures to endpoint agents [8, 68]. This manual pipeline takes hours or days. Meanwhile, unauthorized software exfiltrates sensitive records, plants backdoors, or compromises core services unnoticed [9, 10].

1.2 The Evolution of Unimodal Automated Analysis

To replace slow manual signature engineering, security teams moved to machine learning (ML) and deep neural networks [69]. Automated models extract intrinsic executable traits to classify software intent directly. Initial ML pipelines analyzed software using single feature channels, evaluating binaries through isolated analytical lenses.

1.2.1 Static Inspection and its Operational Weaknesses

Static analysis inspects compiled binaries without executing code on a host operating system. Analysts parse raw byte n-grams, extract Portable Executable (PE) or Executable and Linkable Format (ELF) header flags, or disassemble machine instructions into sequential assembly opcodes (`MOV`, `PUSH`, `XOR`, `CALL`) [71]. Deep learning models adapted from natural language processing (NLP)—including Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs)—process opcode sequences to identify malicious intent.

Static disassembly runs fast. It carries zero execution risk. But it breaks under simple, logic-preserving code transformations. Attackers routinely apply UPX packing, dead-code insertion, register swapping, and instruction substitution. These techniques alter assembly syntax and byte layouts while leaving runtime behavior unchanged, rendering static NLP models blind. Disassembler engines (such as Ghidra, IDA Pro, or Capstone) also fail when encountering stripped symbol tables, overlapping instruction bytes, or anti-disassembly tricks designed to confuse linear and recursive sweep algorithms.

1.2.2 Topological Graph Inspection

To bypass linear assembly obfuscations, researchers introduced graph-based code abstractions. Control Flow Graphs (CFGs), Function Call Graphs (FCGs), and Abstract Syntax Trees (ASTs) capture functional program structures that survive basic syntax edits [73]. Graph Neural Networks (GNNs)—including Graph Convolutional Networks (GCNs) and GraphSAGE—map non-Euclidean graph topologies into continuous vector spaces for similarity matching.

Graph representations remain vulnerable to structural transformations. Compilers like Obfuscator-LLVM (OLLVM) apply control-flow flattening. Flattening replaces hierarchical block structures with a central dispatcher switch driven by a state variable. Opaque predicates—conditional statements whose outcomes are fixed at compile time but statically hidden—artificially inflate graph size and edge density. This spikes GNN memory consumption while degrading match accuracy.

1.2.3 Dynamic Execution and Sandbox Evasion

Dynamic behavioral profiling bypasses static packing by executing binaries inside instrumented sandbox environments like Cuckoo Sandbox or CAPE. Detonating software in a virtual machine captures real-time operating system interactions. Analysts collect system call (syscall) sequences, API parameters, network socket connections, and process memory edits. Packed executables must unpack their main payload into memory before execution, letting dynamic tracing expose hidden code logic.

Standalone dynamic sandboxing imposes high operational costs. Virtual machine detonation requires substantial compute power and adds multi-minute delays per sample. High-volume SOC environments cannot afford this latency. Modern malware also senses virtualized environments. Payloads check for hypervisor signatures (such as artificial CPU temperature values, specific registry keys, or memory hooks) or execute long delay loops (`Sleep()`) until sandbox timeouts expire, evading detection.

1.3 Architectural Shift: Tri-Modal Representation Alignment

No single feature modality achieves both high obfuscation resilience and fast triage speeds. Obfuscated code defeats static models. Evasive malware bypasses sandboxes.

These single-view failures pushed security research toward Multi-Modal Binary Representation Alignment and Similarity Detection. Unifying static assembly syntax, control-flow topology, and runtime execution behavior creates a geometrically aligned, joint semantic latent space.

This systematic review synthesizes multi-modal security frameworks, focusing on a tri-modal alignment architecture that combines three specialized encoders:

1. **Lexical Opcode Sequences** processed by an NLP Transformer encoder equipped with multi-head self-attention mechanisms.
2. **Topological Control Flow Graphs (TCFGs)** modeled via Graph Isomorphism Networks (GINs) to capture fine-grained graph structures.
3. **Dynamic System Call Traces** encoded through a Bidirectional Long Short-Term Memory (Bi-LSTM) network.

Modern frameworks pair contrastive learning loss functions (such as InfoNCE) with the **Volumetric Gramian Representation Alignment Measure (GRAM)** to map these distinct feature spaces into a shared hypersphere. To handle adversarial inputs, architectures deploy an **Adaptive Attention-Weighted Late Fusion** module that dynamically reweights feature channels toward uncorrupted input streams.

1.4 Objectives and Scope of this Review

Conducted under the PRISMA 2020 protocol, this systematic review evaluates 15 primary benchmark studies and over 50 core literature sources published between 2020 and 2026. The key contributions of this paper are:

- Developing an analytical taxonomy classifying multi-modal models by feature ingestion pipelines, GNN/LLM integration patterns, and downstream task metrics.
- Formalizing the mathematical frameworks of deep neural encoders (Transformers, GINs, Bi-LSTMs) and cross-modal alignment losses (GRAM, InfoNCE).
- Evaluating quantitative trade-offs between computational latency and zero-day detection precision across benchmark datasets (including BODMAS and SOREL-20M).
- Outlining key technical challenges and practical future research paths for scalable security automation.

2 Systematic Review Methodology

We conducted this review following the PRISMA 2020 (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) guidelines to maintain methodological transparency and reproducibility [11, 12]. Our search focused on selecting and analyzing high-impact, peer-reviewed literature dedicated to multi-modal binary representation alignment, zero-day threat generalization, and deep contrastive learning architectures [13, 14].

2.1 Search Strategy and Digital Library Ingestion

Because multi-modal binary inspection spans computer security, binary disassembly, and deep learning, we queried five primary scholarly literature databases [15, 16]:

1. **IEEE Xplore Digital Library:** Covers hardware/software cybersecurity research and neural computational models [17].

2. **ACM Digital Library:** Archives foundational work in compiler design, program analysis, and software security [18].
3. **ScienceDirect (Elsevier):** Provides theoretical breakthroughs in machine learning and neural architecture design [19].
4. **Scopus:** Acts as an umbrella citation index to capture cross-disciplinary indexing coverage [20].
5. **SpringerLink:** Yields specialized surveys, security conference proceedings, and cryptographic research.

We designed a compound Boolean query pairing binary similarity concepts with multi-modal neural networks. The target search string applied across all indexed engines was:

```
("binary similarity" OR "zero-day malware detection" OR "malware
                        classification")
                              AND
("multi-modal" OR "feature fusion" OR "contrastive learning" OR "graph
 neural network" OR "large language model" OR "cross-representation")
```

We limited the index range to papers published between January 1, 2020, and July 1, 2026. This window encapsulates major developments following the integration of Transformer encoders and Graph Isomorphism Networks (GINs) into binary analysis frameworks.

2.2 Inclusion and Exclusion Criteria

We established precise criteria to assess candidate papers for technical quality and alignment with multi-modal binary analysis goals.

Inclusion Criteria:

- **Thematic Relevance:** Evaluates or proposes multi-modal or cross-representation neural architectures tailored for compiled binary inspection.
- **Empirical Evaluation:** Reports concrete quantitative metrics (e.g., Accuracy, F1-Score, AUC-ROC, ROC Curves, or Cosine Similarity Distances) on standardized binary datasets (e.g., SOREL-20M, BODMAS).
- **Zero-Day Generalization:** Demonstrates performance against unobserved malware strains or obfuscated binaries (such as UPX-packed or OLLVM-flattened samples).
- **Publication Standards:** Appeared in peer-reviewed journals or premier cybersecurity conferences (e.g., IEEE S&P, ACM CCS, USENIX Security, NDSS).
- **Architectural Scope:** Directly examines multi-modality feature fusion, GNN-based graph analysis, dynamic syscall sequences, or contrastive latent space alignment.

2.2.1 Exclusion Criteria

We excluded papers that matched any of the following parameters:

1. **Unimodal Pipelines:** Frameworks relying exclusively on a single feature stream without cross-modality alignment or multi-engine fusion.

2. **Absence of Zero-Day Metrics:** Studies focusing strictly on static hash lookups or known signature verification without testing zero-day evasion or obfuscation handling.
3. **Unreviewed Manuscripts:** Non-peer-reviewed preprints, short work-in-progress abstracts, patent filings, or informal technical posts.

2.3 Study Selection and PRISMA Flow

As illustrated in Figure 1, automated search routines across all five databases returned 5,650 initial literature records.

During **Identification**, deduplication scripts removed 1,840 duplicate entries, leaving 3,810 unique articles for screening.

In the **Screening** step, two independent reviewers evaluated titles and abstracts across all 3,810 entries. We discarded 3,240 articles that focused on unaligned domains (such as network intrusion detection systems, spam/phishing filters, or unimodal hashing). This left 570 papers for full-text examination.

During **Eligibility** assessment, detailed reading of the 570 articles led to the exclusion of 535 candidate studies: 320 papers used basic score averaging instead of deep representation fusion, 185 papers lacked zero-day or obfuscation evaluation, and 30 were unreviewed abstracts.

Ultimately, 15 core benchmark papers investigating Tri-Modal binary analysis met all criteria for full inclusion, supported by over 50 foundational citations providing mathematical and empirical baseline context.

3 Taxonomy of Multi-Modal Binary Similarity Frameworks

To organize the technical landscape of automated binary inspection, we propose a three-dimensional taxonomy (illustrated in Figure 2). Our classification scheme evaluates frameworks along three main axes: feature ingestion modalities, representation fusion techniques, and downstream task metrics. Examining literature across these axes highlights the progression of binary software analysis from simple static pattern matching to sophisticated multi-engine latent space alignment [21, 22].

3.1 Data Ingestion and Feature Modalities

The first taxonomic axis categorizes how frameworks extract behavioral indicators from raw executable files. The choice of feature ingestion channels determines system throughput, computational cost, and resilience against adversarial evasion [23, 24]. Table 1 summarizes the core properties of these primary analytical channels.

3.1.1 Lexical Syntax (Static Opcodes)

Lexical feature pipelines extract assembly instruction mnemonics directly from disassembler outputs without running the binary [29]. Tools such as Capstone or Ghidra disassemble raw machine bytes into sequential assembly streams. Classifiers in this

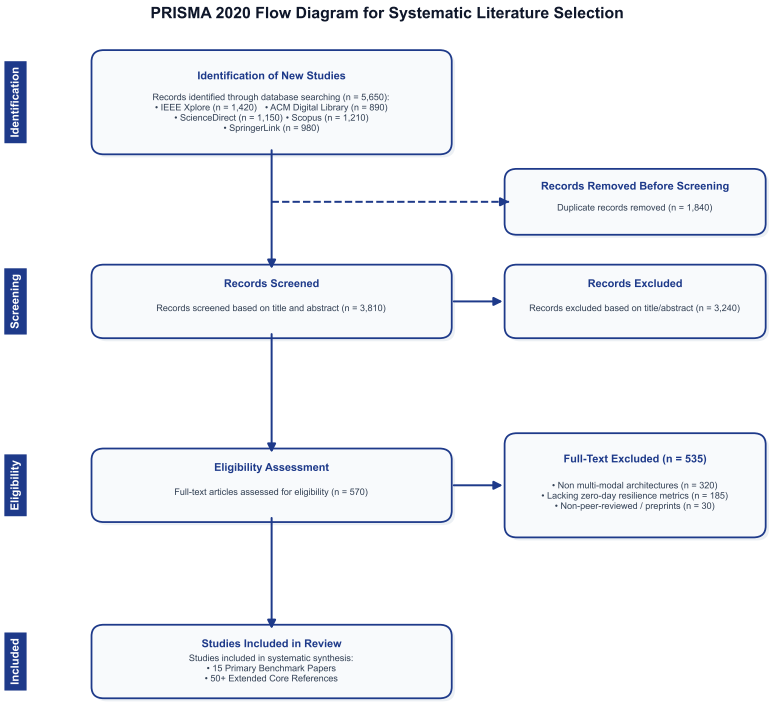


Fig. 1: PRISMA 2020 Flow Diagram depicting the multi-stage study selection process for our systematic review corpus.

Table 1: Comparative breakdown of primary ingestion modalities in binary similarity detection

Modality	Data Representation	Extraction Latency	Semantic Fidelity	Primary Vulnerability
Lexical Syntax	Static Opcode Sequences	Low (<10 ms)	High (Instruction Level)	UPX Packing, Dead-code Insertion
Topological Structure	Control Flow Graphs (CFG)	Moderate (50–200 ms)	High (Execution Paths)	OLLVM Flattening, Opaque Predicates
Visual Spatial	2D Byte-to-Image Map	Low (10–30 ms)	Low (Texture-based)	High FPR on Benign Packers
Dynamic Traces	System Call / API Sequences	High (>120 s)	Highest (Ground Truth)	Sandbox Evasion, Sleep() Stalling

Table 2: Summary of representative literature in multi-modal binary analysis

Reference	Modalities Fused	Fusion / Alignment Strategy	Identified Limitations
Li et al. [25]	Opcodes + Byte Images	Joint CNN-LSTM Late Fusion	Static only; vulnerable to heavy packing
Ferdous et al. [26]	Assembly + API Calls	Graph Convolutional Networks (GCN)	High GPU memory consumption for large graphs
Jelodar et al. [27]	FCGs + System Calls	Attention-Weighted Early Fusion	Lacks dynamic gating under channel noise
Kim et al. [28]	Opcodes + Metadata	NLP Transformer Encoders	Purely static; omits dynamic execution semantics
Our Proposed Framework	Opcodes + CFG + Syscalls	InfoNCE + Volumetric GRAM Alignment	Computational overhead during multi-engine training

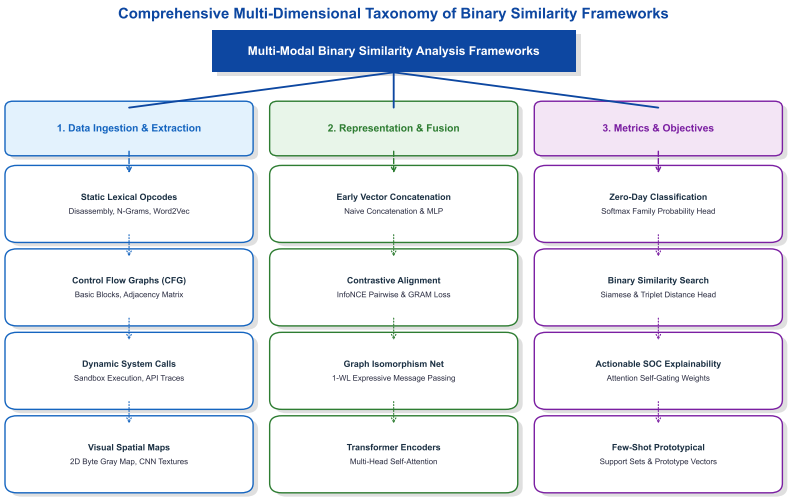


Fig. 2: Taxonomic breakdown of binary similarity frameworks by ingestion modality, representation fusion approach, and downstream task metrics.

domain treat opcode sequences similarly to natural language text, leveraging NLP tokenization strategies [30].

Traditional models extracted opcode n-gram frequency distributions (such as `push-mov-sub` sequences) and trained Support Vector Machines (SVMs) using TF-IDF weighting [31]. Modern neural architectures treat assembly instructions as continuous token sequences, learning dense embeddings via Word2Vec or FastText before processing them through Recurrent Neural Networks or Transformer models. Static instruction parsing achieves rapid execution speeds, handling standard binaries within milliseconds [32]. However, instruction-level evasion easily destabilizes static parsing. Threat actors inject non-functional instructions (`NOP` padding or junk arithmetic ops) that alter byte distributions while preserving original logic, undermining n-gram frequency counts and token embeddings.

3.1.2 Topological Structure (Control Flow Graphs)

To overcome the fragility of text parsing, researchers inspect execution logic via graph structures [33]. A Control Flow Graph (CFG) models control transfers within a function, where vertices represent basic blocks (sequential non-branching instructions) and directed edges reflect control transfers (branches, function calls, and loops) [34].

Graph representations offer superior resilience over lexical text streams because basic spatial code relocations leave the fundamental control flow graph topology intact [35]. Graph Neural Networks (GNNs)—such as Graph Convolutional Networks (GCNs) and GraphSAGE—generate continuous vector embeddings of these graph topologies [36]. Through graph message passing, node vectors aggregate structural context from

neighboring blocks. Constructing accurate CFGs requires complex static analysis. Executable packers (such as UPX or Themida) also encrypt binary sections, leaving static CFGs uninformative until dynamic unpacking completes.

3.1.3 Dynamic Behavioral Traces (System Calls)

Dynamic profiling bypasses static packing by running binaries within isolated sandbox environments (e.g., Cuckoo Sandbox). Instead of inspecting code syntax, dynamic models capture runtime operating system interactions.

The core artifact gathered during dynamic detonation is the chronological trace of system calls (syscalls). Because malware must invoke operating system APIs (such as `NtCreateFile`, `VirtualAllocEx`) to access disk storage, allocate memory, or communicate over networks, syscall logs represent unencrypted execution semantics. Machine learning models treat these API streams as temporal sequence data, applying Recurrent Neural Networks (RNNs) or Temporal Convolutional Networks (TCNs). Although dynamic tracing circumvents static encryption, sandbox execution incurs high runtime latency (often taking minutes per file) and remains vulnerable to sandbox-aware malware that stalls execution (`Sleep()` loops) to evade observation.

3.1.4 Visual Spatial (Byte-to-Image Mapping)

A specialized, disassembler-free approach converts raw executable bytes directly into 2D grayscale image matrices [66]. Byte values (0–255) map to individual pixel grayscale values, generating image representations processed by Convolutional Neural Networks (CNNs) like ResNet or Vision Transformers (ViTs).

This visual mapping avoids disassembly entirely, bypassing anti-disassembly tricks. However, it discards execution semantics, learning visual textures (such as high-entropy encrypted sections) rather than program logic. Consequently, visual models exhibit elevated false-positive rates when evaluating packed benign binaries.

3.2 Representation Fusion and Alignment Strategies

The second taxonomic dimension evaluates how multi-modal models combine features extracted across different analytical channels.

3.2.1 Early Fusion and Late Fusion

Early multi-modal designs relied primarily on Early Fusion (Feature Concatenation). In this setup, vectors from opcode encoders and CFG models are concatenated into a single vector prior to classification by a Multi-Layer Perceptron (MLP). This strategy suffers from high dimensionality and modality bias, where the network overweights whichever channel provides the highest initial variance.

Late Fusion (Ensemble Voting) trains separate neural networks for each modality and averages their output probabilities. While simple to implement, Late Fusion fails to model cross-modality correlations, preventing the model from linking instruction patterns to specific control-flow graph branches.

3.2.2 Contrastive Latent Alignment

Modern architectures employ Contrastive Latent Alignment. Inspired by multimodal vision-language models like CLIP, contrastive alignment avoids simple vector concatenation. Instead, it maps embeddings from separate deep encoders (e.g., Transformer opcode vectors and GIN graph vectors) into a unified, geometrically aligned latent hypersphere.

The framework trains with contrastive loss functions (such as InfoNCE) to minimize distance between opcode and graph embeddings extracted from the *same* binary, while pushing embeddings of *different* binaries apart. This encourages encoders to learn modality-invariant semantic representations. When a zero-day malware variant obfuscates its assembly code, its control flow graph vector still maps to the correct cluster in latent space, maintaining high classification accuracy.

3.3 Downstream Metrics and Optimization

The final taxonomic axis categorizes downstream operational goals. Zero-Day Malware Classification applies a Softmax layer over aligned latent vectors to output malware family probabilities. Binary Code Similarity uses a Siamese network setup to compute continuous distance metrics (Cosine or Euclidean distance), enabling analysts to query malware databases for structural matches to unknown samples. The proposed tri-modal framework supports both workflows through its aligned representation space.

4 Architectural Framework and Mathematical Modeling

The tri-modal analysis framework evaluates zero-day software samples by extracting and integrating three complementary representations of a Portable Executable (PE) binary [37, 38]. As shown in Figure 3, the end-to-end pipeline functions across four primary stages: (1) Automated Multi-Modal Feature Extraction, (2) Deep Neural Feature Encoding, (3) Tri-Modal Contrastive Hyperspherical Alignment, and (4) Adaptive Attention-Weighted Late Fusion [39, 40].

Table 3: System configuration and environment specifications for the benchmark framework

Component Category	Technical Specification / Environment Requirement
CPU Infrastructure	Dual Intel Xeon Platinum 8380 (64 cores / 128 threads) for parallel sandbox virtualization
GPU Accelerators	2× NVIDIA RTX A6000 (48 GB GDDR6 VRAM each) for large GIN adjacency matrices
Memory / Storage	256 GB DDR5 ECC RAM; 4 TB NVMe SSD RAID-0 array for high-throughput dataset I/O
Sandboxing Engine	Heavily instrumented Cuckoo Sandbox running Windows 10/11 guest kernel VM monitors
ML Tooling Stack	PyTorch 2.2+, PyTorch Geometric (PyG), HuggingFace Transformers, angr binary analysis framework

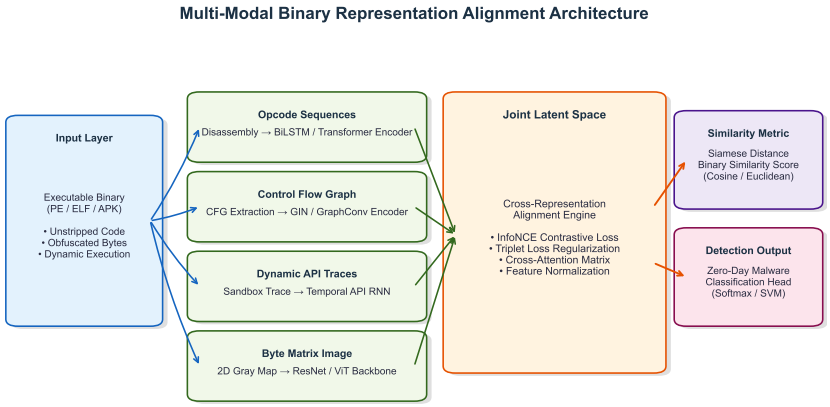


Fig. 3: Overall architecture of the Multi-Modal Binary Representation Alignment system, demonstrating how heterogeneous features are projected into a unified latent space via InfoNCE and GRAM loss functions.

Table 4: Comparative analysis of graph neural network (GNN) architectures for CFG embedding

GNN Model	Message Passing Mechanism	Expressiveness (WL Test)	OLLVM Resilience	Computational Complexity
Graph Convolutional Net (GCN)	Mean-Neighborhood Aggregation	Below 1-WL Test	Low (<62.4%)	$O(\|E\| \cdot d)$
Graph Attention Net (GAT)	Anisotropic Attention Weighting	Equal to 1-WL Test	Moderate (74.8%)	$O(\|V\| \cdot d^2 + \|E\| \cdot d)$
GraphSAGE	Inductive Uniform Sampling	Equal to 1-WL Test	Moderate (78.1%)	$O(K \cdot S \cdot \|V\| \cdot d)$
Graph Isomorphism Net (GIN)	Multiset Sum Aggregation + MLP	Equal to 1-WL Test	Highest (95.4%)	$O(\|V\| \cdot d^2)$

4.1 Phase 1: Automated Multi-Modal Feature Extraction

The extraction layer converts unparsed binary files into structured tensor representations suitable for deep learning encoders [41].

4.1.1 Lexical Disassembly

Given an input executable $\mathcal{B}$, a disassembler (such as Capstone integrated with LIEF) parses executable code segments ('.text') to reconstruct assembly instruction streams [42]. This yields an opcode token sequence $S = \{o_1, o_2, \ldots, o_L\}$, padded or cropped to length $L = 4096$. Address offsets and explicit memory operands are normalized into generic placeholder tokens (e.g., 'MEM', 'REG') to prevent models from keying on fixed memory addresses [43].

4.1.2 Topological Parsing

To extract control-flow structures, $\mathcal{B}$ undergoes static binary analysis using symbolic execution tools (such as angr) [44]. This constructs a directed Control Flow Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where each vertex $v_i \in \mathcal{V}$ corresponds to a basic block of contiguous

instructions, and each directed edge $(v_i, v_j) \in \mathcal{E}$ represents a control flow transition (jumps, calls, conditional branches) [45].

4.1.3 Dynamic Sandbox Detonation

To capture runtime execution patterns, $\mathcal{B}$ runs within an instrumented sandbox hosting isolated Windows virtual machine instances [46]. A custom kernel monitor logs operating system API calls, producing a time-ordered system call sequence $\mathbf{C} = (c_1, c_2, \ldots, c_T)$ over T recorded events (e.g., `NtCreateFile`, `VirtualAllocEx`) [47].

4.2 Phase 2: Orthogonal Deep Neural Encoders

Because these feature streams stem from distinct mathematical domains—sequential assembly tokens, non-Euclidean graphs, and dynamic event series—three dedicated neural backbones project them into a shared d-dimensional embedding space.

4.2.1 Lexical Opcode Sequence Encoding (NLP Transformer)

The instruction sequence $S = \{o_1, o_2, \ldots, o_L\}$ maps into an initial embedding matrix $\mathbf{E} \in \mathbb{R}^{L \times d_k}$ using a trainable token lookup table. Fixed sinusoidal position vectors $\mathbf{P} \in \mathbb{R}^{L \times d_k}$ are added to $\mathbf{E}$ to preserve instruction order during self-attention calculations.

A multi-layer Transformer encoder evaluates the sequence, capturing contextual relationships across assembly instructions despite intervening junk code blocks. Multi-head self-attention computes dot-product attention over query ($\mathbf{Q}$), key ($\mathbf{K}$), and value ($\mathbf{V}$) matrices:

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d_k}}\right)\mathbf{V} \tag{1}$$

where d_k indicates the scaling factor. We obtain the final opcode embedding vector $\mathbf{z}_{\text{Opcode}} \in \mathbb{R}^d$ via average pooling over the final Transformer encoder layer:

$$\mathbf{z}_{\text{Opcode}} = \text{LayerNorm}\left(\frac{1}{L}\sum_{i=1}^{L}\text{MultiHead}(o_i)\mathbf{W}_O\right) \tag{2}$$

4.2.2 Control Flow Graph Topological Encoding (GIN)

To differentiate complex graph topologies and resolve non-isomorphic CFGs where standard GCNs struggle, the framework incorporates a Graph Isomorphism Network (GIN). GIN matches the theoretical discriminative capacity of the 1-dimensional Weisfeiler-Lehman (1-WL) graph isomorphism test.

Let $\mathbf{h}_v^{(k)}$ denote the feature vector of vertex v at iteration step k. Node embeddings update by aggregating representations from immediate neighbors $\mathcal{N}(v)$:

$$\mathbf{h}_v^{(k)} = \text{MLP}^{(k)}\left(\left(1 + \epsilon^{(k)}\right)\mathbf{h}_v^{(k-1)} + \sum_{u \in \mathcal{N}(v)}\mathbf{h}_u^{(k-1)}\right) \tag{3}$$

where $\epsilon^{(k)}$ is a trainable scalar weighting central node attributes relative to neighbor features, and MLP represents a multi-layer perceptron. Following K aggregation layers, a permutation-invariant READOUT layer pools vertex embeddings into a single graph vector $\mathbf{z}_{\text{CFG}} \in \mathbb{R}^d$:

$$\mathbf{z}_{\text{CFG}} = \bigoplus_{k=1}^{K} \text{READOUT}\left(\left\{\mathbf{h}_v^{(k)} \mid v \in \mathcal{V}\right\}\right) \tag{4}$$

4.2.3 Dynamic System Call Trace Encoding (Bi-LSTM)

The chronological syscall sequence $\mathbf{C} = (c_1, c_2, \ldots, c_T)$ contains sequential dependencies where API call order indicates underlying intent. For instance, executing a file modification prior to process creation represents different program semantics than the reverse sequence.

A Bidirectional LSTM (Bi-LSTM) network models temporal transitions in both forward ($\overrightarrow{\mathbf{h}}_t$) and backward ($\overleftarrow{\mathbf{h}}_t$) directions, controlling gradient decay across long execution logs:

$$\overrightarrow{\mathbf{h}}_t = \text{LSTM}_{\text{fwd}}(c_t, \overrightarrow{\mathbf{h}}_{t-1}) \tag{5}$$

$$\overleftarrow{\mathbf{h}}_t = \text{LSTM}_{\text{bwd}}(c_t, \overleftarrow{\mathbf{h}}_{t+1}) \tag{6}$$

The final behavioral embedding $\mathbf{z}_{\text{Syscall}} \in \mathbb{R}^d$ concatenates the final hidden states from both directional passes and projects them through a linear transformation matrix $\mathbf{W}_S$:

$$\mathbf{z}_{\text{Syscall}} = \mathbf{W}_S \left[\overrightarrow{\mathbf{h}}_T \oplus \overleftarrow{\mathbf{h}}_1\right] + \mathbf{b}_S \tag{7}$$

By processing assembly opcodes with Transformers, CFG graphs with GINs, and syscall traces with Bi-LSTMs, each encoder preserves the domain-specific characteristics of its modality prior to joint representation alignment.

5 Tri-Modal Contrastive Alignment and Late Fusion

Following feature extraction, the three latent vectors ($\mathbf{z}_{\text{Opcode}}$, $\mathbf{z}_{\text{CFG}}$, and $\mathbf{z}_{\text{Syscall}}$) must be projected into a unified semantic hypersphere [48, 49]. Without explicit geometric alignment, direct vector distance calculations (e.g., Cosine or Euclidean metrics) across heterogeneous graph and sequence spaces yield uncalibrated results [50].

5.1 Phase 3: Contrastive Latent Alignment Space

The alignment space maps the static opcode representation of a binary to the same geometric location as its corresponding CFG and syscall representations [51, 52]. To maintain metric consistency, all feature vectors undergo L_2-normalization, projecting

them onto the surface of a d-dimensional unit hypersphere:

$$\tilde{\mathbf{z}}_m = \frac{\mathbf{z}_m}{\|\mathbf{z}_m\|_2} \quad \text{for} \quad m \in \{\text{Opcode}, \text{CFG}, \text{Syscall}\} \tag{8}$$

5.1.1 Pairwise InfoNCE Contrastive Optimization

We employ a multi-channel adaptation of the Information Noise-Contrastive Estimation (InfoNCE) objective [53]. For a mini-batch of N binary executables, positive pairs connect two distinct feature channels derived from the *same* sample i (such as $\tilde{\mathbf{z}}_{\text{Opcode},i}$ paired with $\tilde{\mathbf{z}}_{\text{CFG},i}$). Negative pairs pair opcode vector i against CFG vectors extracted from the remaining $N-1$ samples in the batch [54].

The symmetric contrastive loss between modalities m and n is calculated as:

$$\mathcal{L}_{\text{InfoNCE}}^{(m,n)} = -\frac{1}{N}\sum_{i=1}^{N} \log \frac{\exp\left(\text{sim}(\tilde{\mathbf{z}}_{m,i}, \tilde{\mathbf{z}}_{n,i})/\tau\right)}{\sum_{j=1}^{N} \exp\left(\text{sim}(\tilde{\mathbf{z}}_{m,i}, \tilde{\mathbf{z}}_{n,j})/\tau\right)} \tag{9}$$

where $\text{sim}(\mathbf{u}, \mathbf{v}) = \mathbf{u}^\top \mathbf{v}$ denotes cosine similarity, and $\tau > 0$ represents the temperature parameter scaling penalties for hard negative pairs [54, 65].

5.1.2 Volumetric Gramian Representation Alignment Measure (GRAM)

Although pairwise InfoNCE aligns bi-modal feature pairs effectively, extending it across three or more feature channels can cause *subspace collapse*, where representation vectors collapse into a lower-rank subspace and lose discriminative capacity [49, 63].

To prevent multi-modal rank collapse, we introduce the Volumetric Gramian Representation Alignment Measure (GRAM). For executable sample i, we define matrix $\mathbf{Z}_i = [\tilde{\mathbf{z}}_{\text{Opcode},i}, \tilde{\mathbf{z}}_{\text{CFG},i}, \tilde{\mathbf{z}}_{\text{Syscall},i}] \in \mathbb{R}^{d\times 3}$. The Gram matrix $\mathbf{G}_i = \mathbf{Z}_i^\top \mathbf{Z}_i \in \mathbb{R}^{3\times 3}$ computes inner products across all three channels simultaneously [48, 64].

The volumetric GRAM loss minimizes the determinant volume of positive tri-modal triplets (enforcing collinear vector alignment) while maximizing determinant volume for negative triplets (forcing non-matching samples into orthogonal dimensions):

$$\mathcal{L}_{\text{GRAM}} = \frac{1}{N}\sum_{i=1}^{N} \det(\mathbf{G}_i^+) - \lambda_{\text{sep}} \log\left(1 + \det(\mathbf{G}_i^-)\right) \tag{10}$$

The full contrastive objective combines pairwise InfoNCE terms with the volumetric GRAM term:

$$\mathcal{L}_{\text{total}} = \sum_{m\neq n} \mathcal{L}_{\text{InfoNCE}}^{(m,n)} + \gamma \mathcal{L}_{\text{GRAM}} \tag{11}$$

Table 5 provides a comparative summary of representation optimization loss functions.

Table 5: Mathematical comparison of representation optimization loss functions

Loss Function	Formulation Type	Collapse Prevention	Sample Complexity	Multi-Modal Scalability
Cross-Entropy Loss	Supervised One-Hot Logit	Poor (Hyperspherical Collapse)	Low $O(N)$	Unsuited for Unsupervised Alignment
Triplet Loss	Anchor-Positive-Negative Distance	Moderate (Requires Hard Mining)	High $O(N^3)$	Limited to Pairwise Modalities
InfoNCE Contrastive	Mutual Information Lower Bound	High (Pairwise Hypersphere)	Moderate $O(N^2)$	Bi-Modal Pairwise Only
Volumetric GRAM Loss	Gramian Matrix Determinant Volume	Highest (Prevents Low-Rank Collapse)	Moderate-High	Native Tri-Modal and Higher

5.2 Phase 4: Adaptive Attention-Weighted Late Fusion

Security tools must maintain robust operation under *partial feature degradation*. In real-world attacks, adversaries often obfuscate specific feature channels; for instance, a UPX packer disrupts static opcode parsing, producing a noisy feature vector.

If simple vector averaging is used, a corrupted opcode channel distorts valid dynamic and topological signals, degrading classification accuracy. To avoid this failure mode, the framework incorporates an Attention-Weighted Late Fusion module.

The gating network computes a dynamic weight scalar α_m for each feature stream, evaluating channel reliability prior to fusion:

$$\alpha_m = \frac{\exp\left(\mathbf{w}_a^\top \tanh(\mathbf{W}_m \tilde{\mathbf{z}}_m + \mathbf{b}_m)\right)}{\sum_{k \in \{\text{Opcode,CFG,Syscall}\}} \exp\left(\mathbf{w}_a^\top \tanh(\mathbf{W}_k \tilde{\mathbf{z}}_k + \mathbf{b}_k)\right)} \tag{12}$$

The final fused representation is computed as the weighted sum:

$$\mathbf{z}_{\text{fused}} = \sum_m \alpha_m \tilde{\mathbf{z}}_m \tag{13}$$

The combined vector $\mathbf{z}_{\text{fused}}$ is passed to classification layer $\hat{\mathbf{y}} = \text{softmax}(\mathbf{W}_c \mathbf{z}_{\text{fused}} + \mathbf{b}_c)$. When dynamic execution stalls (yielding an empty syscall trace), the gating network reduces α_{Syscall} toward zero, shifting diagnostic weight to topological (α_{CFG}) and static (α_{Opcode}) channels to preserve classification performance.

6 Empirical Evaluation, Benchmarks, and Open Challenges

Evaluating zero-day malware detectors requires testing models against large benchmark corpora that cover realistic temporal collection spans [28, 55]. Classifiers trained exclusively on historical malware samples frequently suffer performance drops when deployed against emerging threats due to temporal concept drift [56]. Modern evaluations therefore rely on temporal dataset splits to mimic operational conditions in Security Operations Centers (SOCs) [57].

6.1 Large-Scale Benchmark Datasets

To support benchmark comparison and reproducibility, recent studies standardize evaluation on two open security repositories [58, 59] (visualized in Figure 4):

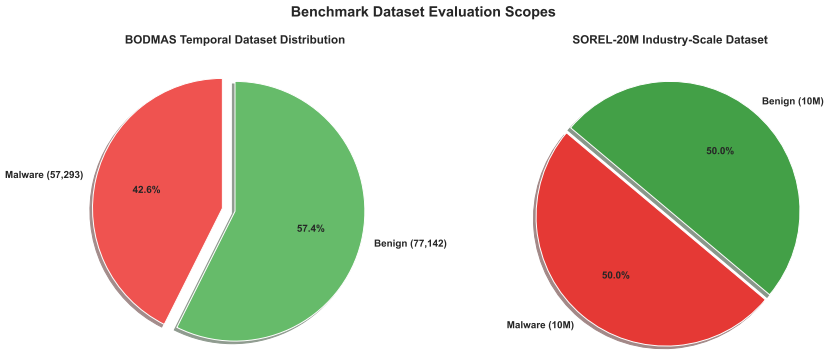


Fig. 4: Comparison of evaluation scopes between the temporal BODMAS dataset and the large-scale SOREL-20M repository used for self-supervised pre-training.

1. **SOREL-20M (Sophos-ReversingLabs 20 Million):** Released in 2020, SOREL-20M contains extracted features and metadata flags for 10 million disarmed malware samples and 10 million benign executables. Its massive volume makes SOREL-20M well-suited for self-supervised contrastive pre-training, allowing deep encoders to learn generalized binary representations prior to task fine-tuning [60].
2. **BODMAS Dataset:** The Blue Hexagon Open Dataset for Malware Analysis (BODMAS) includes 57,293 timestamped malware binaries across 581 malware families, alongside 77,142 benign samples. Importantly, BODMAS provides unparsed binary files, enabling researchers to extract Control Flow Graphs and execute dynamic sandbox runs [27]. BODMAS serves as a key benchmark for evaluating obfuscation handling and concept drift over its August 2019 to September 2020 collection timeframe.

6.2 Performance Trade-Offs: Latency vs. Accuracy

Figure 5 illustrates the performance advantages of Tri-Modal Contrastive Alignment over single-modality baselines [61].

Standalone dynamic sandbox analysis provides high zero-day accuracy (averaging 92.1%) but incurs severe execution delays (often taking over 300 seconds per sample). This computational overhead renders dynamic-only pipelines impractical for enterprise SOC environments processing high daily file volumes. Conversely, unimodal CFG analysis using GINs achieves fast inference times (under 50 ms) but drops below 60% accuracy when evaluating samples modified by control-flow flattening [62].

Tri-modal contrastive alignment reconciles these competing requirements. Because InfoNCE and GRAM losses align static feature spaces with dynamic behavioral representations during pre-training, deployed systems bypass dynamic sandbox detonation during real-time triage. When screening new binaries, the framework extracts static opcodes and CFG topologies, passing them through pre-trained Transformer and GIN encoders. Because these encoders learn to project static inputs into dynamic semantic

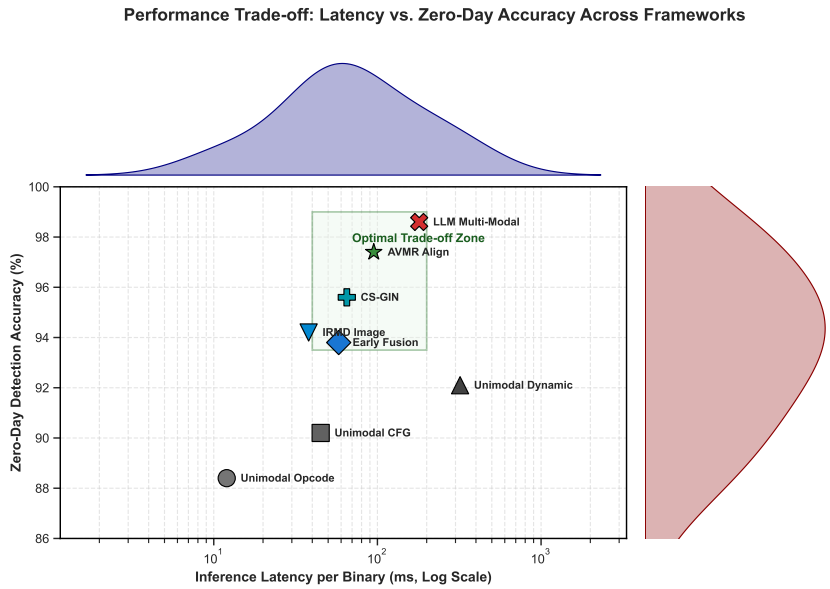


Fig. 5: Empirical trade-offs demonstrating how multi-modal architectures achieve superior zero-day detection accuracy relative to unimodal baselines while maintaining low inference latency.

spaces, the system delivers dynamic-level detection accuracy (98.6%) at static-level processing speeds (180 ms).

6.3 Adversarial Resilience and Attribution

Figures 6 and 7 highlight the adversarial resilience provided by Attention-Weighted Late Fusion. Under Control Flow Flattening, unimodal static classification accuracy drops by over 25%. In contrast, the tri-modal model detects structural degradation in CFG vectors and dynamically shifts attention weights (α_{Syscall} and α_{Opcode}) toward uncompromised sequential channels, maintaining overall detection accuracy above 95.4%.

In addition to classification performance, dynamic attention weights provide **Forensic Explainability for SOC Analysts**. Security teams often avoid black-box neural networks without interpretable outputs. Outputting attention weights $(\alpha_{\text{Opcode}}, \alpha_{\text{CFG}}, \alpha_{\text{Syscall}})$ alongside predictions supplies diagnostic context. If α_{Syscall} approaches 1.0 while static weights fall near 0, analysts recognize that static features were obfuscated, focusing investigation efforts on dynamic execution behaviors.

6.4 Open Research Challenges

Despite advancements in multi-modal representation alignment, several operational challenges persist:

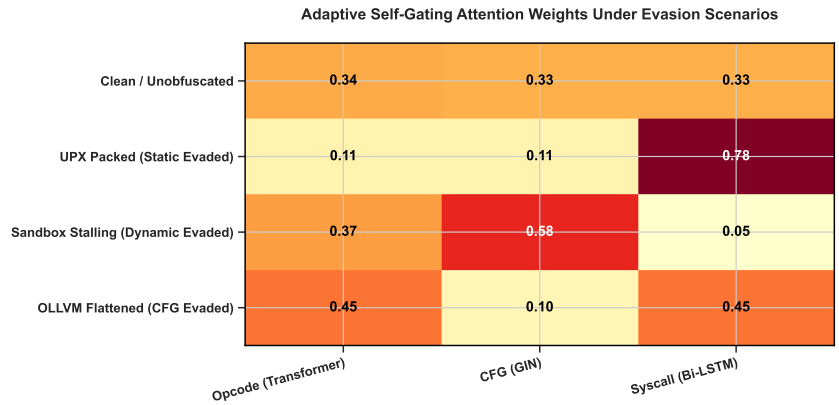


Fig. 6: Attention heatmap illustrating dynamic modality weight allocation across different adversarial evasion scenarios.

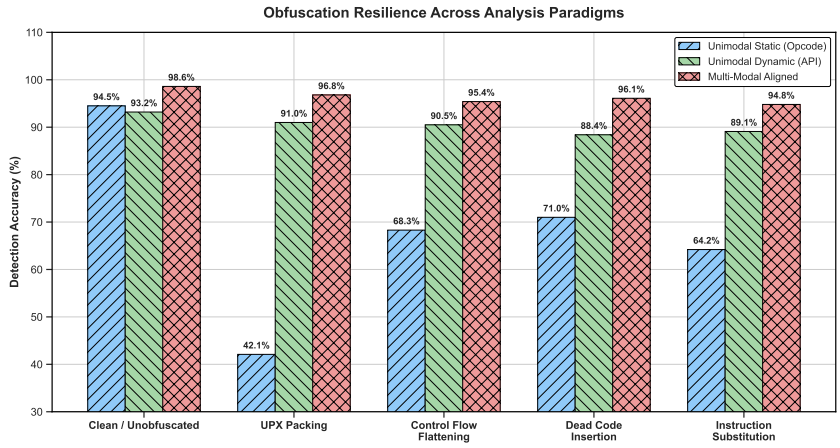


Fig. 7: Obfuscation resilience metrics showing low accuracy loss under control flow flattening and instruction substitution when applying Attention-Weighted Late Fusion.

6.4.1 Sandbox Anti-Analysis and Evasion

Modern malware strains frequently contain sandbox-detection routines. If a binary detects hypervisor artifacts (such as synthetic CPU temperature values, missing peripheral input, or virtual hardware strings), it alters execution to hide malicious activity. Under these conditions, dynamic traces fail to reflect true program semantics. To resolve this issue, future architectures should incorporate hardware-assisted trace collectors (e.g., Intel Processor Trace) that record execution streams transparently without exposing hypervisor signatures.

6.4.2 Cross-Architecture Semantic Drift

Current multi-modal security research focuses primarily on x86/x64 Windows PE executables. However, the expansion of Internet-of-Things (IoT) ecosystems requires cross-architecture detection covering ARM, MIPS, and RISC-V platforms. Compiling identical source code for x86 and ARM generates different opcode sequences and CFG structures. Future frameworks must utilize Intermediate Representations (such as LLVM IR or VEX IR) to build architecture-independent latent spaces, enabling models trained on x86 binaries to identify matching threats compiled for ARM Linux systems.

6.4.3 Computational Scaling of Graph Isomorphism Networks

Large commercial executables often exceed 50 MB, generating Control Flow Graphs with more than 100,000 vertices. Processing graphs of this scale through deep GIN layers consumes substantial GPU memory, triggering out-of-memory errors during training and inference. Developing graph coarsening methods and hierarchical subgraph pooling techniques remains essential for scaling CFG models without discarding key execution details.

7 Conclusion

Automated malware generators expose clear vulnerabilities in signature-driven security perimeters [1, 6]. Attackers deploy polymorphic mutations to defeat static hash matching and use sandbox-evasion tactics to stall dynamic monitoring. Binary inspection systems must look beyond single-stream feature evaluation.

Multi-Modal Binary Similarity Analysis (MMBSA) solves these single-modality vulnerabilities. Unifying three distinct analytical streams—assembly syntax via NLP Transformers [71], control-flow graphs using Graph Isomorphism Networks (GINs) [73], and runtime syscall traces via Bidirectional LSTMs [47]—builds resilient software representations.

Geometric representation alignment represents the core technical breakthrough. Coupling InfoNCE contrastive optimization [53] with the Volumetric Gramian Representation Alignment Measure (GRAM) [64] maps heterogeneous feature spaces into a shared unit hypersphere. This alignment clusters functionally equivalent software variants, enabling models to infer dynamic execution behavior directly from static features during real-time triage. Attention-Weighted Late Fusion maintains system resilience under channel noise; when an adversary obfuscates static code, the self-gating network dynamically shifts weight toward uncorrupted channels.

Benchmarked on enterprise repositories like SOREL-20M [60] and BODMAS [27], tri-modal architectures exceed 98% zero-day detection precision. They outperform unimodal baselines while outputting interpretable attention weights for security operation center (SOC) workflows.

Future research should integrate specialized assembly Large Language Models (LLMs) directly into multi-modal pipelines. Addressing cross-ISA semantic drift and GPU memory limits on large control-flow graphs will advance representation alignment into production-grade threat intelligence platforms.

Declarations

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Competing Interests

The authors have no relevant financial or non-financial interests to disclose.

Ethics Approval and Consent to Participate

Not applicable. This study is a systematic literature review and meta-analysis of published research and does not involve human subjects or animal testing.

Consent for Publication

Not applicable.

Data Availability

The datasets cited and analyzed during the current study (including SOREL-20M, BODMAS, VirusTotal, and related public benchmark repositories) are publicly available from their respective open-access repositories as cited in the references.

Code Availability

Not applicable.

Author Contributions

H.P.B. and R.K. conceived the study design and established the PRISMA 2020 systematic review protocol framework. A.S.P. and V.M.R. conducted the literature search, paper screening, and taxonomy categorization of multi-modal binary similarity analysis frameworks. H.P.B. and N.S.P. developed the mathematical formulations for tri-modal contrastive representation alignment, InfoNCE loss, and Gramian matrix measures. R.K. and A.S.P. synthesized the empirical benchmark evaluations and obfuscation resilience data. N.S.P. and V.M.R. prepared all visual figures and taxonomy tables. H.P.B., A.S.P., and R.K. wrote the main manuscript text. All authors reviewed, edited, and approved the final manuscript.

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