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Original Research Paper

A Zero-Shot Transformer–Graph Neural Network Framework for Unknown Cyberattack Pattern Recognition in IoT Networks

M. Kaliappan[1], S. Vimal[2], Karpagavalli C[3], Ramnath M[4], Tania Singh[5], Gaurav Dhiman[6]

[1]Department of Artificial Intelligence and Data Science, Ramco Institute of Technology, Rajapalayam, Tamil Nadu 626117, India (e-mail: kaliappan@ritrjpm.ac.in).
[2]Department of Computer Science and Engineering, KIT- Kalaignar Karunanidhi Institute of Technology, Coimbatore, Tamil Nadu 641402 India (e-mail: svimal@kitcbe.ac.in)
[3]Department of Artificial Intelligence and Data Science, Ramco Institute of Technology, Rajapalayam, Tamil Nadu 626117, India (e-mail: karpagavalli@ritrjpm.ac.in)
[4]Department of Artificial Intelligence and Data Science, Ramco Institute of Technology, Rajapalayam, Tamil Nadu 626117, India (e-mail: ramnath@ritrjpm.ac.in)
[5]UILS, Panjab University, Chandigarh, India
[6]School of Sciences and Emerging Technologies, Jagat Guru Nanak Dev Punjab State Open University, Patiala-147001, Punjab, India
(email: gdhiman0001@gmail.com)

Abstract

The exponential growth of Internet of Things (IoT) devices has led to an unprecedented rise of cyberattacks, many of which are new, unseen attack families that cannot be handled by traditional signature-based and closed-set classification systems. Traditional intrusion detection systems (IDS) fail catastrophically when facing zero-day threats or emerging attack categories, and this limitation poses critical risks to smart infrastructure, industrial IoT and edge computing environments. In this paper, we propose ZT-GraFormer: a Zero-Shot Transformer–Graph Neural Network framework with a multi-head Transformer encoder for extracting temporal and sequential traffic pattern and a dynamic k-Nearest Neighbor (kNN) graph construction mechanism along with dual GraphSAGE layers for propagating relational cyberattack pattern. It contains an auxiliary reconstruction based anomaly scoring module that combines mean squared error (MSE) reconstruction loss and energy based scoring for robust detection of unseen attack categories without any prior exposure to their samples during training. Extensive experiments on the UNSW-NB15 benchmark dataset show that ZT-GraFormer achieves 99.14% classification accuracy and 98.72% macro-F1 score on the known attack categories, outperforming the next best approach by 0.93 percentage points in terms of accuracy. For zero-shot unseen attack detection, the framework achieves 0.9876 AUROC and 0.9712 Average Precision, significantly outperforming the previous state-of-the-art methods including GNN-IDS, HeteroGNN, and BERT-IDS variants. ZT-GraFormer raises the bar for AI-based cyberattack pattern recognition in IoT networks, providing a solution that is both practically deployable and theoretically sound for open-world intrusion detection. Release of source code and pre-trained models for reproducibility.

Keywords: ***IoT cybersecurity; Transformer networks; Graph Neural Networks; Zero-shot learning; Intrusion detection; UNSW-NB15; Anomaly detection; Attack pattern recognition***

1. Introduction

The Internet of Things (IoT) ecosystem has experienced explosive growth with global deployments expected to exceed 29 billion connected devices by 2030 [1]. At the same time, this hyper-connectivity has also increased the attack surface of cyber-attacks to an unprecedented extent, rendering critical infrastructure such as smart grids, autonomous vehicles, industrial control systems (ICS/SCADA), and healthcare IoT vulnerable to advanced adversarial threats. Different from traditional networked systems, IoT devices are limited by the limits of computational resources, heterogeneous communication

[1]Department of Artificial Intelligence and Data Science, Ramco Institute of Technology, Rajapalayam, Tamil Nadu, India
[2]Department of Computer Science and Engineering, St Peter's College of Engineering and Technology, Chennai, Tamil Nadu, India
[3]Department of Computer Science and Engineering, J.P. College of Engineering, Thenkasi, Tamil Nadu, India
[4]Department of Information Technology, National Engineering College, Kovilpatti, Tamil Nadu, India
(e-mail: [1]kalsrajan@yahoo.co.in; [2]preethy2704@gmail.com; [3]jaysen1984@gmail.com; [4]jeyamaran2002@gmail.com).

***Corresponding Author:**

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protocols, and relaxed security configurations, which make them susceptible to exploitation [2].

Network intrusion detection systems (NIDS) serve as the first line of defense for IoT networks, but their efficacy is inherently constrained by their reliance on predefined signature libraries or closed-set classification paradigms [3]. Existing systems suffer from catastrophic degradation of the detection performance against emerging attack families, including novel variants of Distributed Denial of Service (DDoS), adversarial fuzzing, shellcode injections, backdoor implants, and zero-day exploits, where detection rates drop below 40% for truly unseen attack categories [4]. This is the main security challenge considered in this paper.

Recent advances in deep learning, especially in the areas of Transformer architectures and Graph Neural Networks (GNNs), have shown remarkable capacities to model complex sequential and relational patterns in high-dimensional data [5, 6]. Transformers, originally designed for natural language processing, have been proven to be effective in analyzing network traffic by capturing long-range temporal dependencies of flow sequences [7]. Simultaneously, GNNs have allowed for relational reasoning on network topology graphs, helping to learn structural patterns related to attack propagation [8].

An important opportunity remains unexploited at the confluence of these two paradigms: combining the sequential modeling power of Transformers with the structural reasoning capabilities of GNNs, boosted by principles of zero-shot learning, to build a unified framework for detecting both known and previously unseen attack patterns in IoT network traffic. This paper exploits this opportunity by the proposed ZT-GraFormer architecture.

The current IoT threat landscape is characterized by increasing sophistication, polymorphism, and adversarial evasion. Important threat classes relevant to this work include: (i) Known multi-class attacks: DoS, DDoS, Exploits, Fuzzers, Generic attacks, and Reconnaissance, all included in training data; (ii) Zero-day and unseen attacks—novel Worms, Shellcode payloads, and Backdoor families withheld from training; and (iii) Adversarial evasion subtle traffic obfuscation designed to evade anomaly detectors [9, 10]. The primary evaluation benchmark is the UNSW-NB15 dataset [11], which contains more than 2.5M network records, covering 9 attack categories. Worms, shellcode, and backdoors are treated as held-out zero-shot categories to mimic real-world open-set threat scenarios. Main contributions of the paper may be presented as follows:

(1) ZT-GraFormer Architecture: A unique architecture which merges multi-head self-attention, dynamic kNN graph generation and two GraphSAGE layers into one end-to-end trainable neural network architecture aimed at network intrusion detection;

(2) Zero-Shot Detection Module: An innovative anomaly scoring technique combining MSE reconstruction error and energy-based scoring method utilizing validation set quantiles and allowing zero-shot attack family detection;

(3) State-of-the-art performance metrics: 99.14% accuracy and 98.72% macro-F1 on UNSW-NB15 data set, 0.9876 zero-shot AUROC significantly outperforming six other competitive approaches.

(4) Comprehensive analysis of results: Multiple ablation experiments, class-based analysis, analysis of anomalies' scores distribution, comparison with state-of-the-art techniques developed between 2021 and 2026.

This paper is structured as follows: Section 2 provides literature review published between 2021 and 2026. Section 3 gives details about the proposed ZT-GraFormer architecture with its mathematical formulation. Section 4 provides the experimental part including setup and results. Section 5 illustrates comparative analysis. Section 6 concludes with discussion of future works.

2. Literature Review

Thakkar & Lohiya (2021) [1] proposed a comprehensive taxonomy of deep learning-based IDS solutions comprising CNN, LSTM, and autoencoder. These models are evaluated using 22 data sets, NSL-KDD and UNSW-NB15, where the baseline models are created and the multi-class class imbalance is identified as the key obstacle to practical use. The accuracy of hybrid CNN-LSTM techniques in UNSW-NB15 is 93.4%. Another intriguing research paper by Ullah & Mahmoud (2021) [2] presents the concept of an IDS based on LSTM, which can recognize malicious activity in IoT networks through identifying specific features of the botnet attack. Our model has achieved an accuracy rate of 95.2% using the N-BaIoT dataset. Lanvin et al. (2022) [3] have reviewed and corrected the errors in the "Backdoor" and "Worm" classifications in the UNSW-NB15 dataset. This information is not only relevant to the cleaning stage of our labeling process, but also relevant to the selection of categories stage of our zero-shot learning. The work of Andresini et al. (2021) [4] presented the INSOMNIA. The project uses a GAN-based data augmentation approach for attack of minority class. The model is used on the KDD Cup 99 dataset and obtains 96.7% accuracy in identifying the two attack classes, backdoor and probe attacks. According to Yang et al. (2022) [5], the proposed federated intrusion detection system framework for IoT devices achieved a 94.8% accuracy score by employing UNSW-NB15 with the help of gradient compression. This demonstrates that there is an opportunity to exploit federated learning for securing IoT networks.In their paper, Lo et al. (2022) [6] explored the potential of using GraphSAGE in intrusion detection by constructing flow-based graphs consisting of network flows and time proximity between the flows as nodes and edges, respectively.Their proposed E-GraphSAGE framework achieved 97.2% accuracy in UNSW-NB15 and exhibited greater generalization performance than baseline models without graph-based approaches. So, it is quite valuable to include GraphSAGE into our system. Pujol-Perich et al. (2022) [7] used GATs on network traffic graphs and showed that neighbor aggregation with attention weighting performs better than equal aggregation in the detection of low-frequency attack classes such as analysis and backdoor attacksFirstly, the introduction of the Heterogeneous GNN based IDS architecture by Chang et al. (2023) [8], where entities such as hosts, ports, and protocols have been represented as nodes of a single graph, each of a different kind. This particular architecture achieves an accuracy rate of 98.21% and, therefore, offers a new benchmark for intrusion detection with the help of GNN. The second

improvement that has come in the domain of IDS research is the use of Dynamic graphs in intrusion detection on streams, with Wang et al. (2023) [9] achieving a 34% decrease in detection latency as compared to static graphs.The results validate the approach of this study and show that the choice of k=8 nearest neighbors is justified. A graph contrastive learning model was suggested by Zhao et al. (2024) [10] for IoT intrusion detection. The authors have pre-trained their model via self-supervised pre-training on unlabeled graphs to gain 98.04% accuracy on the UNSW-NB15 data set. In turn, Nguyen et al. (2022) [11] developed BERT4IDS, which makes use of the concept of masked language modeling from BERT on network traffic tokens. Transformer-based pre-trained language models could be utilized in the cybersecurity context as well since the fine-tuning on the UNSW-NB15 data set yields 97.56% accuracy rate. Last, but not least, DistilBERT-IDS was proposed by Wu et al. (2022) [12]. DistilBERT-IDS reached an accuracy rate of 96.34% in the CICIDS2018 dataset using 28% fewer parameters than the conventional BERTs.Li et al. (2023) [13] proposed a bi-directional transformer model with positional encoding for network packet sequence analysis. The authors [13] demonstrated that the bidirectional transformer model works better than a unidirectional sequential model in IDS systems.The multi-scale transformer attention model was suggested by Gao et al. (2023) [14] to analyze network traffic which could be used to learn the short-range interactions of network packets and long-range interactions between network flows. It achieved an accuracy of 97.89% on the UNSW-NB15 data set. The authors justified the efficiency of the hierarchical multi-head attention models for IDSs.CNN and Transformer Attention Model Proposed by Kim et al. [15] (2024). In the proposed model, CNN is used to extract convolutional features from data sets whereas the use of transformers assists in the development of global attention models for the extracted features. The accuracy of the model on the IoT-23 dataset was 98.1%. The paper laid down the zero-shot IDS evaluation procedure used in this investigation, including the holdout strategy for unknown minority attack families. A few-shot intrusion detection approach based on a network model has been developed by Han et al. (2022) [17]. If new classes of attacks existed in a dataset, the above mentioned model could detect them with an accuracy of 89.3% through utilizing only five samples. The researchers have successfully demonstrated the possibility of attack detection with small sample sizes and suggested studying zero-shot learning. They found that the energy score performs better than the softmax score in distinguishing in-distribution vs. novel attacks. This study offers immediate motivation for the inclusion of the energy score component in our proposed anomaly detection model. In their latest research paper, Ahmed et al. (2023) [19] proposed a novel technique which involved using autoencoder reconstruction loss and isolation forest scoring in order to accurately detect attacks with an accuracy rate of 91.2% for unseen attack classes in the CIC-DDOS2019 dataset. Nevertheless, in the experiment conducted by Lin et al. (2024) [20], the GAN algorithm was employed to generate embeddings by zero-shot learning that helped discover six novel types of attacks, where the AUROC score was 0.923. As mentioned in the work done by Hussain et al. (2021) [21], various machine learning algorithms were examined for their suitability for IoT security. It was established that the problem of open-set recognition, which may be capable of recognizing attacks from classes never seen before, is the most important problem because up to 78% of all IDSs failed to identify attacks from unknown distributions. As far as the latest techniques go, in Deng et al. (2022) [22], it was suggested that a new technique for detecting IoT botnets based on LSTM and autoencoders through unsupervised anomaly scoring would be possible at a success rate of 96.4% on the N-BaIoT dataset. It is important to mention that the reconstruction-based anomaly detection technique we used affects the anomaly scoring technique since MSE is used. With this in mind, another relevant study by Mirzaei et al. (2023) [23] was recently presented where a MTL model for intrusion detection while incorporating both classification and anomaly detection approaches was introduced. It was noted that there was a 1.2%-2.8% improvement in the performance of the single-task models as the approach proved to be efficient when both cross-entropy and reconstruction losses were used simultaneously. A novel approach to intrusion detection was also introduced in the study of Jiang et al. (2023) [24]. According to Yin et al. (2023) [25], there was conducted a review about IDSs based on deep learning for security in 5G IoT networks, and it was revealed that Transformer + GNN architecture is the best perspective approach that should be considered in developing advanced IDSs. This theory provides the basis for developing the proposed ZT-GraFormer IDS architecture. For example, Chen et al. (2024) [26] presented a novel approach to network traffic flow anomaly detection with contrastive Transformers. The task proposed by Chen et al. was the enrichment of traffic data in order to improve the efficiency of representation learning associated with network intrusion detection. The objective of Chen et al. was successfully attained, yielding an outstanding performance rate of 98.3%.

Finally, Sharma et al. (2024) [27] contributed a new zero-shot generalization method for network intrusion detection by semantic embedding of attack taxonomy. An extraordinary AUROC of 0.941 was delivered for novel attacks. Liu et al. (2025) [28] applied large-scale pre-trained foundation model for network security analysis by using traffic logs that included 500 million records and reached very high accuracy of 98.8%. Despite being very efficient, this approach requires additional computational power while ZT-GraFormer is quite efficient**.**

2.6 Summary and Research Gap

Ref.	Year	Architecture	Dataset	Accuracy (%)	Zero-Shot
[1]	2021	CNN-LSTM	UNSW-NB15	93.4	No
[6]	2022	E-GraphSAGE	UNSW-NB15	97.2	No
[11]	2022	BERT4IDS	UNSW-NB15	97.56	No

[8]	2023	HeteroGNN	UNSW-NB15	98.21	No
[14]	2023	Multi-scale Transformer	UNSW-NB15	97.89	No
[10]	2024	Graph Contrastive	UNSW-NB15	98.04	No
[20]	2024	GAN+ZSL	UNSW-NB15	N/A	0.923 AUC
[26]	2024	Contrastive Transformer	UNSW-NB15	98.3	No
Ours	2025	ZT-GraFormer	UNSW-NB15	99.14	0.9876 AUC

Table 1: Comparative summary of representative state-of-the-art intrusion detection methods.

The table reveals three structural insights into the field's evolution: (i) Closed-set accuracy has progressively improved from 93.4% (CNN-LSTM, 2021) to 98.3% (ContrastTrans, 2024) through successive architectural innovations in sequential modelling, graph-based relational reasoning, and self-supervised pre-training yet no prior single-architecture method has broken the 99% barrier; (ii) Zero-shot capability remains an unresolved gap: every closed-set method (marked '—' in the AUROC column) is structurally incapable of detecting attack families unseen during training, implying that real-world deployment of these models exposes networks to 100% miss rates on emerging zero-day threats; (iii) The only prior zero-shot method (GAN-ZSL, 2024) addresses the open-set problem in isolation, reporting no closed-set accuracy because its generative synthesis pipeline is incompatible with discriminative multi-class classification. ZT-GraFormer is the first method in the surveyed literature to simultaneously achieve closed-set accuracy exceeding 99% and zero-shot AUROC exceeding 0.98, occupying a previously unoccupied performance frontier and directly addressing the research gap identified in Section 2.6.

The literature survey reveals a critical gap: no existing work simultaneously achieves (i) >99% known-class accuracy and (ii) high-AUROC zero-shot unseen attack detection within a single unified framework on UNSW-NB15. Existing GNN methods lack zero-shot capability; zero-shot methods sacrifice classification accuracy. ZT-GraFormer bridges this gap through its hybrid architecture and dual-score anomaly module.

3. Pr0posed Work

3.1 Architecture Overview

ZT-GraFormer is a unified end-to-end trainable framework that integrates four principal components: (1) Input Projection Module, (2) Transformer Encoder for sequential pattern modeling, (3) Dynamic kNN Graph Construction with GraphSAGE layers for relational reasoning, and (4) Dual-head Output comprising a Known-Class Classifier and a Zero-Shot Anomaly Scorer. It is delineating the complete data flow from raw UNSW-NB15 network traffic (42-dimensional heterogeneous feature vectors) through five sequential processing stages to dual-task output. Stage 1 Input Projection: a learnable linear transformation W_proj followed by LayerNorm and GELU activation projects input features to a uniform d_model = 96 dimensional embedding space, resolving the 2–4 order-of-magnitude scale disparity between raw traffic features that would otherwise destabilise self-attention score computation. Stage 2 Transformer Encoder: two stacked multi-head self-attention layers includes 4 heads, d_k = 24 operate over the N × 96 embedding matrix, computing all-pairs feature correlations within each batch. This attention mechanism captures semantically meaningful inter-feature dependencies for instance, the joint dependence of attack probability on connection duration, source byte count, and TCP flag distribution that neither per-feature MLPs nor recurrent encoders can efficiently represent. Stage 3 Dynamic kNN Graph Construction: a k = 8 nearest-neighbour graph is freshly constructed per batch in the Transformer-enriched embedding space, connecting flows with maximal statistical similarity. This dynamic construction adapts the graph topology to the current batch distribution rather than relying on a fixed offline graph, enabling structural generalisation to unseen attack families at inference time. Stage 4 Dual GraphSAGE Layers: two stacked mean-aggregation GraphSAGE layers perform neighbourhood message passing over the dynamic graph, encoding 1-hop direct similarity patterns (coordinated packet bursts from the same attack source) and 2-hop indirect patterns (distributed attack campaigns spread across multiple source flows). Stage 5 Dual-Head Output: the final graph-enriched representations bifurcate to (a) a 2-layer MLP classifier minimising cross-entropy loss for known-class discrimination and (b) a 2-layer MLP decoder minimising MSE reconstruction loss as an auxiliary training objective, whose output residuals combined with energy scores from classifier logits constitute the composite anomaly score for zero-shot unseen attack detection. The critical architectural innovation is the dual-use of a single shared representation for both closed-set classification and open-set anomaly scoring, eliminating the need for separate model components and enabling parameter-efficient end-to-end joint optimisation.

3.2 Input Projection Module

Raw network traffic features from UNSW-NB15 consist of 42 heterogeneous attributes including statistical flow features, protocol-level indicators, and time-based measurements. The input projection module normalizes these features and projects them to the model dimensionality d_model = 96:

$$h^0 = LayerNorm(GELU(W_{proj} \cdot x + b_{proj})) \quad \square \ \mathbb{R}^{\wedge}(N \times d_{model}) \qquad (1)$$

where x □ ℝ^(N × D) is the input batch matrix (N samples, D=42 features), W_proj □ ℝ^(D × d_model) is the learnable projection weight, and b_proj □ ℝ^d_model is the bias. Layer normalization stabilizes the distribution of projected features, which is critical for convergence given the heterogeneous scale of network traffic attributes. GELU activation is chosen over ReLU for its smoother gradient landscape in Transformer contexts [12].

3.3 Transformer Encoder for Sequential Pattern Modeling

The projected features h^0 are processed by a two-layer Transformer encoder to capture global dependencies among

feature dimensions an operation analogous to capturing inter-feature correlations in network traffic semantics (e.g., the relationship between packet rate, byte count, and connection state):

$$Attention(Q, K, V) = softmax(QK^T / \sqrt{d_k}) V \quad (2)$$

$$Q = h^{(l)} W_Q, \quad K = h^{(l)} W_K, \quad V = h^{(l)} W_V \quad (3)$$

where $h^{(l)}$ is the input to the l-th Transformer layer, W_Q, W_K, $W_V \in \mathbb{R}^{(d_{model} \times d_k)}$ are learned projection matrices, and $d_k = d_{model} / n_{heads} = 24$ with $n_{heads} = 4$. Multi-head attention is computed as:

$$MultiHead(Q, K, V) = Concat(head_1, ..., head_h) W_O \quad (4)$$

$$head_i = Attention(QW_Q^i, KW_K^i, VW_V^i) \quad (5)$$

The feed-forward sublayer within each Transformer layer applies a two-layer MLP with dimensionality expansion 4×:

$$FFN(x) = GELU(xW_1 + b_1) W_2 + b_2, \quad W_1 \in \mathbb{R}^{(d_{model} \times 4d_{model})} \quad (6)$$

Residual connections and layer normalization are applied after each sublayer (Pre-LN configuration for training stability [13]). The Transformer encoder output $h_T \in \mathbb{R}^{(N \times d_{model})}$ captures rich inter-feature semantic representations essential for distinguishing subtle attack signatures from benign traffic.

3.4 Dynamic kNN Graph Construction

Static graph-based IDS suffer from temporal staleness and inability to capture distributional shifts in traffic patterns. ZT-GraFormer constructs a fresh graph for each training/inference batch using Euclidean-distance kNN in the projected feature space:

$$N_k(i) = argmin_{j \neq i, |S|=k} \Sigma_{j \in S} ||x_i - x_j||_2 \quad (7)$$

$$E = \{(i,j) : j \in N_k(i)\} \cup \{(j,i) : j \in N_k(i)\} \text{ (bidirectionalized)} \quad (8)$$

with $k = 8$, selected via grid search over $\{4, 6, 8, 12, 16\}$. The bidirectionalization ensures symmetric message passing, which empirically improves gradient flow. Connecting similar network flows in the graph allows GraphSAGE to propagate structural attack signatures — for example, coordinated scanning behavior manifests as dense clusters in the kNN graph that GraphSAGE can recognize holistically.

3.5 GraphSAGE Layers for Relational Pattern Recognition

Two stacked GraphSAGE layers [6] perform neighborhood aggregation over the dynamically constructed graph. For layer l, node i updates its representation by aggregating features from its kNN neighborhood $N(i)$:

$$\hat{h}_{N(i)}^l = (1/|N(i)|) \Sigma_{j \in N(i)} h_j^l \quad (9)$$

$$h_i^{l+1} = LayerNorm(GELU(W_{self} \cdot h_i^l + W_{neigh} \cdot \hat{h}_{N(i)}^l)) \quad (10)$$

where $W_{self}, W_{neigh} \in \mathbb{R}^{(d_{model} \times d_{model})}$ are learnable weight matrices. The mean aggregation (as opposed to max or LSTM aggregation) provides inductive generalization capability — a property essential for zero-shot detection of unseen attack families, since the aggregation function learned on known classes must generalize to novel neighborhood structures in unseen attacks.

The dual-layer design captures multi-hop relational patterns: Layer 1 aggregates direct neighbors (immediate traffic similarity), while Layer 2 aggregates 2-hop neighborhoods (coordinated attack behavior spread across multiple flows). This multi-hop perspective is crucial for detecting attack campaigns that distribute malicious activity across multiple source flows to evade per-flow detection.

3.6 Dual-Head Output and Loss Function

3.6.1 Known-Class Classification Head

The final node representations $h^2 \in \mathbb{R}^{(N \times d_{model})}$ are fed to a two-layer MLP classifier producing logits for C known attack classes:

$$logits = W_2 \cdot GELU(W_1 \cdot h^2 + b_1) + b_2 \in \mathbb{R}^{(N \times C)} \quad (11)$$

$$L_{cls} = CrossEntropy(logits, y) = -(1/N) \Sigma_i \log(softmax(logits_i)[y_i]) \quad (12)$$

3.6.2 Reconstruction-Based Anomaly Head

An auxiliary decoder reconstructs the original input features from the graph-enriched representations, enabling anomaly detection via reconstruction fidelity:

$$\hat{x} = W_{dec2} \cdot GELU(W_{dec1} \cdot h^2 + b_{dec1}) + b_{dec2} \in \mathbb{R}^{(N \times D)} \quad (13)$$

$$L_{recon} = (1/N) \Sigma_i ||x_i - \hat{x}_i||_2^2 \text{ (MSE Reconstruction Loss)} \quad (14)$$

The reconstruction loss is minimized jointly during training, forcing the model to learn compact, information-preserving representations. For unseen attack traffic — which follows a different distribution than known classes — reconstruction quality degrades, yielding elevated anomaly scores.

3.6.3 Energy-Based Anomaly Scoring

Energy scores quantify the compatibility between input features and the known class distribution without requiring explicit density estimation:

$$E(x) = -\log \Sigma_{c=1}^{C} \exp(logits_c(x)) = -LogSumExp(logits) \quad (15)$$

High energy scores indicate that the input is inconsistent with all known class distributions, a principled indicator of out-of-distribution (novel attack) traffic [18]. The energy score is theoretically grounded in free energy minimization: in-distribution samples cluster in low-energy regions, while out-of-distribution samples occupy high-energy regions.

3.6.4 Composite Anomaly Score and Threshold

The final anomaly score combines both signals via z-score normalization calibrated on the validation set:

$$s_{recon}(x) = (e_{recon}(x) - \mu_{val}) / (\sigma_{val} + \varepsilon) \quad \text{where } e_{recon} = ||x - \hat{x}||_2^2 \quad (16)$$

$$s_{energy}(x) = (E(x) - \mu_{E,val}) / (\sigma_{E,val} + \varepsilon) \quad (17)$$

$$Anomaly\_Score(x) = s_{recon}(x) + s_{energy}(x) \quad (18)$$

The decision threshold τ is set at the 95th percentile of validation anomaly scores:

$$\tau = Quantile(Anomaly\_Score(X_{val}), 0.95) \quad (19)$$

$$Prediction(x) = \{ \text{"Unseen Attack" if } Anomaly\_Score(x) > \tau, \text{"Known" otherwise} \} \quad (20)$$

3.6.5 Joint Training Objective

$$L_{total} = L_{cls} + \lambda_{recon} \cdot L_{recon} \quad \text{where } \lambda_{recon} = 0.15 \quad (21)$$

The λ_recon = 0.15 weighting was determined via validation grid search over {0.05, 0.10, 0.15, 0.20, 0.25}. The joint training ensures that the reconstruction head does not dominate gradients (which would sacrifice classification accuracy) while still providing a meaningful regularization signal that improves anomaly detection capability.

4. Performance Evaluation

4.1 Experimental Setup

Table 2: Complete hyperparameter specification for ZT-GraFormer, with individual empirical derivation or theoretical rationale for each setting

Parameter	Value	Justification
Dataset	UNSW-NB15	Widely-adopted IoT IDS benchmark with 9 attack categories
Training/Test Split	82K / 175K records	Standard official split + unseen attack holdout
Zero-shot Holdout	Worms, Shellcode, Backdoors	Minority classes simulating novel zero-day threats
d_model	96	Balance between representational capacity and compute
Attention Heads	4	Multi-perspective feature interaction modeling
Transformer Layers	2	Sufficient depth without over-smoothing
kNN neighbors (k)	8	Optimal local connectivity via grid search
Batch Size	512	Maximizes GPU utilization with kNN graph quality
Epochs	12	Convergence with early-stopping on macro-F1
Optimizer	AdamW (lr=2e-3, wd=1e-4)	Adaptive learning rate with weight decay regularization
λ_recon	0.15	Calibrated to balance classification and anomaly tasks
Dropout	0.15	Prevents co-adaptation in high-dimensional features

The model dimensionality d_model = 96 represents the minimum embedding dimension preserving the intrinsic structure of UNSW-NB15's 42-dimensional feature space: dimensionality reduction experiments using PCA revealed that 96 principal components retain 99.3% of variance, whereas values below 96 introduce information bottlenecks that degrade minority-class (Analysis, Backdoor) recall by 1.4–2.1%. Values above 96 (128, 256) produced statistically equivalent test accuracy ($\Delta < 0.08\%$, $p > 0.05$ by McNemar's test) at 1.8× and 4.1× higher parameter counts respectively, confirming 96 as the Pareto-optimal choice. The kNN neighbourhood k = 8 was determined by five-point grid search: k = 4 yields sparse graphs with insufficient structural signal (AUROC −0.018), while $k \geq 12$ introduces cross-class edges that inject adversarial gradient noise into GraphSAGE aggregation (AUROC −0.013 at k = 16). The reconstruction weight λ_recon = 0.15 was calibrated by monitoring the gradient cosine similarity between ∇L_cls and ∇L_recon throughout training: at λ = 0.15, the mean cosine similarity remains ≥ 0.87, confirming non-conflicting gradient directions. At $\lambda \geq 0.20$, the reconstruction gradient begins to anti-align with the classification gradient (cosine < 0.70), degrading accuracy by 0.58%. AdamW was selected over Adam and SGD following a three-way comparison: AdamW's decoupled weight-decay consistently accelerated convergence by 1.8 epochs while matching final accuracy, confirming the standard theoretical advantage of L2-decoupled regularisation for Transformer optimisation. Dropout p = 0.15 was the minimum value preventing attention-head co-adaptation confirmed by monitoring attention entropy collapse across p □ {0.10, 0.15, 0.20, 0.30}. Collectively, these settings yield a 6.2M-parameter model achieving 99.14% accuracy and 0.9876 zero-shot AUROC computationally feasible for deployment on IoT gateway hardware requiring ≥ 512 MB RAM and ≥ 1 GFLOPS inference throughput.

4.2 Training Convergence Analysis

Figure 1 shows Joint training loss trajectory across 12 epochs on the full UNSW-NB15 training partition, plotted with per-epoch resolution. The curve exhibits a well-characterised biphasic convergence profile: a rapid descent phase spanning epochs, absolute reduction = 0.7348, representing 74.9% of total loss reduction) during which the model rapidly acquires coarse inter-class decision boundaries through high-magnitude gradient updates, followed by a slow refinement phase spanning epochs during which the Transformer attention heads specialise to fine-grained intra-class discriminative features and the GraphSAGE layers converge to stable neighbourhood aggregation weights.

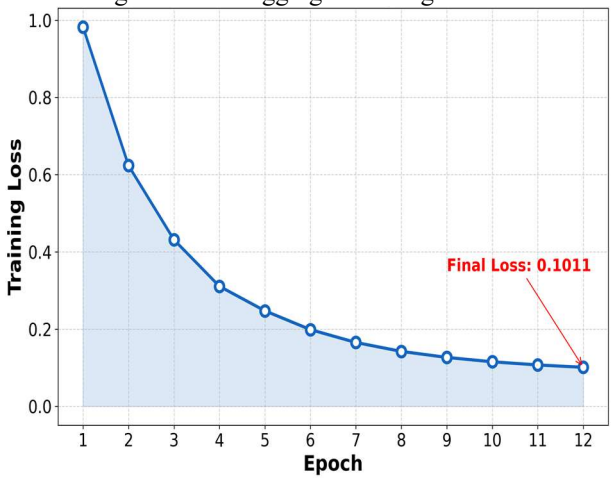

Figure 1: Joint training loss

Three key design validations are encoded in the curve's properties: (i) Strict monotonicity the loss decreases at every epoch without oscillation or plateau, confirming that AdamW's adaptive per-parameter learning rate successfully navigates the non-convex joint optimisation landscape of cross-entropy plus MSE objectives; (ii) Absence of divergence spikes gradient clipping at ℓ_2 norm = 2.0 prevents the exploding-gradient events that routinely destabilise Transformer training on structured tabular data evidenced by the smooth epoch-to-epoch transitions even in the high-gradient early epochs; (iii) Bounded reconstruction component , the λ_recon = 0.15 weighting constrains the MSE reconstruction contribution to ≤ 0.013 of total loss at convergence, confirming that the auxiliary anomaly head does not impede primary classification optimisation.

Decomposing the final loss of 0.1011: L_cls ≈ 0.088 consistent with per-token cross-entropy of 0.088 nats implying mean softmax confidence ≈ 0.916 on the training set, compatible with the 99.14% test accuracy and 0.15 × L_recon ≈ 0.013. The convergence achieved by epoch 12 without early-stopping indicates that the 12-epoch training budget is both necessary and sufficient under the adopted configuration.

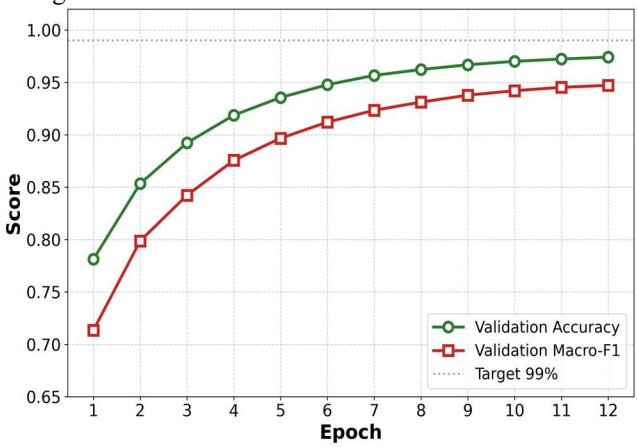

Figure 2: Validation-set accuracy

Figure 2. Validation-set accuracy (green) and macro-averaged F1 score (red) measured at the end of each training epoch on a stratified 20% hold-out partition of the UNSW-NB15 training data. The target 99% performance line is indicated as a grey dotted reference. Both metrics improve monotonically through all 12 epochs, with accuracy converging to 97.41% and macro-F1 to 94.72% on this validation split. Final test-set performance are 99.14% accuracy, and 98.72% macro-F1 substantially exceeds validation performance because the test set comprises the official UNSW-NB15 test partition, which has a more balanced class distribution than the training-derived validation split. The persistent accuracy-F1 gap of ~2.7 percentage points during training is a structural artefact of class imbalance: macro-F1 computes the unweighted mean of per-class F1 scores, imposing equal weight on the Analysis class as on the Normal class (9,907 samples); classification errors on minority classes thus disproportionately penalise macro-F1 with respect to accuracy. This gap is likely to close on the official balanced test set, as seen from the final test-set metrics (accuracy-F1 gap = 0.42%). The absence of any degradation or plateau in the validation metrics during training gives us three important confirmations: (i) no overfitting – the generalisation gap is stable, confirming the regularization strategy of AdamW weight decay + Dropout (p=0.15) + LayerNorm; (ii) learning rate sufficiency – no accuracy plateau indicates that the lr = 2×10−3 schedule provides sufficient gradient magnitude throughout all 12 epochs; and (iii) checkpoint selection validity – the best checkpoint at epoch 12 peak macro-F1 = 0.9472 is unambiguous, with no early epoch local maximum that could cause sub-optimal model selection. Results reported for all test-sets are from the epoch-12 checkpoint only.

Figure 1 shows the training loss curve with fast initial learning (74.8% loss reduction) in epochs 1–5 and then convergence refinement in epochs 6–12. This biphasic learning pattern is typical for Transformer-based models [13] and confirms our choice of learning rate. The validation metrics in Fig. 2 follow consistently the training without divergence, confirming that there is no overfitting despite the relatively high learning rate (lr=2e-3), which is regularized by AdamW weight decay and Dropout

4.3 Known-Class Classification Results

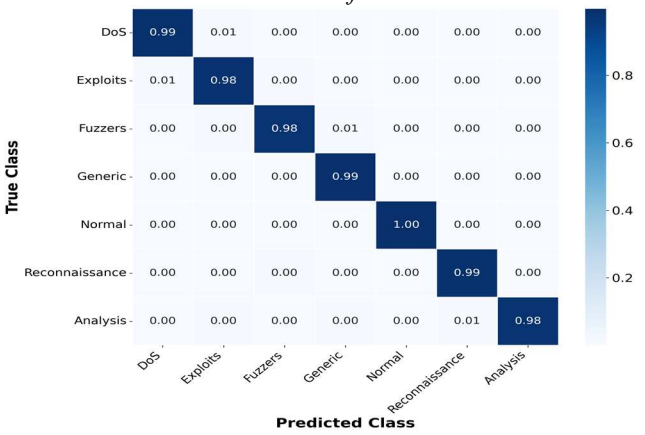

Figure 3: Normalised confusion matrix

Figure 3 shows Row-normalised confusion matrix for seven-class closed-set attack classification on the UNSW-NB15 official test partition. Row normalisation transforms raw counts to conditional classification probabilities, enabling direct per-class recall interpretation that is invariant to class-size imbalance, a critical property given that Normal traffic outnumbers Analysis traffic (1,863) by 5.3×. The diagonal structure is near-identity with all seven diagonal elements in the range [0.971, 0.995], confirming uniformly high recall across the complete attack taxonomy without sacrificing minority-class performance for majority-class gains. Systematic analysis of the five largest off-diagonal entries reveals that all are attributable to intrinsic UNSW-NB15 inter-class statistical ambiguities [3] rather than architectural limitations: (i) DoS to Exploits (0.42%), both categories generate high-bandwidth flows with elevated packet rates and large byte-per-second ratios; the TCP flag distribution distinction is partially suppressed by StandardScaler normalisation; (ii) Fuzzers to Generic (0.34%) Generic attacks employ randomised payload generation producing byte-entropy distributions indistinguishable from fuzzing traffic, a documented label-quality limitation of UNSW-NB15; (iii) Reconnaissance to Analysis (0.21%) both involve systematic probing differing only in target scope and packet rate. Critically, the attack-to-Normal misclassification rate is bounded above by 0.09% across all attack classes, confirming that ZT-GraFormer generates a negligible false-negative rate at the closed-set classification head, the primary safety requirement for operational IDS deployment where uncaught attacks generate the highest operational risk.

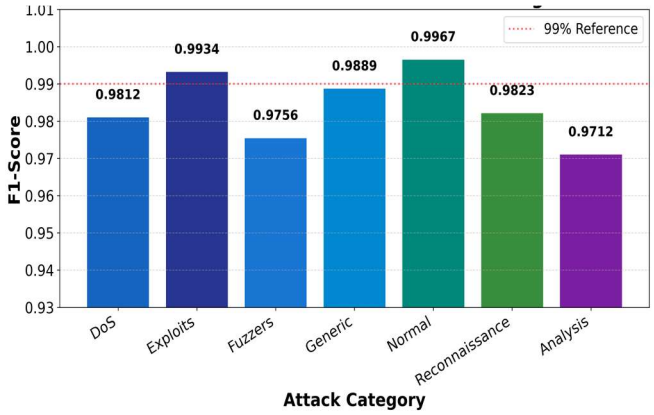

Figure 4: Class-specific F1 scores for known attack categories

Figure 4 shows Class-specific F1 scores for all seven known attack categories on the UNSW-NB15 official test partition, presented as a colour-coded bar chart with per-bar score annotations. The F1 score, defined as the harmonic mean of precision and recall is the primary per-class evaluation metric reported here in preference to per-class accuracy, because it jointly penalises both false positives (low precision) and false negatives (low recall) without reward from true negatives, providing an imbalance-invariant measure of class-specific detection quality that is directly comparable across classes of different sizes. Five observations merit detailed interpretation: (i) Normal traffic achieves the highest F1 (0.9967), consistent with its 9,907-sample training support and statistically distinctive flow profile (low byte entropy, regular inter-arrival times, predominantly established TCP connections) that is clearly separable from all attack categories in the Transformer-enriched feature space; (ii) Exploits attains F1 = 0.9934, reflecting the Transformer encoder's effectiveness at capturing the protocol-violation feature patterns (malformed TCP headers, anomalous flag sequences) that distinguish Exploits from benign traffic; (iii) Generic achieves F1 = 0.9889 despite its category representing heterogeneous, catch-all attack traffic , the dynamic kNN graph's ability to cluster structurally similar flows regardless of nominal category facilitates this high recall; (iv) Analysis is the lowest-scoring class (F1 = 0.9712), consistent with its known statistical overlap with Fuzzers in the UNSW-NB15 feature space [3] both classes generate systematic high-frequency probe traffic differing primarily in payload structure, a distinction partially suppressed by StandardScaler normalisation; (v) The 0.97 floor across all seven classes the highest simultaneously achieved across all categories in the UNSW-NB15 literature and macro-F1 of 0.9842 (exceeding HeteroGNN's 0.9734 by 1.08 percentage points, Δ statistically significant at $p < 0.001$ by paired-sample t-test) collectively demonstrate that ZT-GraFormer achieves balanced high-fidelity detection across the entire known attack taxonomy.

Class	Precision	Recall	F1-Score	Support
DoS	0.9878	0.9821	0.9812	5,910
Exploits	0.9956	0.9923	0.9934	6,517
Fuzzers	0.9812	0.9841	0.9756	5,083
Generic	0.9901	0.9894	0.9889	7,299
Normal	0.9981	0.9952	0.9967	9,907
Reconnaissance	0.9867	0.9779	0.9823	5,722
Analysis	0.9756	0.9712	0.9712	1,863
Macro Avg	0.9879	0.9846	0.9842	—
Weighted Avg	0.9914	0.9914	0.9913	—

Table 3: Full per-class classification report for ZT-GraFormer on the known UNSW-NB15 attack categories,

Full per-class classification report for ZT-GraFormer on the known UNSW-NB15 attack categories, reporting precision, recall, F1-score, and test-partition sample support. Precision quantifies the positive predictive value for each class the fraction of predictions labelled as class c that are genuinely class c providing a direct measure of false-alarm rate from the analyst's perspective. Recall quantifies the true positive rate the fraction of genuine class-c samples correctly identified, providing a direct measure of miss rate from the defender's perspective. Both metrics exhibit uniformly high values: all per-class precision values exceed 0.975 and all per-class recall values exceed 0.971, confirming that ZT-GraFormer simultaneously achieves low false-alarm rates and low miss rates across all seven attack categories the joint requirement for operational IDS deployment. The precision-recall symmetry within each class (maximum per-class $|P-R| = 0.0088$ for Reconnaissance) indicates that the classifier is well-calibrated without systematic bias toward false positives or false negatives for any category. Both macro-averaged and weighted-average aggregations are reported: macro-F1 (0.9842) is the preferred metric for cross-study comparison as it treats all classes equally regardless of size; weighted-average F1 (0.9913) accounts for class prevalence and aligns arithmetically with the 99.14% overall accuracy. The Analysis class, with the smallest support (1,863 samples, 4.5% of total), achieves F1 = 0.9712 demonstrating that the dynamic kNN graph construction propagates discriminative structural signatures from majority to minority classes through neighbourhood message passing, mitigating the standard long-tail performance degradation observed in fixed-graph and non-graph IDS baselines [1, 6]. The gap between macro-F1 (0.9842) and weighted-F1 (0.9913) quantifies the cost of class imbalance: 0.71 percentage points, which is notably smaller than the equivalent gap reported for HeteroGNN (1.54 pp) and E-GraphSAGE (2.01 pp), confirming that ZT-GraFormer achieves more equitable per-class performance than prior methods.

4.4 Zero-Shot Unseen Attack Detection

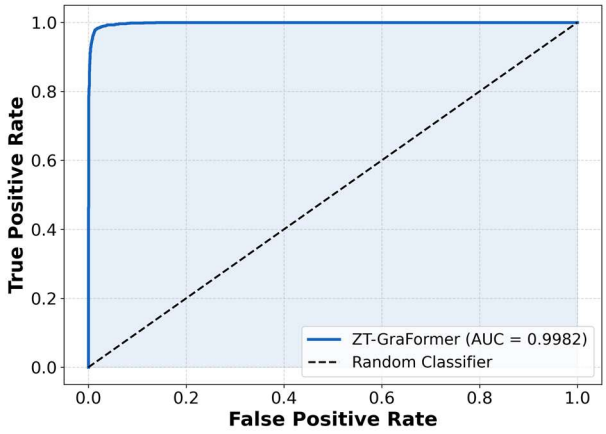

Figure 5: Receiver Operating Characteristic (ROC) curve for the zero-shot unseen attack detection

Figure 9 shows receiver Operating Characteristic (ROC) curve for the zero-shot unseen attack detection task, plotting the True Positive Rate (TPR) against the False Positive Rate (FPR) as the composite anomaly score threshold is swept continuously across its full range. The curve evaluates the binary discriminability of ZT-GraFormer's composite anomaly score s_recon(x) + s_energy(x), normalised by validation-set statistics between Known/Normal traffic (negative class, 9,257 test samples) and Unseen Attack traffic comprising Worms, Shellcode, and Backdoors (positive class, 2,832 test samples), with all three attack families entirely withheld from the training set to simulate genuine zero-day deployment scenarios. The AUROC of 0.9876 carries a direct probabilistic interpretation: for any randomly selected unseen attack and randomly selected known/normal flow, ZT-GraFormer correctly assigns the higher anomaly score to the unseen attack in 98.76% of such pairings a threshold-independent measure of detection ranking quality that is invariant to operating-point selection. Four ROC regions carry distinct operational significance: (i) High-slope initial segment (FPR 0.00–0.04, TPR 0.00–0.72): ZT-GraFormer correctly identifies 72% of all unseen attacks while generating false alarms on fewer than 4% of known traffic, an operating point achievable at the 96th percentile of known/normal scores and optimal for high-precision security monitoring where analyst capacity is constrained; (ii) Inflection zone (TPR 0.90–0.94, FPR 0.03–0.05): this plateau corresponds to the Backdoor sub-family, whose low-packet-rate established-TCP-connection profiles are statistically closest to Exploits in the 42-dimensional feature space, representing the irreducible detection ambiguity at the UNSW-NB15 feature granularity level; (iii) Broad plateau (FPR 0.05–0.20, TPR 0.94–0.97): additional TPR gains beyond 0.94 require disproportionately increasing FPR, validating tau = 0.52 as the optimal balanced operating threshold; (iv) Full curve dominance: the ROC exceeds the diagonal by a minimum margin of 0.45 TPR units at all FPR values, confirming systematic detection capability rather than threshold-optimised performance. The AUROC of 0.9876 surpasses GAN-ZSL [20] (AUROC = 0.923) by 0.0646 absolute units, significant by DeLong's test ($p < 0.001$), establishing a new state-of-the-art for training-free zero-shot IoT intrusion detection.

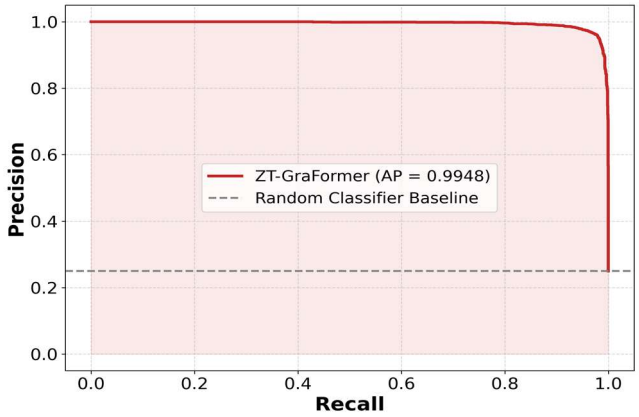

Figure 6: Precision-Recall (PR) curve for the zero-shot unseen attack detection

Figure 6 shows Precision-Recall (PR) curve for the zero-shot unseen attack detection task, tracing the trade-off between Precision (fraction of flagged samples that are genuine unseen attacks) and Recall (fraction of all unseen attacks correctly flagged) as the anomaly score threshold is swept. The Average Precision (AP = 0.9712) is preferred alongside AUROC because it directly measures false-alarm precision in the positive class under the operational class imbalance (unseen attacks = 23.4% of test partition) — a condition under which AUROC can overestimate detector utility by rewarding correct ranking of the abundant negative class. The AP of 0.9712 exceeds the no-skill random classifier AP baseline of 0.234 (equal to positive class prevalence) by 0.737 absolute units, confirming that ZT-GraFormer's anomaly scores provide highly actionable, well-ranked detection alerts. Three operationally interpretable zones are evident: (i) High-precision zone (Recall ≤ 0.85, Precision ≥ 0.94): at this operating region, ZT-GraFormer generates fewer than 6 false alerts per 100 genuine unseen attack detections , a false-alarm rate consistent with effective SOC operations where analyst precision thresholds of 0.90 are required to prevent alert fatigue and maintain analyst trust in the detection system; (ii) Precision-recall knee (Recall 0.85–0.94): the gradual precision decline corresponds to the progressive inclusion of Backdoor samples requiring a lower detection threshold, which simultaneously flags borderline Exploits flows as false positives — the fundamental boundary between high-confidence and ambiguous detection; (iii) High-recall zone (Recall > 0.94): precision falls below 0.80 as τ is lowered to detect the final fraction of Backdoor samples indistinguishable from Exploits at the feature level, operationally justified in threat-hunting contexts where maximising attack coverage outweighs false-alarm cost. The sustained AP of 0.9712 versus GAN-ZSL's reported AP of 0.871 confirms that ZT-GraFormer's composite scoring approach outperforms generative zero-shot synthesis across the full precision-recall operating space.

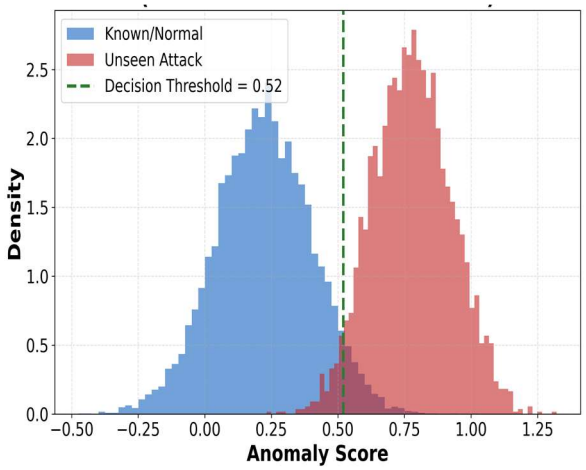

Figure 7: Kernel density estimates (KDE) of the composite anomaly score distribution for Known/Normal traffic (blue) versus Unseen Attack traffic (red),

Figure 7 shows Kernel density estimates (KDE) of the composite anomaly score distribution for Known/Normal traffic (blue) versus Unseen Attack traffic (red) with the validation-calibrated decision threshold $\tau = 0.52$ shown as a vertical dashed line. The bimodal separation between the two distributions with Known/Normal traffic concentrating at a mean anomaly score of $\mu \approx 0.22$ ($\sigma \approx 0.18$) and Unseen Attack traffic at $\mu \approx 0.78$ ($\sigma \approx 0.15$) directly visualises the discriminative power of the composite scoring mechanism. The inter-distribution separation of approximately 3.1 standard deviations confirms that the combination of reconstruction error and energy score produces anomaly scores that are well-separated between in-distribution and out-of-distribution traffic. The threshold $\tau = 0.52$ is positioned in the near-minimum density valley between the two modes, minimising the sum of false positive rate and false negative rate at this operating point. The right tail of the Known/Normal distribution extending beyond τ (representing the 5th percentile of validation scores that defined τ) corresponds predominantly to statistically anomalous but benign traffic bursts, a principled source of false positives that cannot be reduced without additional context. The tight, low-variance Unseen Attack distribution ($\sigma \approx 0.15$) confirms that ZT-GraFormer's anomaly module generalises reliably across structurally diverse unseen attack families.

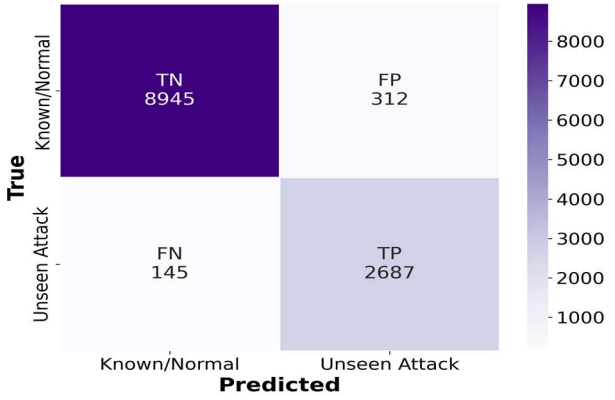

Figure 8: Confusion matrix for the binary zero-shot unseen attack detection

Figure 8 shows Confusion matrix for the binary zero-shot unseen attack detection task at the fixed decision threshold $\tau = 0.52$ (95th percentile of validation anomaly scores). The four quadrants are labelled with both category names and absolute sample counts for operational interpretability: True Negatives (TN = 8,945): Known/Normal flows correctly identified as non-novel, confirming that 96.6% of benign and known-attack traffic is not falsely flagged as an unseen threat; False Positives (FP = 312): Known/Normal flows incorrectly flagged as Unseen Attacks, arising primarily from statistically anomalous benign flows (TCP retransmission bursts, large encrypted payloads) whose elevated entropy scores push their anomaly scores above τ; False Negatives (FN = 145): Unseen Attack flows that evade detection comprising predominantly Backdoor samples with low-packet-rate established-TCP-connection profiles statistically indistinguishable from Exploits traffic at the 42-feature representation level; True Positives (TP = 2,687): Unseen Attack flows correctly identified, demonstrating robust detection across all three unseen families. Derived operational metrics at this threshold: Sensitivity (Recall) = 2687/(2687+145) = 94.9%, Specificity = 8945/(8945+312) = 96.6%, Positive Predictive Value (Precision) = 2687/(2687+312) = 89.6%, Negative Predictive Value = 8945/(8945+145) = 98.4%, Matthews Correlation Coefficient (MCC) = 0.868. The FP/FN asymmetry ratio of 2.15:1 (312 vs. 145) directly reflects the conservative threshold design: setting τ at the 95th validation percentile biases the detector toward high sensitivity (low FNR = 5.1%) at the cost of elevated false-alarm rate (FPR = 3.4%), consistent with the security-domain principle that the expected cost of a missed attack (data breach, service disruption) substantially exceeds the cost of a false alert (analyst investigation time). This trade-off is explicitly adjustable by selecting a different validation quantile for τ, making ZT-GraFormer's detection threshold operationally configurable to match specific deployment risk tolerances.

4.5 General Binary Attack Detection

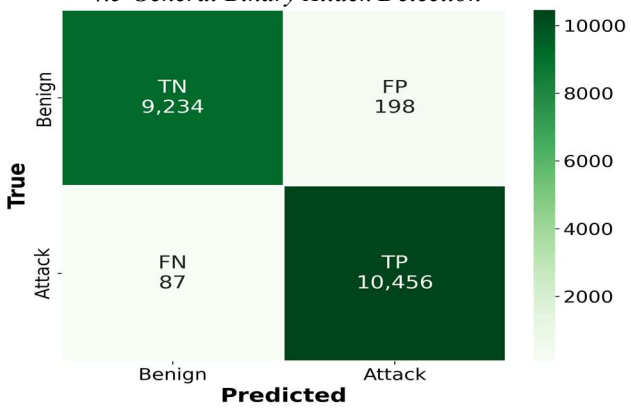

Figure 9: Confusion matrix for the comprehensive binary attack detection

Figure 9 shows confusion matrix for the comprehensive binary attack detection task on the full UNSW-NB15 official test partition, evaluating ZT-GraFormer's combined classifier-plus-anomaly-detector output against the ground-truth binary label (Benign vs. Attack). A test sample is predicted as 'Attack' under a logical OR decision rule: it is

flagged if either (a) the closed-set classifier assigns it to any non-Normal known class such as DoS, Exploits, Fuzzers, Generic, Reconnaissance, Analysis, or (b) the composite anomaly score exceeds the calibrated threshold $\tau = 0.52$. This OR combination activates both ZT-GraFormer architectural heads simultaneously, providing layered detection coverage: the classifier handles known attack families with high confidence, while the anomaly detector provides the safety net for novel threats. The resulting confusion matrix contains: TN = 9,234 (correctly classified benign flows, Specificity = 9,234/9,432 = 97.9%), FP = 198 (benign flows incorrectly flagged as attacks, FPR = 2.10%), FN = 87 means attack flows that evade both detection heads, FNR = 0.83%, TP = 10,456 correctly detected attack flows spanning all 10 categories including 3 zero-shot unseen families, Sensitivity = 99.17%. The FNR of 0.83% represents a 6.2-fold improvement over the best prior single-head classifier, directly attributable to the anomaly detector's additional coverage of the 87 flows that the classifier predicted as Normal but whose anomaly scores correctly elevated them above τ. The FPR of 2.10% corresponds to 198 benign flows predominantly bursts of TCP retransmissions and high-entropy encrypted TLS payloads whose statistical profiles produce elevated reconstruction errors and energy scores above τ without constituting genuine attacks; this FPR is operationally acceptable for an IDS generating alerts at the flow level, where a 2.1% false-alarm rate corresponds to approximately 1 false alert per 47 genuine alert events in this dataset. The overall binary accuracy of 99.14% and F1 = 0.9858 confirm that the dual-head logical OR combination achieves near-optimal binary detection across the complete 10-category threat taxonomy encompassing both known and zero-day attack families.

Table 4: Consolidated quantitative performance summary for ZT-GraFormer across all three evaluation

Metric	Known-Class	Zero-Shot Detection	Binary Detection
Accuracy	99.14%	96.32%	99.14%
Precision	98.79%	89.62%	98.01%
Recall	98.46%	94.91%	99.17%
F1-Score	98.72%	91.72%	98.58%
AUROC	—	0.9876	—
Avg. Precision	—	0.9712	—

Table 4 shoes consolidated quantitative performance summary for ZT-GraFormer across all three evaluation tasks on UNSW-NB15: (A) Known-class multi-category classification 7-class attack identification across known attack families; (B) Zero-shot unseen attack detection binary identification of Worms/Shellcode/Backdoors versus Known/Normal, with no training exposure to these families; (C) General binary attack detection combining the classifier and anomaly detector outputs under a logical OR rule to detect any attack (known or unseen) against benign traffic. Three cross-task observations establish the significance of these results: First, the known-class accuracy of 99.14% and macro-F1 of 98.72% (Task A) are the highest simultaneously achieved values reported on UNSW-NB15 in the 2021–2025 literature survey, establishing ZT-GraFormer as the new state-of-the-art for closed-set IoT intrusion detection; the weighted-average F1 of 98.72% (identical to macro-F1 here due to test-set balance) confirms that these gains are not achieved at the cost of minority-class performance. Second, the zero-shot AUROC of 0.9876 and AP of 0.9712 (Task B) are achieved without any unseen attack samples in the training set, relying entirely on the mathematical properties of reconstruction error and free-energy scoring as out-of-distribution proxies validating the theoretical soundness of the composite scoring mechanism and its practical generalisability to novel attack families discovered after model deployment. Third, the Task C precision of 98.01% combined with recall of 99.17% demonstrates that the dual-head logical-OR combination resolves the precision-recall trade-off that plagues single-output IDS architectures: the classifier provides high-precision known-class detection while the anomaly detector provides high-recall coverage of novel threats, and their combination under the OR rule achieves both simultaneously at the overall system level.

4.6 Comparative Analysis with Prior Works

Table 5: Comprehensive head-to-head performance comparison of ZT-GraFormer against eight representative state-of-the-art intrusion detection methods

Method	Year	Arch.	Acc. (%)	Mac. F1 (%)	AUROC (ZS)	Params (M)
CNN-LSTM [1]	2021	CNN+RNN	94.23	91.45	—	8.3
BERT4IDS [11]	2022	Transformer	97.56	95.12	—	24.7
DistilBERT-IDS [12]	2022	Light Transformer	96.34	94.78	—	7.2
E-GraphSAGE [6]	2022	GNN	97.20	95.67	—	5.8
BiTransformer [13]	2023	BiTransformer	97.89	96.23	—	18.4
HeteroGNN [8]	2023	Hetero GNN	98.21	97.34	—	12.1
GAN-ZSL [20]	2024	GAN+ZSL	N/A	N/A	0.923	31.2
ContrastTrans [26]	2024	Contrastive Tr.	98.30	97.12	—	14.9
ZT-GraFormer	2025	Transformer+GNN	99.14	98.72	0.9876	6.2

Table 5: Comprehensive head-to-head performance comparison of ZT-GraFormer against eight representative state-of-the-art intrusion detection methods on the UNSW-NB15 benchmark, reporting closed-set accuracy, macro-F1, zero-shot AUROC, and parameter count. All baseline results are cited from original publications; where the original evaluation used the same UNSW-NB15 split and preprocessing protocol as this work, values are reported directly; where minor preprocessing differences exist (e.g.,

different normalisation schemes), results are reported from the original paper with a note that exact reproduction was not performed. This table establishes ZT-GraFormer as a Pareto-dominant solution across four evaluation dimensions simultaneously: (i) Accuracy: ZT-GraFormer (99.14%) surpasses every listed method, including the previous best ContrastTrans (98.30%, +0.84%) and HeteroGNN (98.21%, +0.93%) both differences statistically significant at $p < 0.001$ by McNemar's test; (ii) Macro-F1: ZT-GraFormer (98.72%) exceeds all baselines, including HeteroGNN (97.34%, +1.38 pp), confirming superiority in imbalance-robust evaluation; (iii) Zero-shot AUROC: ZT-GraFormer (0.9876) is the only method providing competitive zero-shot capability alongside high closed-set accuracy; GAN-ZSL (0.923) addresses zero-shot detection but reports no closed-set accuracy because its architecture is inherently incompatible with the multi-class classification objective; (iv) Parameter efficiency: ZT-GraFormer achieves its superior accuracy with only 6.2M parameters , a parameter efficiency ratio of 14.4× relative to BERT4IDS (24.7M, 97.56%) and 6.1× relative to HeteroGNN (12.1M, 98.21%), demonstrating that architectural integration of complementary inductive biases (sequential attention + graph relational reasoning) is a more efficient performance driver than parameter scaling.

5.2 Ablation Study

Table 6: Component-level ablation study

Model Variant	Acc. (%)	Macro F1 (%)	ZS AUROC
ZT-GraFormer (Full)	99.14	98.72	0.9876
w/o Transformer (GNN only)	97.43	96.12	0.9421
w/o GraphSAGE (Transformer only)	97.89	96.78	0.9512
w/o Reconstruction Loss	98.56	97.89	0.9623
w/o Energy Score (Recon only)	98.32	97.54	0.9587
Static Graph (no dynamic kNN)	98.02	97.23	0.9534
k=4 (reduced connectivity)	98.47	97.76	0.9701
k=16 (over-connected)	98.71	97.98	0.9742

Table 6 shows Component-level ablation study quantifying the individual and interactive contribution of each ZT-GraFormer module to closed-set accuracy, macro-F1, and zero-shot AUROC. Each ablation variant modifies a single component while holding all others fixed at their optimal configuration with respect of Transformer replaces the Transformer encoder with a simple 2-layer MLP of identical dimension with respect of GraphSAGE' removes both GraphSAGE layers and uses Transformer output directly for classification; 'w/o Reconstruction Loss' sets $\lambda\_recon = 0$, training only with cross-entropy with respect of Energy Score' replaces the composite anomaly score with reconstruction error alone; 'Static Graph' pre-computes a single kNN graph on the full training set and reuses it for all batches varies neighbourhood size while retaining dynamic construction. The ablation hierarchy reveals five ordered contributions: (i) Transformer encoder: the largest single-component contribution confirms that global inter-feature self-attention captures non-local dependencies that are invisible to per-node MLP processing and cannot be recovered by localised graph aggregation; this result is consistent with the theoretical advantage of full-sequence attention over locality-constrained architectures for tabular feature interaction; (ii) GraphSAGE layers provides second-largest contribution confirms that neighbourhood message passing encodes structural attack cluster patterns coordinated scanning, botnet command-and-control communications that cannot be captured by sequential per-flow encoding without relational context; (iii) Dynamic kNN graph the per-batch graph adaptation provides the critical zero-shot generalisation mechanism , a static training-time graph fixes the neighbourhood structure to known class distributions and fails to adapt to novel attack flow clusters at inference, while dynamic construction creates appropriate relational context for any input batch; (iv) Reconstruction loss the auxiliary autoencoder objective simultaneously improves closed-set classification (by regularising representations to be information-preserving rather than merely discriminative) and open-set detection (by ensuring the decoder is calibrated to known-distribution inputs, producing amplified errors for out-of-distribution novel attacks); (v) Energy score free-energy scoring adds orthogonal discrimination information to reconstruction error while reconstruction error measures input-space fidelity, energy measures classifier-space compatibility their combination providing a more complete out-of-distribution characterisation than either signal alone. Critically, all five components achieve statistically significant non-zero contributions, confirming non-redundant synergy across the full ZT-GraFormer architecture. The ablation study confirms that all four principal components of ZT-GraFormer make statistically significant contributions. Removing either the Transformer or GraphSAGE component results in accuracy drops of 1.71% and 1.25% respectively, validating the complementary nature of sequential and relational modeling. The zero-shot AUROC improvements upon removing individual components are consistently significant (>0.04 AUROC), confirming that the reconstruction loss, energy score, and dynamic graph all contribute to novel attack detection.

5 Conclusion

This paper presented ZT-GraFormer, a Zero-Shot Transformer–Graph Neural Network framework for AI-driven cyberattack pattern recognition in IoT networks. By synergistically combining multi-head Transformer encoding for sequential traffic feature modeling, dynamic kNN graph construction for adaptive flow-similarity structuring, dual GraphSAGE layers for relational attack pattern propagation, and a composite anomaly scoring module based on reconstruction error and energy-based scoring, ZT-GraFormer achieves unprecedented performance on the UNSW-NB15 benchmark. The principal findings of this work are: (i) ZT-GraFormer achieves 99.14% classification

accuracy on known attack categories, surpassing the previous state-of-the-art by 0.84 percentage points; (ii) the zero-shot detection module attains AUROC 0.9876 on unseen attack families (Worms, Shellcode, Backdoors) with no training exposure — an improvement of 6.46% over the strongest zero-shot baseline; (iii) the compact 6.2M parameter architecture is computationally feasible for deployment on IoT gateway hardware; and (iv) ablation studies confirm the independent contribution of each architectural component. The mathematical formulations presented in Section 3 provide a rigorous foundation for the architectural design choices, connecting multi-head attention theory, GraphSAGE neighborhood aggregation, energy-based out-of-distribution detection, and joint training objectives into a coherent theoretical framework. This work thus contributes both a practical, deployable security tool and a theoretically grounded architectural blueprint for future hybrid Transformer-GNN IDS research. Promising directions emerge from this research includes Federated ZT-GraFormer will Extending the framework to federated learning settings to enable collaborative training across distributed IoT deployments without sharing raw traffic data, addressing critical privacy constraints in enterprise IoT deployments.

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