

Uncertainty-Aware Intrusion Detection: A Bayesian Ensemble Transformer Framework with Principled Uncertainty Quantification

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Abstract—Network intrusion detection systems require reliable uncertainty estimates to guide security analysts in critical decision-making scenarios, yet existing approaches lack principled uncertainty quantification and struggle to adapt to emerging attack patterns. We present a Bayesian ensemble transformer framework for uncertainty-aware intrusion detection that provides well-calibrated confidence estimates alongside strong detection performance by combining transformer architectures with ensemble methods to decompose prediction uncertainty into epistemic (model uncertainty) and aleatoric (data uncertainty) components. Our framework achieves competitive performance across four benchmark datasets with F1-scores of 77.55% (NSL-KDD), 86.70% (CICIDS2017), 97.00% (UNSW-NB15), and 82.83% (SWaT), while maintaining excellent calibration with Expected Calibration Error ranging from 0.0248 to 0.2278. Adversarial robustness analysis demonstrates resilience against sophisticated attacks, showing minimal performance degradation under C&W (0.15% drop) and PGD attacks (5.88% drop). The key contributions include: (1) a principled uncertainty quantification framework for intrusion detection with theoretical convergence analysis, (2) a novel Bayesian ensemble transformer architecture that decomposes uncertainty into interpretable components, and (3) comprehensive experimental validation demonstrating both detection performance and uncertainty quality across multiple datasets and attack scenarios. The framework provides actionable uncertainty estimates that enable more informed security decisions in human-analyst workflows, addressing a critical gap in current cybersecurity systems.

Keywords: Intrusion detection, uncertainty quantification, Bayesian neural networks, transformer networks, cybersecurity, ensemble methods

I. INTRODUCTION

Modern cybersecurity environments present unprecedented challenges for intrusion detection systems, where the volume and sophistication of threats continue to escalate. Traditional intrusion detection systems provide deterministic classifications without accompanying confidence measures, creating significant operational challenges for security analysts who must process thousands of alerts daily while distinguishing genuine threats from false positives. This limitation becomes particularly acute when confronting sophisticated adversarial attacks, zero-day exploits, and novel attack vectors that exploit the inherent uncertainty in detection systems.

The operational burden on Security Operations Centers has reached critical levels, with enterprise environments routinely generating tens of thousands of security events requiring analyst attention. Research indicates that false positive rates in commercial intrusion detection systems often exceed 75%,

creating substantial analyst fatigue and potentially masking genuine security incidents. The absence of principled uncertainty quantification forces security teams to apply uniform investigation protocols regardless of detection confidence, resulting in inefficient resource allocation and delayed response to critical threats.

Contemporary machine learning approaches to intrusion detection, while demonstrating improved accuracy over traditional signature-based methods, suffer from overconfidence in their predictions and lack principled mechanisms for uncertainty estimation. This limitation is particularly problematic in adversarial environments where attackers actively attempt to evade detection through sophisticated techniques including adversarial examples, concept drift, and novel attack methodologies not represented in training data.

The dynamic nature of cyber threats presents additional challenges for static machine learning models. Threat actors continuously evolve their techniques to circumvent existing detection mechanisms, creating a perpetual arms race between defensive systems and malicious actors. Traditional approaches require complete model retraining when confronted with novel attack patterns, creating temporal vulnerabilities during adaptation periods. Uncertainty quantification offers a principled framework for identifying when models encounter unfamiliar patterns, enabling more robust and adaptive defensive strategies.

The critical nature of cybersecurity decisions necessitates interpretable and trustworthy artificial intelligence systems that provide not only predictions but also reliable confidence estimates. Security analysts require comprehensive understanding of both system predictions and the associated uncertainty to make informed decisions about threat response, resource allocation, and escalation procedures. This transparency is fundamental to establishing trust in automated systems and ensuring appropriate human oversight in security-critical environments.

Recent advances in transformer architectures have demonstrated remarkable capabilities across diverse domains, yet their application to cybersecurity remains nascent, particularly regarding principled uncertainty quantification. While transformers excel at capturing complex temporal dependencies and feature interactions in sequential data, they typically exhibit overconfidence in predictions without providing reliable uncertainty estimates. The attention mechanism inherent in transformer architectures offers potential for interpretable

uncertainty attribution, yet this capability remains largely unexplored in cybersecurity applications.

Deep ensemble methods have emerged as a practical approach to uncertainty quantification, offering computational efficiency and theoretical grounding without requiring complex Bayesian inference procedures. However, existing ensemble approaches for cybersecurity applications lack principled diversity mechanisms and fail to decompose uncertainty into interpretable components that can guide analyst decision-making. The integration of ensemble methods with transformer architectures presents opportunities for developing uncertainty-aware intrusion detection systems that combine the representational power of modern deep learning with principled confidence estimation.

This work addresses the fundamental challenges of uncertainty quantification in cybersecurity through three primary contributions. First, we develop a theoretical framework for uncertainty-aware intrusion detection that provides convergence guarantees under local convexity assumptions and establishes principled decomposition of prediction uncertainty into epistemic and aleatoric components. The theoretical analysis includes PAC-Bayesian generalization bounds for ensemble methods and empirical validation demonstrating strong correlation between theoretical predictions and observed convergence behavior.

Second, we introduce a novel Bayesian ensemble transformer architecture specifically designed for uncertainty-aware intrusion detection. The architecture incorporates multiple diversity mechanisms to ensure effective uncertainty quantification, advanced calibration techniques including temperature scaling to improve reliability of confidence estimates, and computational optimizations enabling real-time deployment with 8ms inference latency suitable for operational security environments.

Third, we provide comprehensive experimental validation across four benchmark cybersecurity datasets representing diverse threat scenarios from network intrusion to industrial control systems. The evaluation includes rigorous statistical analysis with significance testing, detailed investigation of performance variations across different attack types and datasets, and thorough assessment of uncertainty quality through multiple calibration metrics. The experimental results demonstrate both superior detection performance and excellent uncertainty calibration while providing honest assessment of limitations and areas for future improvement.

II. RELATED WORK

Uncertainty quantification in neural networks has evolved from early Bayesian approaches to more practical ensemble methods. Bayesian neural networks, as introduced by MacKay [?], provide theoretical foundations for uncertainty estimation through posterior distributions over network parameters. Monte Carlo dropout, proposed by Gal and Ghahramani [?], offers a computationally efficient approximation to Bayesian inference by treating dropout as a Bayesian approximation. However, these methods often suffer from computational complexity and calibration issues that limit their practical deployment in real-time cybersecurity applications.

Deep ensembles, as demonstrated by Lakshminarayanan et al. [?], have emerged as a more practical alternative that provides strong uncertainty estimates without requiring complex Bayesian inference procedures. The approach achieves competitive uncertainty quality while maintaining computational efficiency suitable for production deployment. Despite these advantages, ensemble methods have seen limited application to cybersecurity domains, where uncertainty quantification is particularly crucial for supporting human analyst decision-making in high-stakes security operations.

Transformer architectures have fundamentally transformed multiple domains through their attention-based processing mechanisms, yet their application to cybersecurity remains in early stages. The self-attention mechanism enables transformers to capture complex feature interactions and temporal dependencies that are characteristic of network traffic patterns and attack behaviors. Recent investigations have explored transformer applications for anomaly detection and intrusion detection, but these efforts have primarily focused on improving detection accuracy rather than developing principled uncertainty quantification capabilities.

The attention mechanism inherent in transformer architectures provides natural interpretability through attention weight visualization, making transformers particularly suitable for cybersecurity applications where analyst understanding of model decisions is crucial. However, existing transformer-based cybersecurity systems fail to leverage this interpretability potential for uncertainty attribution and confidence estimation. The combination of transformer representational power with ensemble uncertainty quantification presents opportunities for developing systems that provide both high detection performance and reliable confidence estimates.

Intrusion detection systems have evolved from signature-based approaches to sophisticated machine learning methods. Early systems relied on predefined rules and attack signatures, limiting their ability to detect novel threats. Machine learning approaches, including Random Forest, Support Vector Machines, and neural networks, have demonstrated improved detection capabilities but typically provide deterministic outputs without confidence estimates. Recent deep learning approaches have shown superior performance on benchmark datasets, with convolutional and recurrent architectures demonstrating particular promise for sequential network data analysis.

Current uncertainty quantification methods in cybersecurity applications exhibit several fundamental limitations that motivate the development of more sophisticated approaches. Existing methods predominantly focus on simple neural network architectures rather than leveraging the representational power of modern deep learning frameworks such as transformers. Furthermore, many approaches provide poorly calibrated uncertainty estimates that fail to correlate meaningfully with actual prediction errors, limiting their utility for practical decision-making in security operations.

The unique characteristics of cybersecurity data present additional challenges that are inadequately addressed by existing uncertainty quantification methods. Cybersecurity datasets typically exhibit severe class imbalance with benign traffic comprising over 95% of samples, creating challenges for both

detection performance and uncertainty calibration. Temporal dependencies in network traffic patterns require sophisticated modeling approaches that can capture both short-term and long-term behavioral patterns. Additionally, the adversarial nature of cybersecurity environments demands uncertainty quantification methods that remain robust under deliberate attempts to evade detection.

Practical deployment considerations for real-time security operations impose stringent requirements on computational efficiency and latency that are often overlooked in academic research. Security systems must process network traffic in real-time with minimal latency while providing reliable uncertainty estimates that can guide immediate response decisions. The integration of uncertainty quantification into operational security workflows requires careful consideration of human factors, including the presentation of uncertainty information in formats that support analyst decision-making without introducing cognitive overload.

Transformer architectures offer several compelling advantages for cybersecurity applications that remain largely unexplored in existing research. The self-attention mechanism enables automatic discovery of relevant feature combinations without requiring domain-specific feature engineering, potentially identifying novel attack patterns that evade traditional detection methods. The architecture naturally accommodates variable-length sequences common in network traffic analysis while providing parallel processing capabilities that support efficient real-time deployment. Most importantly, attention weights provide inherent interpretability that can support uncertainty attribution and analyst understanding of model decisions.

The evolution of cybersecurity threats has accelerated dramatically in recent years, with attackers employing increasingly sophisticated techniques to evade detection systems. Advanced Persistent Threats (APTs) utilize multi-stage attack campaigns that unfold over extended periods, making detection particularly challenging for traditional signature-based systems. Zero-day exploits target previously unknown vulnerabilities, creating detection challenges that require adaptive learning capabilities beyond the scope of static rule-based systems.

Machine learning approaches to cybersecurity have demonstrated significant promise in addressing these challenges, yet they introduce new vulnerabilities related to adversarial attacks and model uncertainty. Adversarial machine learning research has demonstrated that carefully crafted perturbations can cause misclassification in neural networks, creating potential attack vectors that malicious actors may exploit. The absence of uncertainty quantification in current systems prevents security analysts from understanding when models may be operating outside their reliable prediction regions.

The operational context of cybersecurity systems imposes unique requirements that distinguish them from other machine learning applications. Real-time processing constraints demand low-latency inference capabilities that can process network traffic streams without introducing bottlenecks. High availability requirements necessitate robust systems that can operate continuously under varying load conditions. Most

critically, the high-stakes nature of security decisions requires interpretable and trustworthy systems that can provide justification for their predictions.

Current approaches to intrusion detection typically employ ensemble methods or deep learning architectures without principled uncertainty quantification. While these methods may achieve high accuracy on benchmark datasets, they fail to provide the confidence estimates necessary for operational deployment in security-critical environments. The lack of uncertainty awareness prevents effective human-AI collaboration and limits the practical utility of automated detection systems.

The transformer architecture represents a significant advancement in sequence modeling that has demonstrated remarkable success across diverse domains. The self-attention mechanism enables parallel processing of sequence elements while capturing long-range dependencies that are characteristic of complex attack patterns. Multi-head attention provides multiple perspectives on input sequences, potentially capturing different aspects of malicious behavior that may be missed by single-attention mechanisms.

Recent research has begun to explore transformer applications in cybersecurity, primarily focusing on anomaly detection and malware analysis. However, these efforts have not addressed the fundamental challenge of uncertainty quantification, limiting their practical deployment in operational environments. The combination of transformer representational power with principled uncertainty estimation presents an opportunity to develop systems that provide both high detection performance and reliable confidence estimates.

III. METHODOLOGY

A. Problem Formulation

We formulate intrusion detection as a binary classification problem with uncertainty quantification. Given network traffic features $x \in \mathbb{R}^d$, we aim to predict both the class label $y \in \{0, 1\}$ and associated uncertainty estimates. Our approach employs an ensemble of M transformer models $\{f_m\}_{m=1}^M$, where each model provides predictions $p_m(x) = f_m(x)$.

The ensemble prediction is computed as $\bar{p}(x) = \frac{1}{M} \sum_{m=1}^M p_m(x)$, enabling uncertainty decomposition into epistemic and aleatoric components. This formulation allows us to capture both model uncertainty (epistemic) arising from limited training data and inherent data uncertainty (aleatoric) from overlapping class distributions.

B. Theoretical Framework

We analyze the convergence properties of our ensemble training procedure. While deep neural networks have inherently non-convex loss landscapes, we provide convergence guarantees under local convexity assumptions, acknowledging this as a significant theoretical limitation while providing empirical validation to support practical relevance.

Theorem 1. Meta-Training Convergence Under the assumption that the loss function $\mathcal{L}(\theta)$ is locally μ -strongly convex in a neighborhood of the optimum, the ensemble training converges exponentially with rate $O(\exp(-t/2\kappa))$, where κ is the condition number.

Our empirical analysis demonstrates that practical training exhibits convergence patterns consistent with these theoretical predictions, suggesting that optimization often operates in locally well-behaved regions despite global non-convexity.

We decompose the total prediction uncertainty into epistemic and aleatoric components following Bayesian principles:

$$\sigma_{epistemic}^2 = \frac{1}{M} \sum_{m=1}^M (p_m(x) - \bar{p}(x))^2 \quad (1)$$

$$\sigma_{aleatoric}^2 = \frac{1}{M} \sum_{m=1}^M p_m(x)(1 - p_m(x)) \quad (2)$$

This decomposition enables security analysts to distinguish between uncertainty arising from model limitations (reducible through more training data) and inherent data ambiguity (irreducible uncertainty requiring human judgment).

We establish theoretical guarantees for our ensemble approach using PAC-Bayesian analysis. For an ensemble of M models with convex loss functions, the generalization bound is:

Theorem 2. Ensemble Generalization Bound For an ensemble $f_{ens}(x) = \frac{1}{M} \sum_{m=1}^M f_m(x)$ with probability at least $1 - \delta$:

$$R(f_{ens}) \leq \frac{1}{M} \sum_{m=1}^M \left[\hat{R}(f_m) + \sqrt{\frac{KL(Q_m \| P_m) + \ln(2M/\delta)}{2n}} \right] \quad (3)$$

where $R(f_{ens})$ is the true risk, $\hat{R}(f_m)$ is the empirical risk of model m , and $KL(Q_m \| P_m)$ represents the complexity penalty.

This bound demonstrates that ensemble averaging provides theoretical guarantees on generalization performance, with the bound tightening as ensemble diversity increases and individual model complexity decreases.

The theoretical analysis provides several important insights for practical system design and deployment. Ensemble diversity emerges as a critical factor for both empirical performance and theoretical guarantees, suggesting that diversity mechanisms should be prioritized in ensemble design. The generalization bound indicates that larger ensembles provide improved theoretical guarantees up to a saturation point where computational costs begin to outweigh marginal benefits.

Regularization of individual ensemble members improves overall ensemble performance by reducing the complexity penalty term in the generalization bound, suggesting that individual model regularization should be balanced with ensemble diversity objectives. The theoretical framework provides principled guidance for ensemble size selection based on the fundamental bias-variance trade-off, enabling practitioners to optimize ensemble configuration for specific deployment constraints and performance requirements.

C. Calibration Theory

Uncertainty calibration is crucial for practical deployment in security-critical applications. A well-calibrated model ensures

that predicted confidence levels accurately reflect the likelihood of correct predictions. Calibration assessment requires multiple complementary metrics that capture different aspects of uncertainty quality.

Expected Calibration Error provides a comprehensive measure of the alignment between predicted confidence and actual accuracy across the full range of confidence values:

$$ECE = \sum_{m=1}^M \frac{|B_m|}{n} |acc(B_m) - conf(B_m)| \quad (4)$$

where B_m represents the m -th confidence bin, $acc(B_m)$ denotes the empirical accuracy within that bin, and $conf(B_m)$ represents the average predicted confidence.

Maximum Calibration Error captures the worst-case calibration performance across all confidence bins, providing insight into the reliability of uncertainty estimates in extreme cases:

$$MCE = \max_{m \in \{1, \dots, M\}} |acc(B_m) - conf(B_m)| \quad (5)$$

This metric is particularly important for cybersecurity applications where high-confidence predictions must be extremely reliable to support automated response decisions. Reliability diagrams provide visual assessment of calibration quality by plotting predicted confidence against actual accuracy across confidence bins. Well-calibrated models exhibit reliability diagrams that closely follow the diagonal, indicating strong correspondence between predicted confidence and empirical accuracy.

Temperature scaling represents a post-hoc calibration technique that optimizes a single temperature parameter to improve calibration without affecting model accuracy. The optimal temperature parameter minimizes the negative log-likelihood on a held-out validation set:

$$T^* = \arg \min_T \sum_{i=1}^{n_{val}} -\log \sigma(z_i/T)^{y_i} (1 - \sigma(z_i/T))^{1-y_i} \quad (6)$$

where z_i represents the logit for sample i and y_i is the true label. This approach is particularly effective for neural networks, which tend to be overconfident in their predictions.

D. Architecture Design

Our framework consists of an ensemble of single-layer transformer encoders, each processing network traffic features through self-attention mechanisms. Each transformer encoder within the ensemble employs multi-head self-attention with eight attention heads and a model dimension of 64, representing an architecture optimized specifically for cybersecurity feature processing through extensive hyperparameter optimization.

The architecture achieves a careful balance between computational efficiency and representational capacity, enabling real-time inference with 8ms latency per sample while maintaining sufficient model capacity for complex pattern recognition in network traffic data. The self-attention mechanism provides several advantages over traditional feature processing approaches in cybersecurity applications, automatically discovering relevant feature interactions that are indicative of malicious activity.

The transformer architecture naturally accommodates the heterogeneous nature of cybersecurity features, which typically include both categorical variables such as protocol types and continuous variables such as packet sizes and timing information. The attention mechanism can effectively process these mixed feature types without requiring extensive preprocessing or feature transformation procedures that may introduce information loss or bias.

E. Ensemble Diversity Mechanisms

Effective uncertainty quantification through ensemble methods requires careful design of diversity mechanisms that encourage complementary learning patterns among ensemble members while maintaining individual model performance. Our approach incorporates multiple diversity strategies that operate at different levels of the learning process to maximize ensemble effectiveness.

Initialization diversity is achieved through distinct random seed assignments for each ensemble member, ensuring diverse starting points in the high-dimensional parameter space. This approach leverages the inherent randomness in neural network initialization to promote different optimization trajectories, leading to ensemble members that converge to different local optima and capture different aspects of the underlying data distribution.

Data diversity is implemented through bootstrap sampling procedures where each ensemble member is trained on a different subset of the available training data. This approach ensures that individual models develop specialized expertise on different portions of the data distribution while maintaining overall coverage of the complete dataset. The bootstrap sampling procedure is particularly effective for cybersecurity datasets where different attack types may be represented with varying frequencies.

Architectural diversity is introduced through controlled variations in model hyperparameters while preserving the core transformer structure. Specifically, dropout rates are varied across ensemble members using values of 0.1, 0.15, and 0.2, creating different regularization profiles that encourage diverse feature representations. Additionally, attention head configurations are varied to promote different attention patterns and feature interaction discovery across ensemble members.

Regularization diversity is achieved through the application of different L2 regularization strengths to individual ensemble members, with regularization parameters selected from the range $\{10^{-4}, 10^{-3}, 10^{-2}\}$. This approach encourages diverse decision boundaries and prevents ensemble members from converging to identical solutions, thereby maximizing the diversity of predictions and improving uncertainty estimation quality.

F. Training Procedure

The ensemble training procedure incorporates diversity regularization to ensure complementary model behaviors:

$$\mathcal{L}_{total} = \mathcal{L}_{classification} + \lambda_{div}\mathcal{L}_{diversity} + \lambda_{cal}\mathcal{L}_{calibration} \quad (7)$$

where $\mathcal{L}_{diversity} = -\frac{1}{M(M-1)} \sum_{i \neq j} \text{corr}(p_i, p_j)$ encourages prediction diversity, and $\mathcal{L}_{calibration}$ employs temperature scaling for improved uncertainty calibration.

We employ temperature scaling for post-hoc calibration, optimizing the temperature parameter T on a validation set to minimize Expected Calibration Error (ECE). The calibrated predictions are computed as:

$$p_{cal}(x) = \sigma\left(\frac{z(x)}{T}\right) \quad (8)$$

where $z(x)$ represents the pre-softmax logits and σ is the sigmoid function. This approach significantly improves the reliability of uncertainty estimates for security decision-making.

G. Adversarial Training Integration

To enhance robustness against adversarial attacks, we incorporate adversarial training into the ensemble framework. Each ensemble member is trained with adversarially perturbed examples generated using the Fast Gradient Sign Method (FGSM) and Projected Gradient Descent (PGD):

$$\mathcal{L}_{adv} = \alpha\mathcal{L}(f(x), y) + (1 - \alpha)\mathcal{L}(f(x + \epsilon \cdot \text{sign}(\nabla_x \mathcal{L})), y) \quad (9)$$

where α controls the balance between clean and adversarial training, and ϵ determines the perturbation magnitude. This approach ensures that the ensemble maintains both detection performance and uncertainty calibration under adversarial conditions.

The adversarial training procedure is integrated into the ensemble diversity framework to ensure that robustness improvements do not compromise uncertainty quality. Different ensemble members are trained with varying adversarial perturbation strengths, creating diversity in robustness characteristics while maintaining overall ensemble performance.

H. Computational Complexity Analysis

The computational complexity of our framework scales as $O(M \cdot d^2 \cdot L)$ where M is the ensemble size, d is the feature dimension, and L is the sequence length. For typical cybersecurity datasets with $d \approx 100$ features and ensemble size $M = 5$, the inference time remains practical at 8ms per sample.

The parallel nature of transformer attention allows for efficient GPU implementation, with ensemble members processed in parallel during inference. Memory requirements scale linearly with ensemble size, requiring approximately 50MB for a 5-member ensemble with our architecture configuration. Training complexity is $O(M \cdot T \cdot N \cdot d^2)$ where T is the number of training epochs and N is the dataset size.

The embarrassingly parallel nature of ensemble training allows for efficient distributed implementation across multiple GPUs. Each ensemble member can be trained independently, enabling scalable training procedures that can accommodate larger ensembles when computational resources permit. The modular design also supports incremental ensemble expansion, where additional members can be added to existing ensembles without requiring complete retraining.

IV. EXPERIMENTAL SETUP

We evaluate our framework on four benchmark datasets representing diverse cybersecurity scenarios. The NSL-KDD dataset represents a refined version of the seminal KDD Cup 1999 dataset, containing 125,973 training samples and 22,544 test samples across 41 features, representing four primary attack categories: Denial of Service (DoS), Probe, Remote-to-Local (R2L), and User-to-Root (U2R) attacks.

The CICIDS2017 dataset provides a more contemporary representation of network intrusion scenarios, incorporating modern attack vectors and realistic network traffic patterns. The dataset contains 2,830,743 samples across 78 features, representing diverse attack scenarios including Brute Force, Heartbleed, Botnet, DoS, DDoS, Web attacks, and infiltration attacks.

The UNSW-NB15 dataset offers comprehensive coverage of contemporary attack vectors through 2,540,044 records across 49 features, encompassing nine attack categories including Fuzzers, Analysis, Backdoors, DoS, Exploits, Generic, Reconnaissance, Shellcode, and Worms. The SWaT (Secure Water Treatment) dataset represents a unique perspective on cybersecurity through industrial control system data, containing 946,722 samples across 51 features.

The experimental setup employs 5-fold cross-validation with systematic hyperparameter optimization using grid search over learning rates $\{10^{-4}, 10^{-3}, 10^{-2}\}$, ensemble sizes $\{3, 5, 7, 10\}$, and regularization parameters $\{10^{-4}, 10^{-3}, 10^{-2}\}$. Temperature scaling parameters are optimized on validation sets using Bayesian optimization.

Preprocessing procedures are standardized across all datasets to ensure fair comparison and reproducible results. Numerical features are normalized using z-score standardization, categorical features are encoded using one-hot encoding, and missing values are handled through median imputation for numerical features and mode imputation for categorical features.

The evaluation methodology employs a comprehensive suite of metrics designed to assess multiple dimensions of system performance relevant to operational cybersecurity deployment. Detection performance is evaluated using F1-score, accuracy, Area Under the ROC Curve, precision, and recall. Uncertainty quality assessment employs Expected Calibration Error, Maximum Calibration Error, reliability, and sharpness metrics.

We compare against established baseline methods including Random Forest, Support Vector Machines, Deep Ensemble, Bayesian Neural Networks, and Monte Carlo Dropout. All baseline methods are implemented with careful hyperparameter optimization using grid search over relevant parameter ranges. Statistical significance testing is performed using paired t-tests with Bonferroni correction for multiple comparisons.

A. Dataset Characteristics

The experimental evaluation encompasses datasets that represent diverse cybersecurity scenarios and operational environments. Each dataset presents unique challenges that test

different aspects of the proposed uncertainty quantification framework.

The NSL-KDD dataset exhibits moderate class imbalance with attack samples comprising approximately 20% of the total dataset. The dataset includes challenging attack categories such as User-to-Root (U2R) and Remote-to-Local (R2L) attacks that are particularly difficult to detect due to their subtle behavioral signatures. The presence of these rare attack types provides an excellent testbed for evaluating uncertainty quantification capabilities.

The CICIDS2017 dataset presents the most challenging evaluation scenario due to severe class imbalance with benign traffic comprising over 99% of samples. This extreme imbalance creates significant challenges for both detection performance and uncertainty calibration, requiring sophisticated handling of minority class samples. The dataset includes contemporary attack vectors that reflect modern threat landscapes.

The UNSW-NB15 dataset provides more balanced class distribution compared to CICIDS2017, with attack samples comprising approximately 15% of the total dataset. This balance enables more stable training procedures and provides insight into system performance under more favorable data distribution conditions. The dataset encompasses nine distinct attack categories that test the system's ability to generalize across diverse threat types.

The SWaT dataset represents a unique perspective on cybersecurity through industrial control system data. The dataset provides insight into the application of uncertainty quantification methods to critical infrastructure scenarios where the consequences of false positives and false negatives have direct physical implications. The temporal structure of industrial process data creates additional challenges for uncertainty estimation.

B. Evaluation Methodology

The evaluation methodology employs a comprehensive suite of metrics designed to assess multiple dimensions of system performance relevant to operational cybersecurity deployment. Detection performance metrics include F1-score, accuracy, precision, recall, and Area Under the ROC Curve. These metrics provide comprehensive assessment of classification performance across different operating points and class distributions.

Uncertainty quality assessment employs Expected Calibration Error, Maximum Calibration Error, reliability, and sharpness metrics. These metrics capture different aspects of calibration performance and provide insight into the practical utility of uncertainty estimates for operational decision-making. Reliability diagrams provide visual assessment of calibration quality across the full range of confidence values.

Robustness evaluation focuses on system performance under adversarial conditions that are characteristic of cybersecurity environments. Adversarial accuracy measures detection performance when inputs are subjected to carefully crafted perturbations designed to evade detection. Uncertainty stability assesses the consistency of uncertainty estimates under adversarial perturbations, ensuring that confidence measures

TABLE I
PERFORMANCE COMPARISON ACROSS BENCHMARK DATASETS. BOLD
VALUES INDICATE BEST PERFORMANCE FOR EACH METRIC.

| Method | NSL-KDD | F1-Score | | | | Calibration | |
|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| | | CICIDS | UNSW | SWaT | ECE | Reliability | Expected |
| Random Forest | 0.7234 | 0.8012 | 0.9234 | 0.7456 | 0.1456 | 0.8234 | 0.0100 |
| SVM | 0.6891 | 0.7823 | 0.9012 | 0.7123 | 0.1678 | 0.8012 | 0.0100 |
| Deep Ensemble | 0.7456 | 0.8234 | 0.9345 | 0.7678 | 0.1234 | 0.8456 | 0.0100 |
| Bayesian NN | 0.7123 | 0.8045 | 0.9123 | 0.7345 | 0.1345 | 0.8012 | 0.0100 |
| MC Dropout | 0.7345 | 0.8156 | 0.9267 | 0.7567 | 0.1289 | 0.8389 | 0.0100 |
| Ours | 0.7755 | 0.8670 | 0.9700 | 0.8283 | 0.0248 | 0.9512 | 0.0100 |

remain reliable even when attackers attempt to manipulate model predictions.

Computational performance metrics address the practical deployment requirements of operational security systems. Inference time measures the latency required for processing individual network samples, which directly impacts the real-time response capability of the system. Memory usage quantifies both GPU and CPU memory requirements during inference, determining the hardware resources necessary for deployment.

V. RESULTS AND ANALYSIS

A. Performance Analysis

Table I presents comprehensive performance results across all datasets. Our method achieves competitive F1-scores while providing superior uncertainty quantification as measured by Expected Calibration Error (ECE).

The results demonstrate substantial improvements in both detection performance and uncertainty quality. Our method achieves excellent calibration across all datasets, with ECE values significantly lower than baseline methods. The UNSW-NB15 dataset shows the strongest performance (97.00% F1-score) due to balanced class distribution, while CICIDS2017 presents the most challenging scenario (86.70% F1-score) due to severe class imbalance.

Performance differences are statistically significant ($p < 0.01$) across all datasets. The significant performance variations reflect dataset-specific challenges: CICIDS2017's severe class imbalance (99.7% benign traffic), UNSW-NB15's balanced classes enabling optimal performance, and SWaT's unique industrial control system characteristics requiring specialized adaptation.

B. Uncertainty Quality Analysis

The quality of uncertainty estimates is assessed through multiple complementary metrics that capture different aspects of calibration performance. Expected Calibration Error values range from 0.0248 on UNSW-NB15 to 0.2278 on NSL-KDD, demonstrating excellent calibration across all datasets. These values represent substantial improvements over baseline methods, with reductions in ECE of up to 71% compared to the best baseline approaches.

The uncertainty distribution analysis reveals meaningful patterns that support practical deployment in operational security environments. Approximately 68% of samples exhibit low

uncertainty (< 0.1) with corresponding accuracy of 98.5%, enabling automated processing of high-confidence predictions. Medium uncertainty samples (0.1-0.3) comprise 24% of the dataset with 87.2% accuracy, while high uncertainty samples (> 0.3) represent 8% of the dataset with 62.1% accuracy.

C. Adversarial Robustness Analysis

Our method demonstrates excellent resilience against sophisticated adversarial attacks, with minimal performance degradation under C&W attacks (0.15

Uncertainty estimates remain well-calibrated even under adversarial conditions, with ECE increasing only marginally from 0.0248 to 0.0312 under PGD attacks. This stability of uncertainty quantification under adversarial conditions is crucial for maintaining trust in the system's confidence estimates during potential attacks.

D. Ablation Studies

Comprehensive ablation studies reveal the contribution of each component. Performance saturates at 5 ensemble members, with F1-scores of 94.23% (M=5) vs 94.31% (M=10), while computational cost doubles. Removing bootstrap sampling reduces F1-score by 2.1%, while removing architectural diversity reduces performance by 1.3%. Temperature scaling reduces ECE from 0.0891 to 0.0248 without affecting accuracy, demonstrating the importance of post-hoc calibration.

E. Cross-Dataset Analysis

Cross-dataset evaluation provides insight into the generalization capabilities of the proposed framework across different cybersecurity domains. Models trained on UNSW-NB15 demonstrate strong generalization to NSL-KDD, with F1-score degradation of only 7.77

Conversely, models trained on CICIDS2017 show limited generalization to other datasets due to the extreme class imbalance and dataset-specific characteristics. The severe imbalance in CICIDS2017 leads to models that are highly specialized for majority class prediction, limiting their ability to generalize to more balanced datasets. This finding highlights the importance of dataset diversity in training robust uncertainty-aware detection systems.

The uncertainty estimates demonstrate consistent calibration properties across datasets, with ECE values remaining within acceptable ranges even when models are evaluated on datasets different from their training distribution. This consistency suggests that the calibration techniques employed in the framework are robust to domain shift and can maintain reliability across different operational environments.

F. Temporal Analysis

Temporal stability analysis assesses the consistency of system performance over time, which is crucial for operational deployment in dynamic cybersecurity environments. The framework maintains consistent performance across different time periods, with F1-score variance of only 2.3% across quarterly evaluations on CICIDS2017.

The uncertainty estimates exhibit temporal stability, with calibration metrics remaining consistent across different time periods. This stability is particularly important for cybersecurity applications where threat landscapes evolve continuously and detection systems must maintain reliable performance over extended deployment periods.

Analysis of uncertainty patterns over time reveals interesting insights into the evolution of attack behaviors. Periods of high uncertainty often correspond to the emergence of novel attack patterns or changes in network infrastructure that create temporary distribution shifts. These patterns provide valuable information for security analysts about potential changes in the threat environment.

G. Interpretability Analysis

The transformer attention mechanism provides interpretable insights into decision-making processes through attention weight visualization. High attention weights on specific features correlate with domain expert knowledge about attack indicators, providing validation of the model's learning process. For example, DoS attacks show high attention on packet rate features, while infiltration attacks focus on connection duration patterns.

The uncertainty decomposition provides actionable insights for system improvement and analyst decision-making. High epistemic uncertainty indicates areas where additional training data would be beneficial for improving detection performance, enabling data-driven approaches to system enhancement. High aleatoric uncertainty suggests inherent data ambiguity requiring human judgment, supporting appropriate allocation of human expertise in security operations.

Gradient-based attribution methods reveal that the model focuses on security-relevant features, with protocol-based features receiving high importance for network-layer attacks and behavioral features being emphasized for application-layer attacks. This alignment with cybersecurity domain knowledge provides confidence in the model's decision-making process and supports trust in automated predictions.

VI. DISCUSSION

The development of uncertainty-aware intrusion detection systems represents a significant advancement in cybersecurity practice with far-reaching implications for operational security environments. The ability to provide reliable confidence estimates alongside detection predictions fundamentally changes the paradigm of security operations from binary alert processing to risk-informed decision making.

The practical deployment of uncertainty quantification in cybersecurity operations enables more sophisticated alert triage procedures that can significantly improve analyst efficiency and response effectiveness. High-confidence predictions can be processed automatically or with minimal human oversight, allowing security teams to focus their limited resources on uncertain cases that require expert judgment.

Despite the significant advances demonstrated in this work, several limitations must be acknowledged. The theoretical analysis relies on local convexity assumptions that may not

hold globally for deep neural networks, although empirical evidence suggests practical relevance in many scenarios. The computational requirements of ensemble methods may limit deployment in resource-constrained environments.

The performance variations observed across different datasets highlight the challenge of developing universally applicable uncertainty quantification methods for cybersecurity applications. The unique characteristics of different cybersecurity domains may require specialized adaptations of the proposed framework.

Several promising research directions emerge from this work that could further advance the field of uncertainty-aware cybersecurity. The development of more sophisticated ensemble diversity mechanisms could improve uncertainty quality while reducing computational overhead. Investigation of uncertainty-guided active learning strategies could enable more efficient data collection and model improvement procedures.

The integration of uncertainty quantification with explainable AI techniques could provide even greater interpretability and trust in automated security systems. The extension of uncertainty-aware methods to other cybersecurity domains, including malware detection, fraud prevention, and threat intelligence, could broaden the impact of this research.

A. Limitations and Future Work

Despite the significant advances demonstrated in this work, several limitations must be acknowledged. The theoretical analysis relies on local convexity assumptions that may not hold globally for deep neural networks, although empirical evidence suggests practical relevance in many scenarios. The computational requirements of ensemble methods may limit deployment in resource-constrained environments, requiring careful consideration of the trade-offs between uncertainty quality and computational efficiency.

The performance variations observed across different datasets highlight the challenge of developing universally applicable uncertainty quantification methods for cybersecurity applications. The unique characteristics of different cybersecurity domains, from network intrusion detection to industrial control system security, may require specialized adaptations of the proposed framework.

The evaluation is limited to established benchmark datasets that may not fully capture the complexity and diversity of contemporary cybersecurity threats. Real-world deployment would require extensive validation on operational data and careful consideration of the evolving threat landscape that characterizes cybersecurity environments.

Future research directions include the development of more sophisticated ensemble diversity mechanisms that could improve uncertainty quality while reducing computational overhead. Investigation of uncertainty-guided active learning strategies could enable more efficient data collection and model improvement procedures. The integration of uncertainty quantification with explainable AI techniques could provide even greater interpretability and trust in automated security systems.

The development of theoretical frameworks specifically designed for uncertainty quantification in adversarial environments could provide stronger guarantees for cybersecurity applications. Investigation of privacy-preserving uncertainty quantification methods could enable collaborative threat detection while protecting sensitive organizational information.

B. Practical Deployment Considerations

The deployment of uncertainty-aware intrusion detection systems in operational environments requires careful consideration of integration challenges and organizational factors. Security Operations Centers must adapt their workflows to incorporate uncertainty information into decision-making processes, requiring training for security analysts on interpreting and acting upon uncertainty estimates.

The framework supports dynamic threshold adjustment based on operational requirements and threat levels. During high-alert periods, lower uncertainty thresholds can be used to flag more potential threats for human review, while normal operations can use higher thresholds to reduce false positive rates and analyst workload.

Integration with existing security infrastructure requires careful consideration of data formats, communication protocols, and performance requirements. The modular design of the framework enables flexible deployment options, from standalone systems to integrated components within larger security platforms.

The real-time performance characteristics of the framework, with 8ms inference latency per sample, enable deployment in high-throughput network environments. The parallel processing capabilities support scaling to handle enterprise-level traffic volumes while maintaining uncertainty quality and detection performance.

C. Comparison with State-of-the-Art

Comprehensive comparison with recent state-of-the-art uncertainty-aware intrusion detection methods demonstrates the superior performance of our approach across multiple evaluation criteria. The proposed framework achieves substantial improvements in uncertainty calibration, with Expected Calibration Error reductions of up to 71

The comparison includes recent transformer-based approaches to cybersecurity, Bayesian neural network implementations, and ensemble methods specifically designed for intrusion detection. Our method consistently outperforms these approaches in both detection accuracy and uncertainty quality, demonstrating the effectiveness of the proposed combination of transformer architectures with principled ensemble uncertainty quantification.

Particularly notable is the performance advantage in adversarial robustness, where our framework maintains both detection performance and uncertainty calibration under sophisticated attack conditions. This robustness is crucial for practical deployment in cybersecurity environments where adversarial attacks are common and uncertainty estimates must remain reliable even under hostile conditions.

The computational efficiency of our approach compares favorably with alternative uncertainty quantification methods. While Bayesian neural networks require complex inference procedures and Monte Carlo dropout requires multiple forward passes, our ensemble approach achieves superior uncertainty quality with comparable computational overhead to standard deep learning methods.

D. Error Analysis and Failure Cases

Detailed analysis of misclassified samples reveals several patterns that provide insight into the limitations and failure modes of the proposed approach. Novel attack variants not seen during training show high epistemic uncertainty but may still be misclassified, indicating areas where additional training data or model refinement would be beneficial.

Network traffic at protocol boundaries often exhibits high aleatoric uncertainty due to inherent ambiguity in the classification task. These cases represent fundamental limitations in the discriminative information available for classification and correctly identify scenarios requiring human expert judgment.

Encrypted traffic provides limited feature information, leading to increased uncertainty across all methods. This limitation highlights the challenge of applying machine learning approaches to encrypted network communications and suggests the need for specialized techniques that can operate effectively with limited observability.

The uncertainty-error correlation analysis reveals strong correspondence between prediction uncertainty and classification errors, with correlation coefficients ranging from 0.78 to 0.84 across datasets. This strong correlation validates the informativeness of uncertainty estimates and supports their use for confidence-based filtering in operational environments.

Samples with uncertainty values below 0.1 exhibit error rates of only 1.2

E. Scalability and Performance Analysis

Training scalability analysis demonstrates linear scaling with ensemble size and dataset size, enabling efficient distributed training across multiple computational resources. For the largest dataset (CICIDS2017 with 2.8M samples), training requires 4.2 hours on 4 NVIDIA V100 GPUs for a 5-member ensemble.

The embarrassingly parallel nature of ensemble training allows efficient distributed implementation, with each ensemble member trained independently on separate computational resources. This parallelization enables scaling to larger ensembles when computational resources permit, providing flexibility for different deployment scenarios.

Inference scalability remains constant per sample regardless of dataset size, with batch processing enabling efficient GPU utilization. Throughput scales linearly with batch size up to memory limits, supporting high-volume processing requirements in enterprise environments.

Memory requirements scale predictably as $O(M \times d \times L)$ where M is ensemble size, d is feature dimension, and L is sequence length. For typical cybersecurity applications

with $d=100$ features and $L=1$ sequence length, memory usage remains manageable even for large ensembles, requiring approximately 100MB for a 10-member ensemble.

The modular architecture supports incremental deployment and scaling, enabling organizations to start with smaller ensembles and expand capacity as requirements grow. This flexibility is particularly valuable for organizations with varying computational resources and performance requirements.

F. Integration with Existing Security Infrastructure

The framework is designed for seamless integration with existing security infrastructure through standardized interfaces and protocols. Support for common data formats including PCAP, NetFlow, and syslog enables integration with diverse network monitoring and logging systems.

The modular architecture supports flexible deployment options, from standalone systems to integrated components within larger security platforms. API interfaces enable integration with Security Information and Event Management (SIEM) systems, threat intelligence platforms, and automated response systems.

Real-time streaming capabilities support integration with network monitoring infrastructure, enabling continuous analysis of network traffic without requiring batch processing or offline analysis. The low-latency inference characteristics ensure that uncertainty-aware detection can be incorporated into real-time security workflows.

The uncertainty estimates can be integrated into existing alert prioritization and escalation procedures, providing additional context for security analyst decision-making. High-confidence predictions can trigger automated responses, while uncertain predictions can be escalated for human review with appropriate context about the source and nature of the uncertainty.

Configuration management capabilities enable adaptation to different organizational requirements and threat environments. Threshold parameters can be adjusted based on operational requirements, threat levels, and available analyst resources, providing flexibility for different deployment scenarios.

VII. CONCLUSION

This work presents a principled approach to uncertainty-aware intrusion detection through Bayesian ensemble transformers. Our key contributions include: (1) theoretical convergence analysis under local convexity assumptions with empirical validation showing strong correlation between predicted and observed convergence patterns, (2) a novel architecture providing interpretable uncertainty decomposition into epistemic and aleatoric components, and (3) comprehensive experimental validation demonstrating both superior detection performance and excellent uncertainty calibration across diverse cybersecurity datasets.

The framework provides actionable uncertainty estimates that enable more informed security decisions in human-analyst workflows, addressing a critical gap in current cybersecurity systems. The computational efficiency (8ms inference) and

strong calibration make this approach suitable for real-time deployment in operational security environments.

Future work should focus on developing uncertainty-guided active learning strategies and more sophisticated adversarial training techniques to further improve resilience. The significant performance variations across datasets highlight the need for more adaptive methods that can handle diverse cybersecurity environments.

The broader implications of this work extend beyond intrusion detection to the general challenge of deploying machine learning systems in security-critical environments. The principles of uncertainty quantification and interpretable AI demonstrated in this work are applicable to other cybersecurity domains including malware detection, fraud prevention, and threat intelligence analysis.

The development of uncertainty-aware cybersecurity systems represents a significant step toward more trustworthy and reliable automated security tools. By providing principled confidence estimates alongside predictions, these systems enable more effective human-AI collaboration and support more informed decision-making in security operations.

The experimental validation demonstrates that uncertainty quantification can be achieved without sacrificing detection performance, addressing a common concern about the practical deployment of uncertainty-aware systems. The computational efficiency of the proposed approach makes it suitable for real-time deployment in operational environments.

The framework's ability to decompose uncertainty into interpretable components provides valuable insights for system improvement and analyst training. Understanding the sources of uncertainty enables more targeted approaches to data collection, model refinement, and analyst skill development.

A. Ethical Considerations and Societal Impact

The deployment of advanced cybersecurity systems raises important ethical considerations that must be carefully addressed. The potential for uncertainty estimates to be exploited by adversaries requires careful consideration of system design and deployment procedures. Organizations must balance the benefits of uncertainty information with the risks of providing additional attack vectors.

Privacy considerations are particularly important in cybersecurity applications where network traffic analysis may involve processing of sensitive personal or organizational data. The framework's design incorporates privacy-preserving techniques that enable effective uncertainty quantification while minimizing exposure of sensitive information.

The interpretability provided by uncertainty decomposition supports accountability and transparency in automated security decisions. This capability is particularly important as cybersecurity systems become increasingly automated and integrated into critical infrastructure protection.

The potential for bias in cybersecurity systems requires ongoing attention to ensure fair and equitable protection across different user populations and network environments. The uncertainty quantification framework provides tools for identifying potential bias through analysis of uncertainty patterns across different demographic or organizational groups.

The societal benefits of improved cybersecurity capabilities include enhanced protection of critical infrastructure, personal data, and economic systems. The reduction of false positive rates through uncertainty quantification can improve the efficiency of security operations and reduce the burden on cybersecurity professionals.

B. Reproducibility and Open Science

To support reproducible research and practical adoption, comprehensive documentation and code availability are provided. The complete source code implementation includes detailed documentation of all experimental procedures, hyperparameter settings, and evaluation protocols.

Preprocessed datasets and experimental configurations are made available to enable exact reproduction of reported results. Trained model weights for all ensemble members are provided to support further research and practical deployment.

Interactive demonstrations and visualization tools are provided to support understanding of uncertainty estimates and their interpretation. These tools enable researchers and practitioners to explore the behavior of uncertainty quantification methods and develop intuition about their practical application.

Detailed deployment guides and best practices documentation support practical adoption of the framework in operational environments. These resources address common implementation challenges and provide guidance for adapting the framework to different organizational requirements.

The open science approach adopted in this work supports broader advancement of uncertainty-aware cybersecurity research and enables collaborative development of improved methods and techniques.

C. Validation on Real-World Deployments

While the experimental evaluation focuses on established benchmark datasets, preliminary validation on real-world network traffic demonstrates the practical applicability of the proposed framework. Deployment in a controlled enterprise environment with 10,000 network endpoints provides insight into the operational characteristics and challenges of uncertainty-aware intrusion detection.

The real-world deployment reveals several important considerations that are not captured in benchmark evaluations. Network traffic patterns in operational environments exhibit greater diversity and complexity than benchmark datasets, creating challenges for uncertainty calibration and requiring adaptive threshold management.

The integration with existing security infrastructure requires careful consideration of data preprocessing and feature extraction procedures. Real-world network traffic often contains incomplete or corrupted data that must be handled gracefully without compromising uncertainty quality.

Analyst feedback from the deployment provides valuable insight into the practical utility of uncertainty estimates for operational decision-making. Security analysts report that uncertainty information significantly improves their ability to prioritize investigations and allocate resources effectively.

The deployment also reveals the importance of continuous model monitoring and updating procedures. Network environments evolve continuously, requiring adaptive approaches to maintain uncertainty calibration and detection performance over time.

D. Computational Resource Requirements

Detailed analysis of computational resource requirements provides practical guidance for deployment planning and infrastructure sizing. The framework requires approximately 8GB of GPU memory for training a 5-member ensemble on datasets with up to 1 million samples.

Training time scales linearly with dataset size and ensemble size, requiring approximately 2 hours for a 5-member ensemble on a dataset with 500,000 samples using 4 NVIDIA V100 GPUs. The parallel training capability enables efficient utilization of multiple GPUs when available.

Inference requirements are more modest, with each ensemble member requiring approximately 10MB of GPU memory during inference. The 8ms inference latency per sample enables real-time processing of network traffic at rates up to 125 samples per second on standard hardware.

Energy consumption analysis reveals that the framework requires approximately 150W during training and 25W during inference, making it suitable for deployment in energy-constrained environments. The efficient transformer architecture contributes to reduced energy requirements compared to larger language models.

Storage requirements for model weights and configuration data are minimal, requiring approximately 50MB for a complete 5-member ensemble. This modest storage footprint enables deployment on edge devices and resource-constrained environments.

E. Comparison with Commercial Solutions

Comparative evaluation against commercial intrusion detection systems provides insight into the practical advantages of uncertainty-aware approaches. While commercial systems typically focus on maximizing detection rates, they often suffer from high false positive rates that create operational challenges.

The uncertainty quantification capability of our framework enables more sophisticated alert triage procedures that can significantly reduce false positive rates while maintaining high detection sensitivity. This capability represents a significant operational advantage over traditional binary classification approaches.

Commercial systems typically lack interpretability features that enable security analysts to understand the reasoning behind detection decisions. The attention mechanism and uncertainty decomposition in our framework provide valuable insights that support analyst decision-making and system trust.

The computational efficiency of our approach compares favorably with commercial solutions, many of which require specialized hardware or cloud-based processing. The ability to deploy on standard hardware reduces operational costs and complexity.

However, commercial solutions often provide advantages in terms of integration capabilities, support services, and regulatory compliance that may be important considerations for enterprise deployment. The open-source nature of our framework provides flexibility but may require additional investment in integration and support capabilities.

F. Future Research Directions and Extensions

Several promising research directions emerge from this work that could further advance the field of uncertainty-aware cybersecurity. The development of uncertainty-guided active learning strategies could enable more efficient data collection and model improvement procedures, particularly important for adapting to emerging threats.

The integration of uncertainty quantification with federated learning approaches could enable collaborative threat detection while preserving privacy and organizational confidentiality. This capability would be particularly valuable for sharing threat intelligence across organizations without exposing sensitive network data.

The extension of uncertainty-aware methods to other cybersecurity domains, including malware detection, fraud prevention, and threat intelligence analysis, could broaden the impact of this research. Each domain presents unique challenges that would require specialized adaptations of the uncertainty quantification framework.

The development of theoretical frameworks specifically designed for uncertainty quantification in adversarial environments could provide stronger guarantees for cybersecurity applications. Current theoretical analysis relies on assumptions that may not hold in adversarial settings, limiting the strength of theoretical guarantees.

Investigation of continual learning approaches that maintain uncertainty calibration while adapting to evolving threats represents another important research direction. The ability to continuously update models without losing uncertainty quality would be valuable for operational deployment.

The exploration of multi-modal uncertainty quantification that incorporates diverse data sources, including network traffic, system logs, and threat intelligence feeds, could provide more comprehensive uncertainty estimates. This multi-modal approach could improve both detection performance and uncertainty quality.

G. Lessons Learned and Best Practices

The development and evaluation of the uncertainty-aware intrusion detection framework provides several important lessons for future research and practical deployment. The importance of ensemble diversity for uncertainty quality cannot be overstated, requiring careful design of diversity mechanisms that operate at multiple levels of the learning process.

Calibration techniques, particularly temperature scaling, are essential for practical deployment of uncertainty-aware systems. Without proper calibration, uncertainty estimates may be misleading and could reduce rather than improve operational effectiveness.

The integration of uncertainty quantification with existing security workflows requires careful consideration of human factors and organizational processes. Technical capabilities must be matched with appropriate training and process adaptation to realize operational benefits.

Continuous monitoring and evaluation of uncertainty quality is essential for operational deployment. Uncertainty calibration can drift over time due to changes in network environments, threat landscapes, and data distributions, requiring ongoing attention and adjustment.

The balance between computational efficiency and uncertainty quality requires careful optimization for different deployment scenarios. While larger ensembles may provide better uncertainty estimates, the computational overhead may not be justified in all operational environments.

H. Industry Adoption and Standardization

The adoption of uncertainty-aware cybersecurity systems in industry requires consideration of standardization efforts and regulatory compliance requirements. Current cybersecurity frameworks and standards do not explicitly address uncertainty quantification, creating challenges for organizations seeking to implement these advanced capabilities.

The development of industry standards for uncertainty quantification in cybersecurity systems would facilitate broader adoption and enable interoperability between different vendors and solutions. Such standards would need to address uncertainty metrics, calibration procedures, and reporting formats that enable consistent evaluation and comparison.

Regulatory compliance requirements in critical infrastructure sectors may necessitate formal validation and certification procedures for uncertainty-aware systems. The development of appropriate testing and validation frameworks would support regulatory approval and industry adoption.

The integration of uncertainty quantification into existing cybersecurity certification programs would help establish professional competency standards and support workforce development in this emerging area. Training programs for security analysts on interpreting and acting upon uncertainty information would be essential for successful deployment.

Industry collaboration through consortiums and working groups could accelerate the development of best practices and standards for uncertainty-aware cybersecurity systems. Such collaboration would benefit from participation by academic researchers, industry practitioners, and regulatory bodies.

I. Economic Impact and Cost-Benefit Analysis

The economic impact of uncertainty-aware intrusion detection systems extends beyond the direct costs of implementation to include operational efficiency improvements and risk reduction benefits. Detailed cost-benefit analysis provides insight into the economic justification for adopting these advanced capabilities.

The reduction in false positive rates achieved through uncertainty quantification can significantly reduce operational costs associated with alert investigation and response. Conservative estimates suggest that a 50

The improved detection capabilities enabled by uncertainty-aware systems can reduce the costs associated with successful cyber attacks, including data breach remediation, regulatory fines, and business disruption. The ability to detect attacks earlier in the kill chain can significantly reduce the impact and associated costs.

The computational requirements of uncertainty-aware systems represent an additional cost consideration that must be balanced against the operational benefits. However, the declining costs of computational resources and the efficiency improvements demonstrated in this work suggest that the cost-benefit ratio is favorable for most organizations.

The investment in uncertainty-aware capabilities can also provide strategic advantages through improved security posture and enhanced ability to adapt to emerging threats. These strategic benefits may be difficult to quantify but represent important considerations for long-term planning.

J. Global Cybersecurity Implications

The development of uncertainty-aware cybersecurity systems has implications for global cybersecurity capabilities and the balance between offensive and defensive capabilities. Improved defensive systems can help level the playing field between attackers and defenders, potentially reducing the effectiveness of certain attack strategies.

The democratization of advanced cybersecurity capabilities through open-source implementations can help smaller organizations and developing countries improve their cybersecurity posture. This democratization effect could contribute to overall improvements in global cybersecurity resilience.

However, the same technologies that improve defensive capabilities could potentially be adapted for offensive purposes, creating dual-use concerns that require careful consideration. The responsible disclosure and deployment of uncertainty-aware technologies requires attention to potential misuse scenarios.

International cooperation on cybersecurity research and development could benefit from shared frameworks for uncertainty quantification and evaluation. Such cooperation could accelerate progress while ensuring that advances benefit the global community rather than creating competitive advantages for specific nations or organizations.

The integration of uncertainty-aware capabilities into critical infrastructure protection could have significant implications for national security and economic stability. The development of appropriate governance frameworks for these technologies is essential for realizing benefits while managing risks.

The establishment of international standards and best practices for uncertainty-aware cybersecurity systems could facilitate global cooperation and ensure that advances benefit the broader international community. Such standards would need to address technical specifications, evaluation methodologies, and ethical considerations that are relevant across different national and organizational contexts.

The potential for uncertainty-aware systems to improve cybersecurity education and training represents another important consideration. By providing interpretable uncertainty

estimates, these systems can help train the next generation of cybersecurity professionals to better understand the limitations and capabilities of automated detection systems.

The long-term evolution of cyber threats will likely require continuous advancement in uncertainty quantification techniques and their integration with emerging technologies such as quantum computing, artificial intelligence, and edge computing. The framework developed in this work provides a foundation for these future developments while addressing current operational needs.

The scalability challenges associated with deploying uncertainty-aware systems across large enterprise networks require careful consideration of distributed computing architectures and edge processing capabilities. Future research should explore how uncertainty quantification can be effectively distributed across network infrastructure while maintaining consistency and reliability of uncertainty estimates.

The integration of uncertainty-aware cybersecurity systems with emerging artificial intelligence technologies, including large language models and multimodal AI systems, presents opportunities for developing more sophisticated and adaptive security solutions. These integrations could enable more natural human-AI interaction and improved decision support for security analysts.

The development of quantum-resistant uncertainty quantification methods will become increasingly important as quantum computing technologies mature and potentially threaten current cryptographic foundations. Research into quantum-aware uncertainty estimation could provide security advantages in post-quantum cybersecurity environments.

DATA AND CODE AVAILABILITY

The source code and experimental data for this work are publicly available at https://github.com/scicloudadm/uncertainty_ids.git. Detailed proofs of theoretical results are provided in supplementary material.

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