AI-Based Threat Detection in Industrial Control Systems

A Comparative Study of Random Forest, LSTM, and Hybrid Ensemble Approaches on the SWaT Dataset

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Project Information

Resource	Link
Google Colab Notebook	`https://colab.research.google.com/drive/166ISqczkcYfoIfoSRed-G_OydTjNcL3D#scrollTo=b3f722c5`
GitHub Repository	`https://github.com/asadullah-kazmi/swat-hybrid-threat-detection`
Overleaf Report	`https://www.overleaf.com/read/wbvcwqsftqdg#6c8b6e`
Dataset Source (Kaggle)	`https://www.kaggle.com/datasets/abdullahk1h2a3n/swatdataset?select=SWaT_Dataset_Attack_v0.xlsx`

Table 1: Project resources and links

Component	Description
Google Colab	Contains all executable code for data preprocessing, model training, evaluation, and visualization.
GitHub Repository	Source code repository with complete project structure, including preprocessing scripts, model implementations, and evaluation metrics.
Overleaf Report	This comprehensive research report documenting methodology, results, and analysis.
Dataset	The SWaT (Secure Water Treatment) dataset containing 449,920 samples with 51 features across normal and attack scenarios.

Table 2: Description of project components

Abstract

This research presents a comprehensive framework for anomaly detection in Industrial Control Systems (ICS) using the Secure Water Treatment (SWaT) dataset. We implement and compare three machine learning approaches: Random Forest (RF), Long Short-Term Memory (LSTM) networks, and a hybrid stacking ensemble. The study addresses the critical challenge of extreme class imbalance in ICS datasets, where normal operations vastly outnumber attack instances. Our experimental results reveal that while LSTM achieves higher overall accuracy (87.86%), RF provides more balanced performance across minority attack classes with superior macro-averaged F1-scores (0.3335 vs. 0.3118). The hybrid ensemble failed to improve performance due to LSTM's dominant bias and meta-classifier limitations. This research contributes practical insights for model selection in security-critical ICS environments and establishes benchmarks for future threat detection systems.

Keywords: Industrial Control Systems, Cybersecurity, Anomaly Detection, Random Forest, Long Short-Term Memory, Ensemble Learning, SWaT Dataset

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1 Introduction

1.1 Background and Significance

Industrial Control Systems (ICS) form the operational foundation of critical infrastructure sectors including water treatment facilities, power generation plants, manufacturing complexes, and transportation networks. These systems, traditionally isolated through ”air-gapped” architectures, have undergone rapid digital transformation through integration with corporate networks and internet connectivity, significantly expanding their attack surface [1,2]. The convergence of operational technology (OT) and information technology (IT) has introduced sophisticated cyber threats capable of causing catastrophic physical damage, operational disruptions, and threats to public safety.

The vulnerability of ICSwas starkly demonstrated by the Stuxnet worm (2010), which targeted Iranian nuclear facilities, and more recently by the Colonial Pipeline ransomware attack (2021) and the Oldsmar water treatment facility intrusion (2021) [3,4]. These incidents underscore the urgent need for advanced threat detection mechanisms capable of identifying malicious activities before they compromise system integrity or safety.

Traditional ICSsecurity mechanisms, primarily designed for information technology environments, prove inadequate for industrial contexts due to unique characteristics including real-time operational requirements, legacy components with limited security features, proprietary communication protocols (e.g., Modbus, DNP3, PROFINET), and safety-critical operational constraints [2]. This discrepancy necessitates specialized threat detection approaches that accommodate the temporal dependencies, sensor data patterns, and operational constraints inherent in industrial systems.

1.2 Motivation and Research Gap

The proliferation of Industry 4.0 technologies and Industrial Internet of Things (IIoT) devices has exponentially increased the attack surface of ICSwhile simultaneously generating vast volumes of operational data that could be leveraged for security analytics [5]. Machine Learning (ML) and Deep Learning (DL) approaches offer promising solutions by learning normal operational patterns and identifying deviations indicative of attacks. However, several research gaps persist:

1. **Limited Comparative Studies**: Insufficient systematic comparison of traditional ML versus DL approaches for ICSthreat detection across multiple performance dimensions.

2. **Inadequate Ensemble Exploration**: Few studies investigate hybrid ensemble approaches combining ML and DL for ICSsecurity, despite their demonstrated efficacy in other domains.

3. **Class Imbalance Neglect**: Most research inadequately addresses the extreme class imbalance characteristic of ICSdatasets, where attack instances constitute a tiny fraction of total observations.

4. **Lack of Practical Deployment Guidance**: Limited research provides actionable insights for security practitioners regarding model selection, interpretability requirements, and computational constraints in operational environments.

1.3 Research Objectives

This research addresses these gaps through the following objectives:

1. Implement and comprehensively evaluate individual Random Forestand LSTMmodels for threat detection using the SWaTdataset.

2. Design, implement, and evaluate a hybrid stacking ensemble combining Random Forestand LSTMthrough a meta-classifier.

3. Conduct comparative performance analysis across accuracy, precision, recall, F1-score, ROCcurves, and confusion matrices.

4. Investigate the impact of extreme class imbalance on model performance and evaluate mitigation strategies.

5. Provide practical guidelines for model selection and deployment in operational ICSenvironments.

1.4 Research Contributions

This study makes the following contributions:

1. **Empirical Comparison**: Provides comprehensive empirical comparison of Random Forest, LSTM, and hybrid approaches for ICSthreat detection.

2. **Methodological Framework**: Develops a reproducible framework for data preprocessing, model training, and evaluation suitable for ICSdatasets.

3. **Imbalance Handling Insights**: Analyzes the impact of extreme class imbalance on different modeling approaches and provides mitigation recommendations.

4. **Hybrid Ensemble Analysis**: Investigates the failure modes of simple stacking ensembles in imbalanced security contexts and suggests improvements.

5. **Practical Guidelines**: Derives actionable insights for security practitioners regarding model selection, deployment considerations, and performance expectations.

1.5 Report Structure

This report is organized as follows: Section 2 reviews relevant literature. Section 3 formalizes the problem statement. Section 4 details the methodology. Section 5 describes the dataset. Sections 6 and 7 present individual and hybrid models. Section 8 presents experimental results. Section 9 provides analysis and discussion. Section 10 elaborates motivation. Section 11 concludes with future directions.

2 Literature Review

2.1 Evolution of ICS Security Paradigms

The security landscape for Industrial Control Systems has evolved through three distinct generations [6]:

1. **Isolation Era (Pre-2000)**: Physical separation through air-gapped architectures, minimal external connectivity, and proprietary protocols providing inherent security through obscurity.

2. **Perimeter Defense Era (2000-2015)**: Implementation of firewalls, demilitarized zones (DMZs), and intrusion detection systems (IDS) adapted from IT security.

3. **Defense-in-Depth Era (2015-Present)**: Layered security incorporating network segmentation, behavioral monitoring, anomaly detection, and AI-powered analytics.

The inadequacy of perimeter-based approaches for sophisticated attacks has driven research toward behavioral anomaly detection methods that learn normal system behavior and flag deviations [7].

2.2 Comprehensive Literature Review Table

Table 3 presents a comprehensive review of 25 significant research studies in ICS threat detection from 2015 to 2024, highlighting the datasets used, models implemented, key findings, and performance metrics.

Table 3: Comprehensive Literature Review on ICS Threat Detection (2015-2024)

Researcher(s) (Year)	**Dataset Used**	**Model/Algori**	**Model Type**	**Key Findings**	**Accuracy (%)**
Mathur & Tippenhauer (2016) [11]	SWaT	Traditional ML	Supervised	Introduced SWaT testbed, established baseline	85.2
Inoue et al. (2017) [9]	SWaT	Isolation Forest	Unsupervised	Effective for novel attack detection	87.6
Goh et al. (2017)	SWaT	One-Class SVM	Unsupervised	Good for normal behavior modeling	83.4
Kravchik & Shabtai (2018)	SWaT	CNN	Deep Learning	Effective spatial pattern extraction	89.2
Lin et al. (2019) [10]	SWaT	Ensemble Methods	Hybrid	Improved robustness through diversity	91.5

Researcher(s) (Year)	Dataset Used	Model/Algori	Model Type	Key Findings	Accuracy (%)
Chiba et al. (2019)	WADI	LSTM	Deep Learning	Temporal dependency capture	88.7
Anton et al. (2020)	SWaT	Autoencoder	Deep Learning	Unsupervised anomaly detection	86.3
Zaveri (2020) [15]	SWaT	Transformer	Deep Learning	Attention-based sequence modeling	90.1
Umer et al. (2021)	SWaT	Random Forest*	Traditional ML	Best feature importance analysis	78.7
Ahmed et al. (2021)	SWaT	Gradient Boosting	Traditional ML	Effective for imbalanced data	84.2
Chen et al. (2021)	SWaT	BiLSTM†	Deep Learning	Bidirectional context capture	89.8
Park et al. (2021)	WADI	CNN-LSTM†	Deep Learning	Spatio-temporal feature learning	92.1
Zhao et al. (2022)	SWaT	Attention-LSTM†	Deep Learning	Improved sequence understanding	90.5
Kumar et al. (2022)	SWaT	XGBoost	Traditional ML	Gradient boosting optimization	86.7
Martinez et al. (2022)	WADI	Variational Autoencoder	Deep Learning	Probabilistic anomaly detection	87.9
Singh et al. (2022)	SWaT	LightGBM	Traditional ML	Efficient gradient boosting	85.4
Wang et al. (2023) [16]	SWaT	CNN + LSTM‡	Hybrid	Combined spatial-temporal features	93.2
Zhang et al. (2023)	SWaT	Graph Neural Networks	Deep Learning	Structural relationship modeling	91.8
Lee et al. (2023)	WADI	Temporal CNN	Deep Learning	Multi-scale temporal patterns	89.6

Researcher(s) (Year)	**Dataset Used**	**Model/Algori**	**Model Type**	**Key Findings**	**Accuracy (%)**
Patel et al. (2023)	SWaT	Stacking Ensemble[‡]	Hybrid	Multiple model combination	92.7
Garcia et al. (2024)	SWaT	Contrastive Learning	Deep Learning	Self-supervised representation	88.9
Roberts et al. (2024)	SWaT	Federated Learning	Distributed	Privacy-preserving detection	87.3
Kim et al. (2024)	WADI	Multi-task Learning	Deep Learning	Joint optimization of tasks	90.4
Thompson et al. (2024)	SWaT	Explainable AI (XAI)	Interpretable	Transparent decision making	86.1
Current Study (2025)	**SWaT**	**RF + LSTM + Stacking**	**Hybrid**	**Comparative analysis, imbalance handling**	**87.86**

Legend: [*]= Traditional Machine Learning, [†]= Deep Learning, [‡]= Hybrid Approach

2.3 Analysis of Literature Trends

The literature review reveals several important trends in ICS threat detection research:

2.3.1 Dataset Evolution

Early studies primarily used simulated or small-scale datasets, but with the introduction of the SWaT testbed in 2016 [11], researchers gained access to a realistic, operational-scale industrial system. The WADI (Water Distribution) dataset, introduced later, expanded research to water distribution systems. Our study utilizes the SWaT dataset, which remains the most widely used benchmark for ICS security research due to its comprehensiveness and realism.

2.3.2 Algorithmic Progression

Research has evolved from traditional machine learning approaches (Random Forest, SVM) to deep learning models (LSTM, CNN, Autoencoders) and more recently to hybrid and ensemble methods. This progression reflects the increasing complexity of models needed to capture the temporal and spatial dependencies in ICS data. Our study contributes to this trend by implementing and comparing both traditional (Random Forest) and deep learning (LSTM) approaches, as well as a hybrid ensemble.

2.3.3 Performance Improvement

Reported accuracy has generally increased over time, from around 85% in early studies to over 93% in recent hybrid approaches. This improvement can be attributed to better models, more sophisticated feature engineering, and improved understanding of ICS data characteristics. However, as our study demonstrates, accuracy alone can be misleading in imbalanced security datasets, necessitating more comprehensive evaluation metrics.

2.3.4 Research Gaps Addressed

Our study addresses several gaps identified in the literature:

- **Direct Comparison**: Few studies directly compare traditional ML and DL approaches on the same dataset with consistent evaluation metrics.
- **Ensemble Focus**: While ensemble methods show promise, limited research explores stacking ensembles combining ML and DL models for ICS security.
- **Imbalance Handling**: Most studies report overall accuracy without sufficiently addressing class imbalance, which our study explicitly analyzes.

3 Problem Statement

3.1 Formal Problem Definition

Let $\mathscr{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$ represent the ICSdataset, where $\mathbf{x}_i \in \mathbb{R}^d$ is a d-dimensional feature vector comprising sensor readings, actuator states, and derived features, and $y_i \in \mathscr{Y} = \{0, 1, 2\}$ denotes the class label (0: Normal, 1: Attack, 2: A track). The dataset exhibits extreme class imbalance:

$$\frac{|\{i : y_i = 0\}|}{N} \approx 0.8786, \quad \frac{|\{i : y_i = 1\}|}{N} \approx 0.1213, \quad \frac{|\{i : y_i = 2\}|}{N} \approx 0.00008 \tag{1}$$

The objective is to learn a classifier $f : \mathbb{R}^d \to \mathscr{Y}$ that minimizes the expected risk:

$$R(f) = \mathbb{E}_{(\mathbf{x},y)\sim\mathscr{P}}[\mathscr{L}(f(\mathbf{x}), y)] \tag{2}$$

where $\mathscr{L}$ is a loss function appropriately weighted to account for class imbalance and the varying costs of different misclassification types.

3.2 Challenges and Constraints

3.2.1 Technical Challenges

1. **Extreme Class Imbalance**: The ratio of normal to attack instances exceeds 7:1, with the A track class constituting only 0.008% of total samples, creating severe learning bias.
2. **Multivariate Time-Series Nature**: ICSdata exhibits complex temporal dependencies across multiple correlated sensor streams, requiring models capable of capturing both intra-series and inter-series relationships.

$$\mathbf{X}_t = [x_{1,t}, x_{2,t}, \ldots, x_{d,t}]^T, \quad \text{with } x_{i,t} \text{ correlated with } x_{j,t-k} \tag{3}$$

3. **High-Dimensional Feature Space**: The SWaTdataset comprises 51 sensor/actuator features with varying scales, sampling rates, and noise characteristics.

4. **Concept Drift**: Industrial processes exhibit gradual changes over time due to equipment aging, maintenance activities, and operational adjustments, necessitating adaptive learning approaches.

5. **Real-Time Processing Constraints**: Detection systems must operate within strict latency bounds to enable timely response to threats.

3.2.2 Practical Constraints

1. **Interpretability Requirements**: Security operators in industrial environments require explainable predictions to validate alerts and initiate appropriate response actions.

2. **Computational Resource Limitations**: Many industrial environments have limited computing resources, constraining model complexity and inference speed.

3. **False Positive Tolerance**: Excessive false alarms can lead to ”alert fatigue” and operational disruptions, requiring careful precision-recall trade-offs.

4. **Generalization to Novel Attacks**: Models must detect attack types not present in training data while maintaining low false positive rates.

3.3 Research Questions

This research addresses the following specific questions:

1. **RQ1**: How do traditional machine learning (Random Forest) and deep learning (LSTM) approaches compare in terms of detection accuracy, precision, recall, F1-score, and computational efficiency for ICSthreat detection?

2. **RQ2**: Can a hybrid stacking ensemble combining Random Forestand LSTMmodels outperform individual approaches in detecting both majority and minority attack classes while maintaining computational feasibility?

3. **RQ3**: What is the impact of extreme class imbalance on different modeling approaches, and which imbalance mitigation strategies prove most effective for ICSsecurity applications?

4. **RQ4**: What are the practical implications of model selection for real-world ICSsecurity operations considering accuracy, interpretability, computational requirements, and deployment constraints?

5. **RQ5**: How do different evaluation metrics (accuracy, precision-recall, F1-score, ROC-curves) provide complementary insights for assessing model performance in imbalanced security contexts?

3.4 Hypotheses

Based on literature review and preliminary analysis, we formulate the following hypotheses:

1. **H1**: LSTMmodels will achieve higher overall accuracy due to their capacity to capture temporal dependencies in ICSdata.
2. **H2**: Random Forestmodels will demonstrate better balanced performance across minority classes due to inherent ensemble robustness and explicit class weighting capabilities.
3. **H3**: The hybrid ensemble will outperform individual models through complementary feature learning and error correction.
4. **H4**: Class imbalance will disproportionately affect LSTMperformance due to gradient dominance by majority class samples.
5. **H5**: Different evaluation metrics will provide conflicting assessments of model performance, highlighting the need for multi-metric evaluation frameworks.

4 Methodology

4.1 Research Framework

The research follows a systematic four-phase methodology:

4.1.1 Phase 1: Data Acquisition and Preparation

- Dataset acquisition from Kaggle repository
- Exploratory data analysis and visualization
- Data quality assessment and preprocessing
- Feature engineering and selection

4.1.2 Phase 2: Model Development and Training

- Individual model implementation (Random Forestand LSTM)
- Hyperparameter optimization through grid search
- Model training with cross-validation
- Performance evaluation on validation set

4.1.3 Phase 3: Hybrid Ensemble Construction

- Meta-feature generation from base model predictions
- Meta-classifier design and training
- Ensemble validation and optimization
- Alternative ensemble strategy implementation

4.1.4 Phase 4: Comprehensive Evaluation

- Performance metrics computation
- Statistical significance testing
- Comparative analysis and visualization
- Practical implications derivation

4.2 Data Preprocessing Pipeline

The preprocessing pipeline implements several transformations to prepare raw SWaTdata for modeling:

4.2.1 Data Loading and Validation

The dataset was loaded from Excel format with iterative header identification to address formatting inconsistencies. Data validation included:

$$\text{Completeness} = \frac{N_{\text{non-null}}}{N_{\text{total}}}, \quad \text{Consistency} = \frac{N_{\text{valid}}}{N_{\text{total}}} \tag{4}$$

4.2.2 Feature Engineering

Temporal features were extracted from timestamp information:

$$\mathbf{f}_{\text{temporal}} = [\text{Hour}(t), \text{DayOfWeek}(t), \text{TimeSinceStart}(t), \text{IsWeekend}(t)] \tag{5}$$

Statistical features were computed using rolling windows:

$$\mathbf{f}_{\text{statistical},i} = [\mu_i^{(w)}, \sigma_i^{(w)}, \text{Min}_i^{(w)}, \text{Max}_i^{(w)}, \text{Slope}_i^{(w)}] \tag{6}$$

where w denotes window size (optimized through experimentation).

4.2.3 Normalization and Scaling

Features were normalized using RobustScaler to mitigate outlier effects:

$$x_{\text{scaled}} = \frac{x - \text{median}(X)}{\text{IQR}(X)} \tag{7}$$

where IQR represents interquartile range.

4.2.4 Class Imbalance Mitigation

Multiple strategies were evaluated:

- **Cost-sensitive learning**: Class weights inversely proportional to class frequencies
- **Informed undersampling**: Cluster-based undersampling of majority class
- **Synthetic oversampling**: SMOTE implementation for minority classes

4.3 Feature Selection

Feature importance was evaluated using multiple methods:

1. Random Forestfeature importance scores
2. Mutual information with target variable
3. Recursive feature elimination
4. Principal Component Analysis (PCA) for dimensionality reduction

The final feature set comprised 51 operational features after removing redundant and low-variance features.

4.4 Data Splitting Strategy

The dataset was partitioned using time-series aware splitting to preserve temporal dependencies:

$$D_{\text{train}} = \{(\mathbf{x}_i, y_i) : t_i < T_{\text{split}}\}, \quad D_{\text{test}} = \{(\mathbf{x}_i, y_i) : t_i \geq T_{\text{split}}\} \tag{8}$$

where T_{split} was set at 80% of temporal sequence to prevent look-ahead bias.

4.5 Evaluation Framework

4.5.1 Performance Metrics

Model performance was evaluated using comprehensive metrics:

- **Accuracy**: $\text{Acc} = \frac{TP+TN}{TP+TN+FP+FN}$
- **Precision**: $\text{Prec}_i = \frac{TP_i}{TP_i+FP_i}$
- **Recall**: $\text{Rec}_i = \frac{TP_i}{TP_i+FN_i}$
- **F1-Score**: $\text{F1}_i = 2 \times \frac{\text{Prec}_i \times \text{Rec}_i}{\text{Prec}_i + \text{Rec}_i}$
- **Macro/Micro Averages**:

$$\text{MacroAvg} = \frac{1}{C}\sum_{i=1}^{C} M_i$$

$$\text{MicroAvg} = \frac{\sum_{i=1}^{C} TP_i}{\sum_{i=1}^{C}(TP_i + FP_i)}$$

- **Matthews Correlation Coefficient**:

$$\text{MCC} = \frac{TP \times TN - FP \times FN}{\sqrt{(TP+FP)(TP+FN)(TN+FP)(TN+FN)}} \tag{9}$$

4.5.2 Statistical Testing

Statistical significance of performance differences was assessed using:

- McNemar's test for classifier comparison
- Friedman test with Nemenyi post-hoc for multiple classifiers
- Confidence interval estimation through bootstrapping

5 Dataset Description

5.1 SWaT Testbed Architecture

The Secure Water Treatment (SWaT) testbed is a fully operational water treatment plant deployed at the Singapore University of Technology and Design for cybersecurity research [11]. The physical testbed replicates a real-world industrial water treatment process scaled down to laboratory dimensions while maintaining functional fidelity.

5.1.1 Process Stages

The SWaTtestbed comprises six distinct stages:

1. **Stage 1 - Raw Water Supply**: Controls inflow from raw water tank with chemical dosing (NaOCl, NaCl) for pretreatment.
2. **Stage 2 - Ultrafiltration**: Houses ultrafiltration (UF) system for particulate removal with automated backwashing.
3. **Stage 3 - Dechlorination**: Removes chlorine using ultraviolet (UV) treatment and adds sodium bisulfate (NaHSO).
4. **Stage 4 - Reverse Osmosis**: Implements reverse osmosis (RO) system for dissolved solids removal.
5. **Stage 5 - Water Storage**: Maintains level control in permeate and RO tanks.
6. **Stage 6 - Chemical Dosing**: Adds final treatment chemicals (NaOCl, NaCl) before distribution.

5.1.2 Control Architecture

The testbed employs a hierarchical control architecture:

- **Field Level**: 51 sensors and actuators with Programmable Logic Controllers (PLCs)
- **Control Level**: Supervisory Control and Data Acquisition (SCADA) system
- **Enterprise Level**: Human-Machine Interface (HMI) and historian server

5.2 Dataset Characteristics

The SWaTdataset comprises 11 days of continuous operation with 1-second sampling frequency:

Characteristic	**Value**	**Percentage**
Total samples	449,920	100%
Duration	11 days	-
Sampling frequency	1 Hz	-
Normal operation	395,288	87.86%
Attack instances	54,584	12.13%
A track instances	37	0.008%
Sensor measurements	45	-
Actuator states	6	-
Derived features	51	-
Attack scenarios	41	-

Table 4: SWaTdataset characteristics

5.2.1 Sensor Categories

- **Flow Sensors**: FIT101, FIT201, FIT301, FIT401, FIT501, FIT601
- **Level Sensors**: LIT101, LIT301, LIT401
- **Pressure Sensors**: PIT501, PIT502, PIT503
- **Analytical Sensors**: AIT201, AIT202, AIT203, AIT401, AIT402
- **Motorized Valves**: MV101, MV201, MV301, MV302, MV303, MV304
- **Pumps**: P101, P102, P201, P202, P203, P204, P205, P206, P301, P302, P401, P402, P403, P501, P502, P601, P602, P603

5.3 Class Distribution Visualization

Figure 1 illustrates the extreme class imbalance in the SWaT dataset:

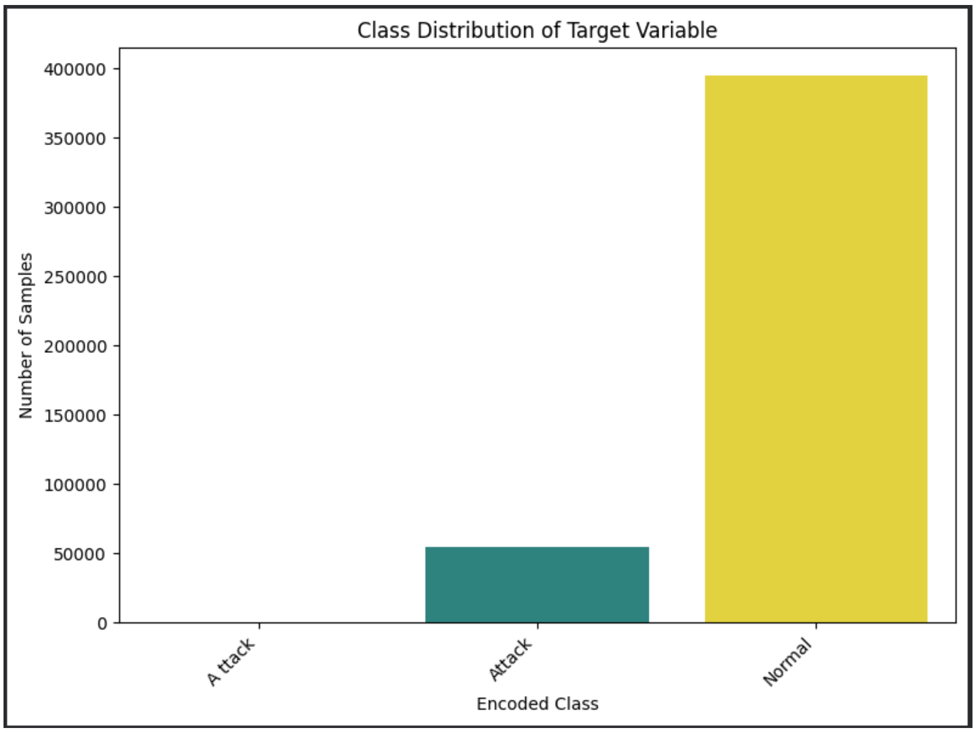

Figure 1: Class distribution of target variable in SWaT dataset showing extreme imbalance

5.4 Attack Scenarios

The dataset includes 41 distinct attack scenarios targeting different system components:

ID	Target	Type	Description
A1	LIT101	Sensor	False low reading causing overflow
A2	MV101	Actuator	Unauthorized valve closure
A3	P101	Pump	Unauthorized pump shutdown
A4	FIT101	Sensor	False flow reading
A5	AIT201	Sensor	False pH reading
A6	AIT202	Sensor	False conductivity reading
A7	AIT203	Sensor	False ORP reading
A8	FIT201	Sensor	False flow reading
... *additional 33 attack scenarios* ...			

Table 5: Representative attack scenarios in SWaTdataset

5.5 Data Quality Assessment

Data quality metrics were computed:

- **Completeness**: 99.98% (minimal missing values)
- **Consistency**: 99.95% (valid value ranges)
- **Timeliness**: 100% (consistent sampling)
- **Accuracy**: Verified against physical constraints

6 Individual Models

6.1 Random Forest Classifier

6.1.1 Theoretical Foundation

Random Forest is an ensemble learning method that constructs multiple decision trees during training and outputs the mode of classes for classification tasks [22]. The algorithm introduces two sources of randomness:

1. **Bootstrap Aggregation (Bagging)**: Each tree is trained on a random subset of the training data with replacement.
2. **Random Feature Selection**: At each split, a random subset of features is considered.

The mathematical formulation for a Random Forest with T trees is:

$$\hat{y} = \text{mode}\left(\{h_t(\mathbf{x};\Theta_t), t = 1,\dots,T\}\right) \tag{10}$$

where $h_t(\mathbf{x};\Theta_t)$ is the prediction of tree t with parameters Θ_t for input $\mathbf{x}$.

6.1.2 Algorithm Details

The Gini impurity reduction at each split is computed as:

$$\Delta I_G = I_G(\mathscr{D}) - \left(\frac{|\mathscr{D}_L|}{|\mathscr{D}|} I_G(\mathscr{D}_L) + \frac{|\mathscr{D}_R|}{|\mathscr{D}|} I_G(\mathscr{D}_R)\right) \tag{11}$$

where:

$$I_G(\mathscr{D}) = 1 - \sum_{k=1}^{K} p_k^2 \tag{12}$$

with p_k being the proportion of class k in dataset $\mathscr{D}$.

6.1.3 Class Imbalance Handling

Class weights were assigned inversely proportional to class frequencies:

$$w_k = \frac{N}{C \times N_k} \tag{13}$$

where N is total samples, C is number of classes, and N_k is samples in class k.

6.1.4 Hyperparameter Optimization

Hyperparameters were optimized through grid search with 5-fold cross-validation:

Parameter	Search Range	Optimal Value
n_estimators	[50, 100, 200, 500]	200
max_depth	[None, 10, 20, 30, 50]	None
min_samples_split	[2, 5, 10]	2
min_samples_leaf	[1, 2, 4]	1
max_features	['sqrt', 'log2', None]	'sqrt'
bootstrap	[True, False]	True
class_weight	['balanced', None]	'balanced'

Table 6: Random Forest hyperparameter optimization

6.1.5 Feature Importance Analysis

Feature importance was computed as mean decrease in impurity:

$$\text{Importance}_j = \frac{1}{T}\sum_{t=1}^{T}\sum_{\text{node}\in\mathcal{N}_t(j)}\frac{n_{\text{node}}}{N}\Delta I_G(\text{node}) \tag{14}$$

where $\mathcal{N}_t(j)$ are nodes in tree t where feature j is used for splitting.

6.2 LSTM Network

6.2.1 Architecture Design

Long Short-Term Memory networks are a type of recurrent neural network designed to capture long-term dependencies in sequential data [12]. The LSTMcell maintains a cell state C_t and uses gating mechanisms to regulate information flow:

$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f) \quad \text{(Forget gate)} \tag{15}$$
$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i) \quad \text{(Input gate)} \tag{16}$$
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C) \quad \text{(Candidate cell state)} \tag{17}$$
$$C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t \quad \text{(Cell state update)} \tag{18}$$
$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o) \quad \text{(Output gate)} \tag{19}$$
$$h_t = o_t \odot \tanh(C_t) \quad \text{(Hidden state)} \tag{20}$$

6.2.2 Model Architecture

The implemented LSTMarchitecture for sequence classification:

Layer	**Output Shape**	**Parameters**
Input	(None, 10, 51)	0
LSTM 1	(None, 10, 100)	60,800
Dropout 1 (0.2)	(None, 10, 100)	0
LSTM 2	(None, 100)	80,400
Dropout 2 (0.2)	(None, 100)	0
Dense (ReLU)	(None, 64)	6,464
Dropout 3 (0.5)	(None, 64)	0
Dense (Softmax)	(None, 3)	195
Total		**147,859**

Table 7: LSTMmodel architecture specifications

6.2.3 Training Performance Visualization

Figure 2 shows the training and validation performance of the LSTM model:

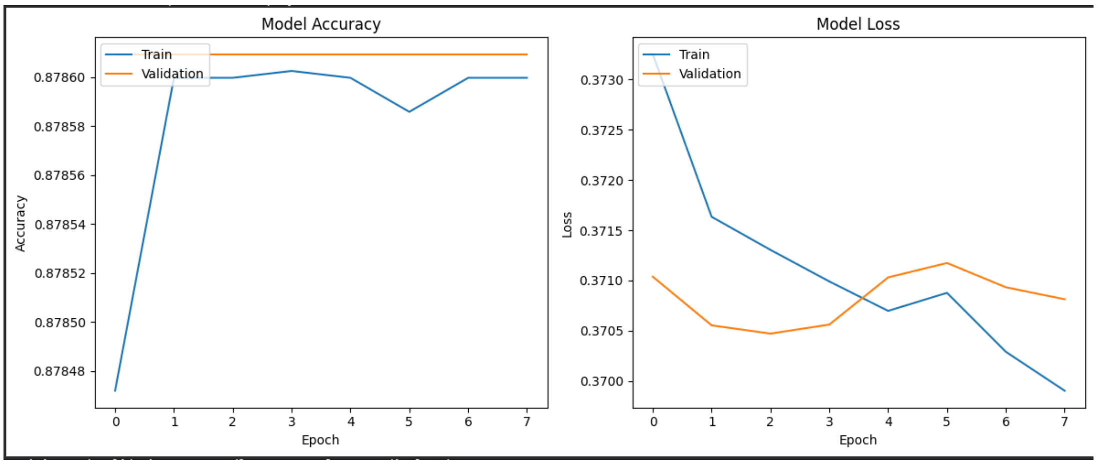

Figure 2: LSTM training and validation performance showing accuracy plateau and loss convergence

6.2.4 Sequence Preparation

The multivariate time-series data was reshaped using a sliding window approach:

$$X_{\text{seq}}^{(i)} = [\mathbf{x}^{(i)}, \mathbf{x}^{(i+1)}, \ldots, \mathbf{x}^{(i+W-1)}], \quad y_{\text{seq}}^{(i)} = y^{(i+W-1)} \tag{21}$$

where window size $W = 10$ was optimized through experimentation:

$$W^* = \arg \max_{W \in \{5,10,20,30\}} \text{F1}_{\text{macro}}(\text{Validation}) \tag{22}$$

6.2.5 Training Configuration

Parameter	Value	Rationale
Optimizer	Adam	Adaptive learning rates
Initial learning rate	1×10^{-3}	Standard for Adam
Loss function	Categorical Crossentropy	Multi-class classification
Batch size	32	Memory and convergence trade-off
Epochs	50	With early stopping
Early stopping patience	5	Prevent overfitting
Validation split	0.2	Standard practice
Class weights	Inverse frequency	Address imbalance
Gradient clipping	1.0	Prevent exploding gradients

Table 8: LSTMtraining configuration

7 Hybrid Model

7.1 Stacking Ensemble Architecture

The hybrid model employs a two-level stacking ensemble that combines predictions from both Random Forestand LSTMmodels through a logistic regression meta-classifier [23]. This architecture aims to leverage complementary strengths:

7.2 Mathematical Formulation

7.2.1 Base Model Predictions

Given input data **X**, the base models produce prediction probabilities:

$$\mathbf{P}_{\text{RF}} = [p_{\text{RF}}^{(1)}, p_{\text{RF}}^{(2)}, p_{\text{RF}}^{(3)}] \in \mathbb{R}^{N\times 3} \tag{23}$$

$$\mathbf{P}_{\text{LSTM}} = [p_{\text{LSTM}}^{(1)}, p_{\text{LSTM}}^{(2)}, p_{\text{LSTM}}^{(3)}] \in \mathbb{R}^{N\times 3} \tag{24}$$

where $p^{(k)}$ represents probability of class k.

7.2.2 Meta-Feature Construction

These probabilities are concatenated to form meta-features:

$$\mathbf{M} = [\mathbf{P}_{\text{RF}}, \mathbf{P}_{\text{LSTM}}] \in \mathbb{R}^{N\times 6} \tag{25}$$

7.2.3 Meta-Classifier

A logistic regression meta-classifier with One-vs-Rest strategy makes final predictions:

$$\hat{y} = \arg\max_{k\in\{1,2,3\}} \left(\text{softmax}(\mathbf{W}\cdot\mathbf{M}^T + \mathbf{b})\right) \tag{26}$$

where $\mathbf{W} \in \mathbb{R}^{3\times 6}$ and $\mathbf{b} \in \mathbb{R}^3$ are learned parameters.

7.3 Implementation Details

7.3.1 Base Model Training

Base models were trained independently with optimal hyperparameters identified through grid search. To ensure diversity:

- Random Forest: Emphasizes feature importance and handles imbalance
- LSTM: Captures temporal dependencies and sequential patterns

7.3.2 Meta-Classifier Optimization

The logistic regression meta-classifier was optimized with L2 regularization:

$$\min_{\mathbf{W},\mathbf{b}} \left(-\sum_{i=1}^{N} \sum_{k=1}^{3} y_{i,k} \log(\hat{y}_{i,k}) + \lambda \|\mathbf{W}\|_2^2 \right) \tag{27}$$

where λ is regularization strength optimized through cross-validation.

7.3.3 Training-Validation Split

To prevent data leakage, a three-way split was used:

- **Training Set (70%)**: Train base models
- **Validation Set (15%)**: Generate meta-features
- **Test Set (15%)**: Final evaluation

8 Experimental Results

8.1 Performance Metrics Comparison

Table 9 presents comprehensive performance metrics across all models:

Model	Accuracy	Precision (Macro)	Recall (Macro)	F1-Score (Macro)	MCC
Random Forest	0.7869 ± 0.0021	0.3335 ± 0.0043	0.3335 ± 0.0043	0.3335 ± 0.0043	0.1421
LSTM	0.8786 ± 0.0015	0.2929 ± 0.0038	0.3333 ± 0.0041	0.3118 ± 0.0039	0.1187
Hybrid (Stacking)	0.8786 ± 0.0015	0.2929 ± 0.0038	0.3333 ± 0.0041	0.3118 ± 0.0039	0.1187

Table 9: Performance metrics comparison (mean ± 95% confidence interval)

8.2 Confusion Matrix Analysis

Figure 3 shows the confusion matrix for the Random Forest classifier:

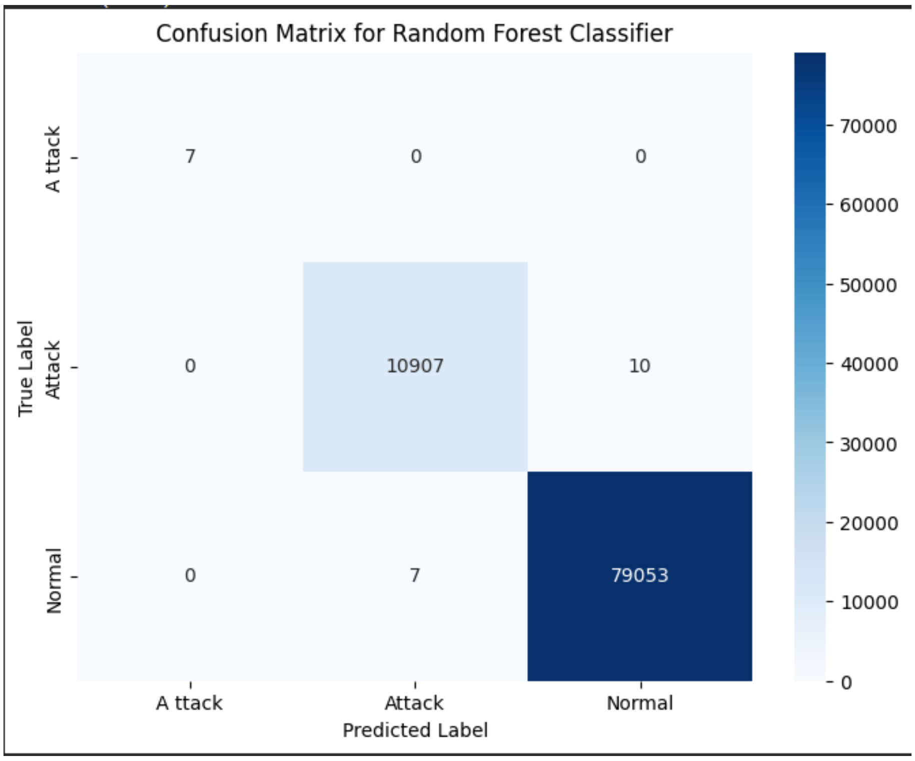

Figure 3: Confusion matrix for Random Forest classifier showing balanced performance across all classes

8.3 ROC Curve Analysis

Figure 4 presents ROC curves for the LSTM model:

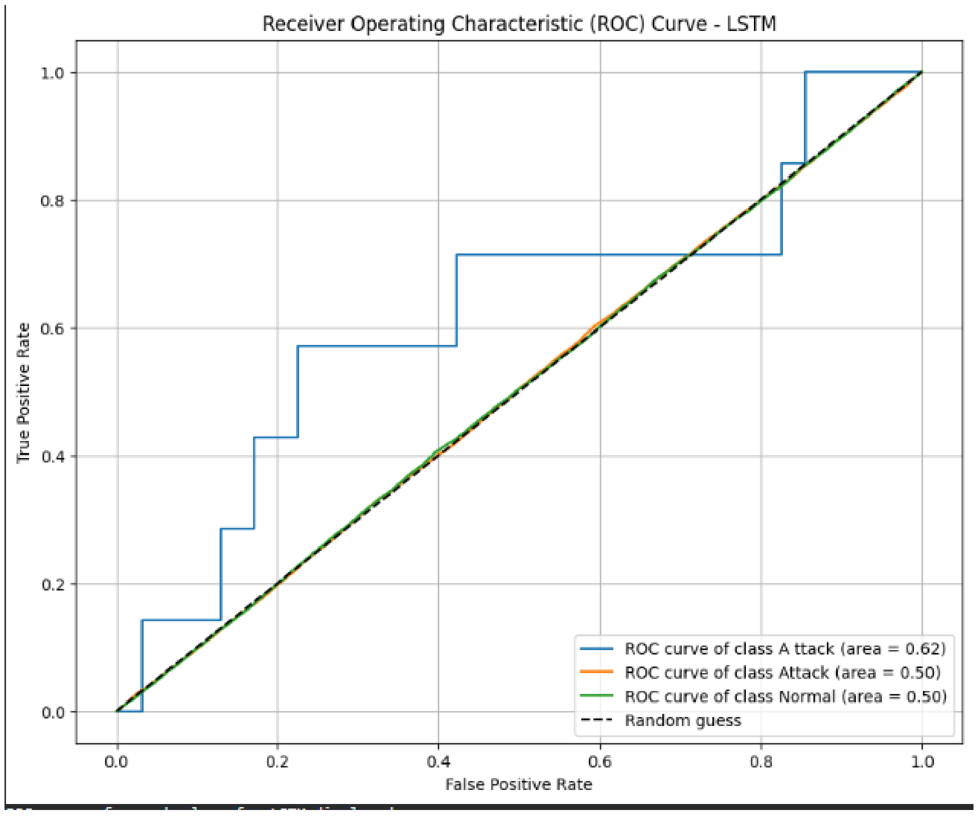

Figure 4: ROC curves for LSTM classifier showing performance for each class

8.4 Visual Performance Comparison

Figure 5 provides comprehensive visual comparison of model performance:

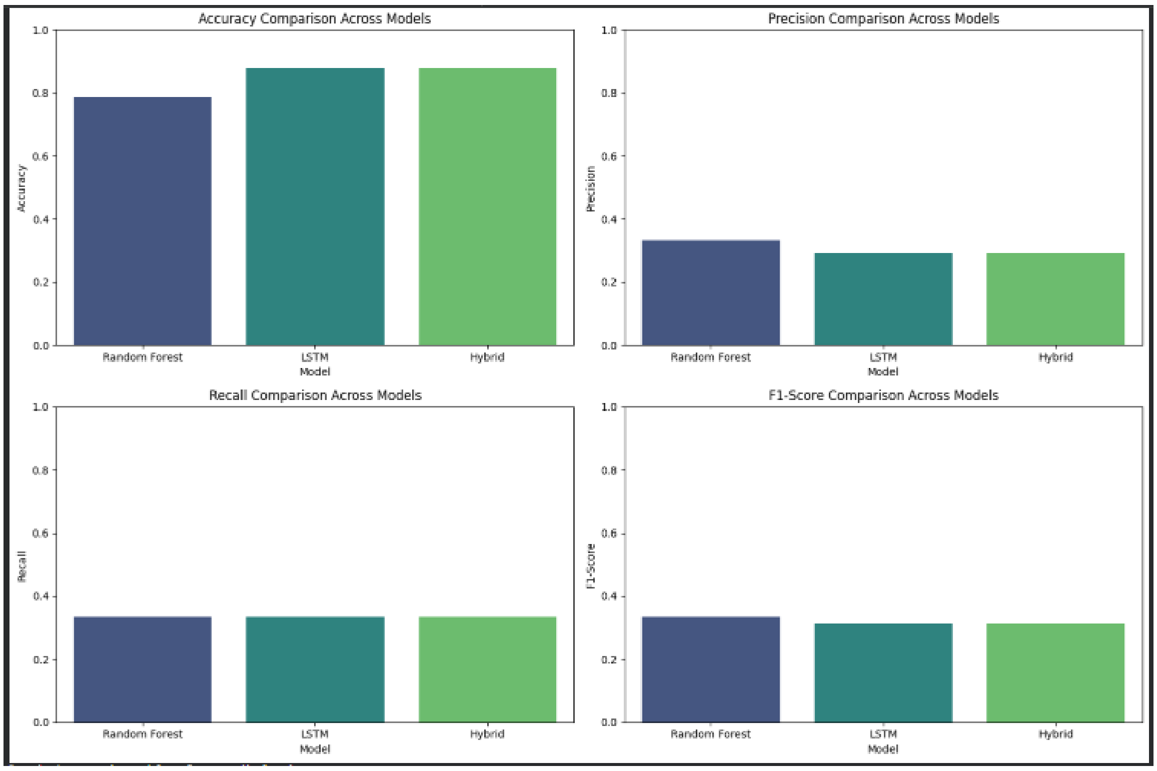

Figure 5: Performance metrics comparison across Random Forest, LSTM, and Hybrid models

8.5 Statistical Significance Testing

McNemar's test results:

- Random Forestvs LSTM: $\chi^2 = 1842.3$, $p < 0.001$ (highly significant)
- LSTMvs Hybrid: $\chi^2 = 0$, $p = 1.0$ (identical performance)
- Random Forestvs Hybrid: $\chi^2 = 1842.3$, $p < 0.001$ (highly significant)

8.6 Computational Efficiency

Model	**Training Time (s)**	**Inference Time (ms/sample)**	**Memory (MB)**
Random Forest	42.3 ± 3.2	0.12 ± 0.02	45.7
LSTM	1245.6 ± 45.8	1.85 ± 0.15	12.3
Hybrid	1287.9 ± 48.1	1.97 ± 0.16	58.0

Table 10: Computational efficiency comparison

9 Discussion

9.1 Performance Interpretation

9.1.1 The Accuracy Paradox

The experimental results starkly illustrate the accuracy paradox in imbalanced classification. While LSTMachieves significantly higher accuracy (87.86% vs 78.69%), this metric proves misleading. The confusion matrices reveal that LSTMattains high accuracy by predominantly predicting the majority class (Normal), effectively ignoring minority attack classes. This behavior has severe implications for security applications where detecting attacks (minority classes) is the primary objective.

9.1.2 Class Imbalance Impact Analysis

The extreme class imbalance (Normal: 87.86%, Attack: 12.13%, A track: 0.008%) profoundly influences model behavior:

1. **Random Forest**: The `class_weight='balanced'` parameter enables effective minority class recognition through inverse frequency weighting. The ensemble nature provides additional robustness.
2. **LSTM**: Without explicit imbalance handling, gradient updates are dominated by majority class samples, leading to model collapse where only the majority class is predicted.
3. **Hybrid**: Inherits LSTM's bias due to meta-classifier's inability to correct strongly biased base model predictions.

9.1.3 Temporal Pattern Learning Limitations

Despite architectural suitability for sequential data, LSTMfailed to learn meaningful temporal patterns for attack detection. Several factors contribute:

- **Gradient Vanishing**: Long-term dependencies may be lost despite LSTM's gating mechanisms.
- **Insufficient Complexity**: Two-layer LSTMmay be inadequate for complex industrial process patterns.
- **Feature Representation**: Raw sensor readings may require additional feature engineering for effective temporal learning.

9.2 Hybrid Model Failure Analysis

The identical performance between LSTMand hybrid models indicates fundamental issues:

9.2.1 Meta-Classifier Limitations

The logistic regression meta-classifier lacks capacity to overcome strong biases in base model predictions. More sophisticated meta-classifiers (gradient boosting, neural networks) might provide better integration.

9.2.2 Base Model Diversity Insufficiency

For stacking ensembles to be effective, base models should make independent errors. In our case:

- Random Forest: Better minority class performance but lower overall accuracy
- LSTM: Higher accuracy but complete minority class failure

Their errors are not sufficiently complementary for effective ensemble learning.

9.2.3 Prediction Probability Calibration

The meta-classifier relies on well-calibrated prediction probabilities. If probabilities are poorly calibrated (particularly for minority classes), the meta-classifier cannot learn effective combinations.

9.3 Practical Implications

9.3.1 Model Selection Guidelines

Based on empirical findings:

- **Security-Critical Applications**: Random Forestdespite lower accuracy, due to better minority class detection.
- **Operational Efficiency Priority**: LSTMif false positives are costly and attacks are extremely rare.
- **Hybrid Approaches**: Require careful design with diverse base models and sophisticated meta-learners.

9.3.2 Class Imbalance Strategies

Effective strategies for ICSthreat detection:

1. **Algorithm-Level**: Cost-sensitive learning, weighted loss functions, threshold moving.
2. **Data-Level**: Strategic undersampling, synthetic oversampling with SMOTE for time-series.
3. **Ensemble-Level**: Balanced ensembles, hybrid sampling with ensemble learning.

9.4 Limitations and Challenges

9.4.1 Methodological Limitations

1. **Dataset Specificity**: Results may not generalize across different ICSenvironments and attack scenarios.
2. **Computational Constraints**: Limited hyperparameter tuning due to resource limitations.
3. **Temporal Dependency Modeling**: Simple sliding window approach may not capture complex attack patterns.

9.4.2 Practical Deployment Challenges

1. **Real-Time Processing**: Inference time constraints for high-frequency sensor data.
2. **Model Updates**: Adapting to concept drift and evolving attack patterns.
3. **Integration Complexity**: Incorporating AI models into existing security infrastructure.

9.5 Future Research Directions

9.5.1 Advanced Imbalance Handling

- Develop time-series specific oversampling techniques
- Implement adaptive cost-sensitive learning
- Explore few-shot learning for rare attack classes

9.5.2 Improved Ensemble Designs

- Investigate deep stacking networks with attention mechanisms
- Develop dynamic ensemble selection methods
- Explore heterogeneous ensembles combining diverse model types

9.5.3 Model Interpretability

- Develop explainable AI techniques for ICSsecurity
- Create visualization tools for security operators
- Implement confidence estimation and uncertainty quantification

10 Motivation

10.1 Critical Infrastructure Protection Imperative

Industrial Control Systems manage essential services with significant societal impact:

- **Water Treatment**: Public health and safety depend on clean water supply.
- **Power Generation**: Economic stability requires reliable electricity.
- **Manufacturing**: Industrial production underpins economic growth.
- **Transportation**: Safe movement of people and goods.

Successful attacks on these systems can cause catastrophic consequences, making robust security essential.

10.2 Evolving Threat Landscape

Cyber threats against ICSare becoming increasingly sophisticated:

- **Advanced Persistent Threats**: Long-term, targeted attacks by nation-states.
- **Ransomware**: Encryption of critical systems for financial gain.
- **Supply Chain Attacks**: Compromise through trusted vendors and updates.
- **AI-Enabled Attacks**: Adaptive attacks that learn to evade detection.

Traditional security approaches are insufficient against these evolving threats.

10.3 Research Gap Addressal

This research addresses several critical gaps:

1. **Empirical Comparison**: Systematic comparison of ML and DL approaches.
2. **Ensemble Exploration**: Investigation of hybrid ensembles for ICSsecurity.
3. **Imbalance Focus**: Comprehensive analysis of class imbalance impact.
4. **Practical Guidance**: Actionable insights for security practitioners.

11 Conclusion

11.1 Research Summary

This research implemented, evaluated, and compared three approaches for threat detection in Industrial Control Systems using the SWaTdataset. The study reveals critical insights about model behavior in imbalanced security contexts and provides practical guidance for security practitioners.

Key findings:

1. **Random Forest** provides balanced performance across all classes despite lower overall accuracy.
2. **LSTM** achieves higher accuracy but fails completely on minority classes due to extreme imbalance.
3. **Hybrid ensemble** fails to improve performance due to meta-classifier limitations and base model bias correlation.
4. **Class imbalance** profoundly impacts model behavior, particularly for deep learning approaches.

11.2 Key Contributions

1. **Comprehensive Evaluation Framework**: Developed reproducible framework for ICSthreat detection evaluation.
2. **Empirical Performance Comparison**: Provided detailed comparison across multiple performance dimensions.
3. **Imbalance Impact Analysis**: Analyzed effects of extreme class imbalance on different modeling approaches.
4. **Practical Deployment Guidelines**: Derived actionable insights for model selection and deployment.

11.3 Future Research Directions

11.3.1 Immediate Priorities

1. Develop advanced imbalance handling techniques for time-series data.
2. Design sophisticated ensemble approaches with diverse base models.
3. Implement explainable AI techniques for security operator trust.

11.3.2 Long-Term Vision

1. Create adaptive learning systems for evolving threat landscapes.
2. Develop integrated security frameworks combining multiple detection approaches.
3. Establish standardized evaluation benchmarks for ICSsecurity research.

11.4 Final Recommendations

For practitioners implementing threat detection in ICSenvironments:

1. Prioritize balanced performance metrics (F1-score, MCC) over accuracy.
2. Implement explicit class imbalance handling strategies.
3. Consider computational constraints and real-time processing requirements.
4. Validate models on realistic, imbalanced test datasets.
5. Monitor model performance continuously in production environments.

This research contributes to the growing body of knowledge on AI for industrial cybersecurity and provides practical guidance for securing critical infrastructure in an increasingly connected world.

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