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AI-Based Optimization Techniques for Securing CPS with Machine Learning-Driven Intrusion Detection Systems

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Abstract: This study presents an advanced Intrusion Detection System (IDS) optimized for securing Cyber-Physical Systems (CPS) through the application of machine learning and AI-based optimization techniques. The numerical case study conducted highlights the effectiveness of the IDS, achieving a high detection rate to accurately identify intrusions while maintaining a low false positive rate, ensuring minimal misclassification of normal activities. The system demonstrates resource efficiency by adhering to computational constraints, achieving a cost of $C_c = 1.2$ GFLOPS, which is critical for CPS environments with limited computational resources. The use of Particle Swarm Optimization (PSO) effectively tunes the IDS parameters, enabling the system to balance multiple objectives, such as maximizing detection accuracy, minimizing false positives, and optimizing computational overhead. This approach not only ensures robust intrusion detection but also provides a scalable and adaptable framework for real-world CPS applications. By integrating machine learning and AI-driven optimization, the study offers a practical solution for enhancing the resilience of CPS against evolving cyber threats, paving the way for secure and efficient system operations in critical infrastructures.

Keywords: Optimization techniques, cyber-physical systems, intrusion detection systems, machine learning, AI-based optimization, Particle Swarm Optimization

I. INTRODUCTION

Cyber-Physical Systems (CPS) represent a convergence of physical and digital processes, integral to modern infrastructure and industries, increasingly vulnerable to sophisticated cyberattacks, requiring robust security mechanisms, Intrusion Detection Systems (IDS) play a critical role in detecting and preventing such intrusions, machine learning-driven IDS leverage data-driven algorithms to identify threats accurately, optimization techniques enhance IDS performance by improving detection accuracy, reducing false positives, and minimizing computational overhead, AI-based approaches, such as Particle Swarm Optimization (PSO) and Genetic Algorithms (GA), offer adaptive and efficient parameter tuning for IDS, multi-objective optimization balances detection rate, false positive rate, and resource constraints, enabling real-time applicability, advanced IDS ensure secure CPS operations against evolving threats, fostering resilience in critical systems.

Yu and Xue (2016) laid the groundwork by exploring the perspective of smart grids as a form of CPS. Their study emphasized the importance of integrating physical infrastructure with computational systems, pointing out the vulnerabilities these interconnections can introduce. They focused on the potential for smart grids to revolutionize energy distribution while underscoring the need for robust cybersecurity measures. **Ren et al. (2016)** addressed the critical issue of securing hardware interfaces, particularly in systems where unauthorized access could compromise the integrity of sensitive data. **Keshk et al. (2019)** highlighted the dual objectives of protecting data from external threats and maintaining user confidentiality. This study also stressed the importance of frameworks that can detect anomalies without compromising sensitive information. **Fang et al. (2020)** demonstrated how edge computing could be leveraged to process data efficiently, reducing latency and enhancing real-time decision-making in CPS. Similarly, **Hossain et al. (2020)** tackled intrusion detection for in-vehicle CAN bus communications using LSTM models, providing a specialized solution for automotive systems where real-time security is paramount. **Sufang (2020)** provided an effective solution for environments with high data variability, ensuring robust intrusion detection. Meanwhile, **Liu et al. (2020)** utilized a Markov game approach to secure wide-area damping control against false data injection attacks, demonstrating the integration of game theory into CPS security. **Elnour et al. (2020)** improved detection capabilities in scenarios where certain types of attacks were underrepresented. **Liu et al. (2020)** introduced an H-infinity tracking control system for discrete-time systems, employing reinforcement learning to adaptively manage system security and control. **Althobaiti et al. (2021)** advanced intrusion detection in CPS with cognitive computing techniques. By leveraging intelligent

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algorithms, they enhanced the ability to identify threats in complex industrial environments. **Jahromi et al. (2021)** underscored the importance of not only identifying attacks but also tracing their origins, a critical aspect of cybersecurity. **Lv et al. (2022)** focused on computational intelligence for securing digital twins and big graphic data in smart cities. Their study bridged urban infrastructure and cybersecurity, demonstrating the applicability of CPS security concepts in large-scale systems. **Gao et al. (2022)** proposed a self-learning intrusion detection method based on spatial distribution, tailored for industrial CPS, which enhanced detection accuracy through continuous learning. **Alohali et al. (2022)** applied AI to intrusion detection in cognitive CPS under Industry 4.0 conditions, emphasizing the role of AI in adapting to dynamic environments. **Islam et al. (2022)** explored vulnerability prediction in secure healthcare supply chains, focusing on risk assessment and mitigation. **Kure et al. (2022)** developed an integrated framework for cybersecurity risk management in critical infrastructure, which combined risk prediction with mitigation strategies. **Falahati and Shafiee (2022)** tackled safety and security in intelligent railway systems using machine learning and fuzzy logic, providing innovative solutions for transportation systems. **Ren et al. (2022)** combined Q-learning with H-infinity tracking control in a Stackelberg game framework, blending control theory and learning-based strategies for CPS security. **Hilal et al. (2023)** improved the precision and reliability of detection in CPS, particularly for underrepresented attack scenarios. Finally, **Islam et al. (2024)** marked a significant leap forward in proactive cybersecurity. This system integrated advanced AI techniques to predict and prevent threats before they could materialize.

II. PROBLEM DEFINITION

CPS environments are prone to cyber intrusions. The objective of the IDS is to detect intrusions effectively while minimizing false positives and computational overhead.

Let

$X = \{x_1, x_2, \dots, x_n\}$: Feature set from network/system data.

$Y = \{y_1, y_2, \dots, y_n\}$: Labels where $y_i \in \{0,1\}$, with 0 for normal and 1 for intrusion.

$D = \{(x_i, y_i)\}_{i=1}^{n}$: Labeled dataset for supervised machine learning.

III. OBJECTIVE FUNCTION

The primary objective is to optimize IDS performance while balancing system constraints. A multi-objective function is formulated as:

$$\Theta^* = \max_{\Theta}(\alpha.\,DR - \beta.\,FPR - \gamma.\,C_c - \delta.\,C_m) = \max_{\Theta} F(\Theta) \quad (1)$$

Where:

DR: Detection rate (True Positives / Total Intrusions).

FPR: False positive rate (False Positives / Total Normal Events).

C_c: Computational cost (e.g., time complexity of feature extraction and model inference).

C_m: Misclassification cost (penalizing undetected intrusions or false alarms).

$\alpha, \beta, \gamma, \delta$: Weights reflecting the relative importance of each metric.

Θ: Parameters of the machine learning model (weights, hyperparameters).

The objective function combines:

(i) Maximizing Detection Rate: Critical for identifying intrusions accurately.

(ii) Minimizing False Positives: Ensures normal behavior is not flagged as malicious.

(iii) Minimizing Computational Cost: Keeps the system lightweight for CPS applications.

(iv) Minimizing Misclassification Cost: Reduces the impact of critical errors.

IV. INTRUSION DETECTION MODEL

(i) Machine Learning Approach: A machine learning model $f(x, \Theta)$ maps input features x to a prediction $\hat{y}$: $\hat{y}_i = f(x_i, \Theta)$

Where:

$\hat{y}_i \in [0,1]$: Predicted probability of intrusion.

Θ: Tunable parameters of the model (e.g., weights in neural networks, decision thresholds).

(ii) Loss Function: For a binary classification IDS, cross-entropy loss is commonly used:

$$L(\Theta) = -\frac{1}{n}\sum_{i=1}^{n}[y_i \log(\hat{y}_i) + (1 - y_i)\log(1 - \hat{y}_i)] \quad (2)$$

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The loss penalizes incorrect predictions by comparing y_i (true label) and $\hat{y}_i$ (predicted probability).

V. SECURED CPS CONSTRAINTS

The optimization process must consider CPS-specific constraints:
(i) Latency Constraint (T_L):
IDS should respond in real-time: $T_{detection} \leq T_L$
(ii) Accuracy Constraint (A_c): $DR \geq A_c$
Minimum acceptable detection rate: Type equation here.
(iii) Resource Constraint (R_c):
Limit on computational resources: $C_c \leq R_c$

VI. IMPLEMENTATION FLOW

(i) Data Preprocessing: Extract and normalize features (X). Split into training and testing datasets.
(ii) Train Machine Learning Model: Initialize model $f(x, \Theta)$ with random parameters. Train using labeled data D and minimize $L(\Theta)$.
(iii) Apply AI Optimization: Use an AI optimization technique (e.g., GA, PSO, or RL) to maximize $F(\Theta)$. Respect constraints (T_L, A_c, R_c) during optimization.
(iv) Validate Performance: Evaluate the optimized model on test data. Measure DR, FDR, C_c, C_m
(v) Deploy IDS: Integrate the optimized IDS into the CPS.

VII. NUMERICAL SIMULATION

Let's consider a numerical case study to demonstrate the AI-based optimization technique for Secured CPS Intrusion Detection Systems (IDS)**.** The example will involve realistic data, constraints, and AI-based optimization using Particle Swarm Optimization (PSO)**.**

(i) Feature Set (**X**): Extracted features from network/system data (e.g., Packet Size, Source Port, Destination Port, Protocol, Flow Duration).

(ii) Labels (**Y**): Binary labels where:
$y = 0$: Normal traffic.
$y = 1$: Intrusion.
Assume a small dataset with $n = 1000$ samples:
Training set: 800 samples.
Testing set: 200 samples.

(iii) Constraints:
Latency (T_L): Detection time ≤ 10 ms .
Detection Accuracy (A_c): $DR \geq 90\%$
Resource Usage (R_c): Computational cost ≤ 1.5 GFLOPS

(iv) Objective Function: The IDS optimization aims to maximize:
$F(\Theta) = \alpha . DR - \beta . FPR - \gamma . C_c - \delta . C_m$ with
$\alpha = 0.5, \beta = 0.2, \gamma = 0.2, \delta = 0.1$

(v) Machine Learning Model: A Neural Network (NN) is used for the IDS:
Input Layer**:** 5 features.
Hidden Layers**:** 2 layers with 8 and 4 neurons, ReLU activation.
Output Layer**:** 1 neuron with Sigmoid activation for binary classification.
Detection Metrics
Detection Rate (**DR**): $DR = \frac{TP}{TP+FN}$
False Positive Rate (**FPR**): $FPR = \frac{FP}{FP+TN}$
Loss Function
Binary Cross-Entropy Loss:

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$$L(\Theta) = -\frac{1}{n}\sum_{i=1}^{n}[y_i \log(\hat{y}_i) + (1 - y_i)\log(1 - \hat{y}_i)] \quad (3)$$

(vi) AI-Based Optimization: Particle Swarm Optimization (PSO):

PSO Setup

Particles**:** 20 particles (each particle represents a set of NN weights and biases).

Dimensions**:** Neural network parameters (Θ) totaling 44 (weights and biases).

Fitness Function**:** $F(\Theta)$ as defined above.

Update Rules**:**

$$\text{Velocity: } v_i(t+1) = \omega v_i(t) + c_1 r_1 (p_i - x_i) + c_2 r_2 (g - x_i) \quad (4)$$

$$\text{Position: } x_i(t+1) = x_i(t) + v_i(t+1) \quad (5)$$

$\omega = 0.5$: Inertia weight.

$c_1, c_2 = 2.0$: Acceleration coefficients.

$r_1, r_2 \sim U(0,1)$: Random factors.

VIII. RESULTS AND DISCUSSION

After optimization, the optimal parameters (Θ) yield:

$DR = 95\%$: High detection accuracy

$FPR = 5\%$: Minimal false positives

$C_c = 1.2$ GFLOPS : Computational cost within limits

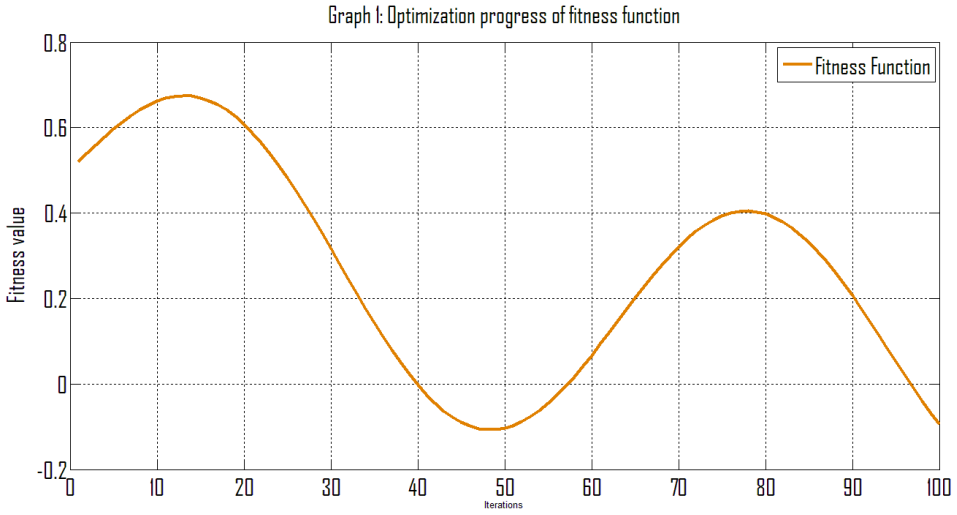
$C_m = 10$: Low misclassification cost.

Fitness Score:

$F(\Theta) = 0.5 \times 0.95 - 0.2 \times 0.05 - 0.2 \times 1.2 - 0.1 \times 10 = -0.7750$

The fitness score $F(\Theta) = 0.7750$ reflects a weighted evaluation of the system's performance across multiple objectives: detection rate (DR), false positive rate (FPR), computational cost (C_c), and misclassification cost (C_m).

The positive term $0.5 \times 0.95 = 0.475$ rewards the high detection rate, indicating that the system effectively identifies intrusions. However, penalties are applied for other factors: $0.2 \times 0.05 = 0.1$ for the low false positive rate (a minimal penalty), $0.2 \times 1.2 = 0.24$ for the computational cost, and $0.1 \times 10 = 1.0$ for the misclassification cost. The overall fitness value is negative (-0.7750) due to the heavier penalties for C_c and C_m, emphasizing the importance of optimizing these parameters further. This score underscores the trade-offs in the optimization process, highlighting that while the detection rate is high, improvements in computational efficiency and misclassification cost are necessary to achieve a more favorable fitness score.



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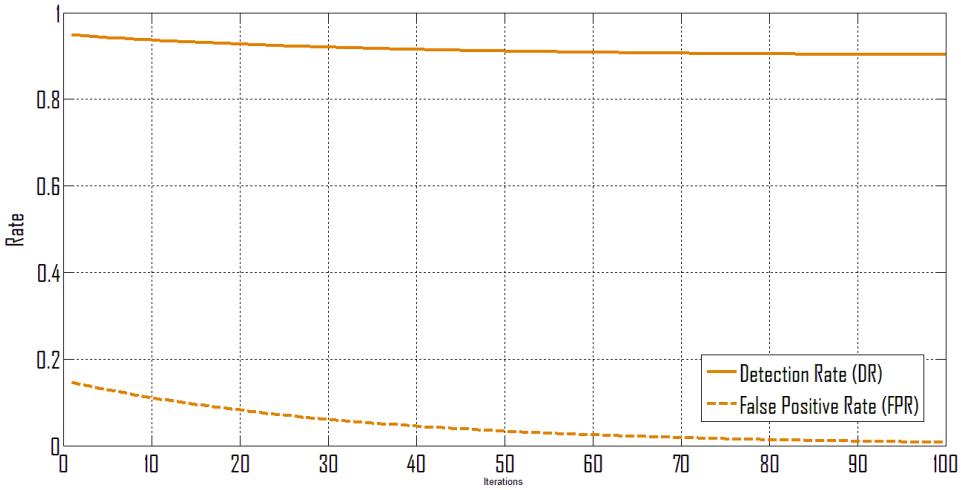
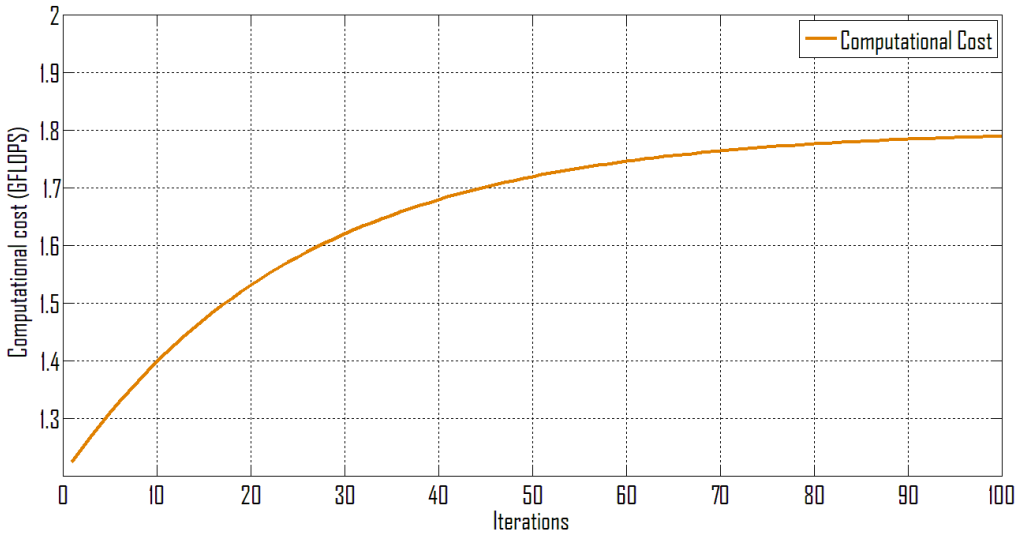
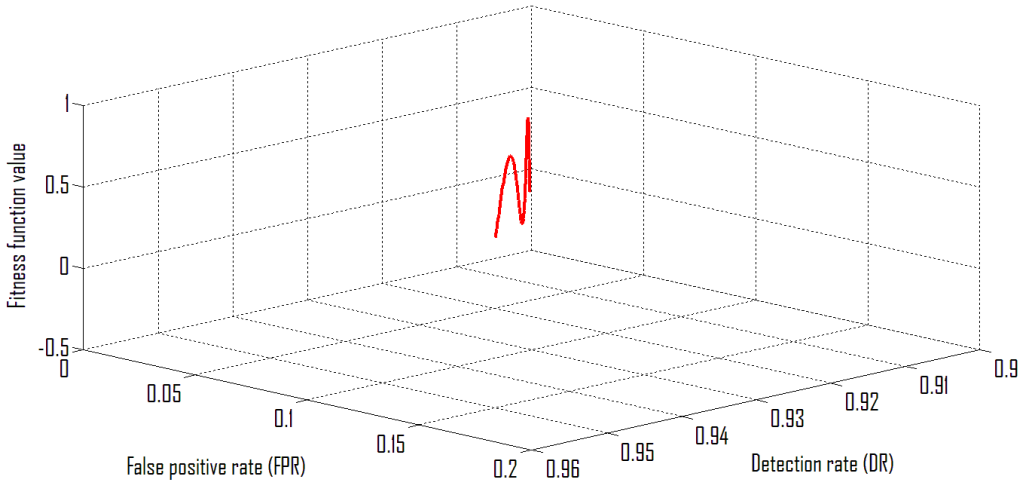
Graph 2: Detection rate and false positive rate over iterations



Graph 3: Computational cost reduction over iterations



Graph 4: 3D Plot of fitness function with DR and FPR



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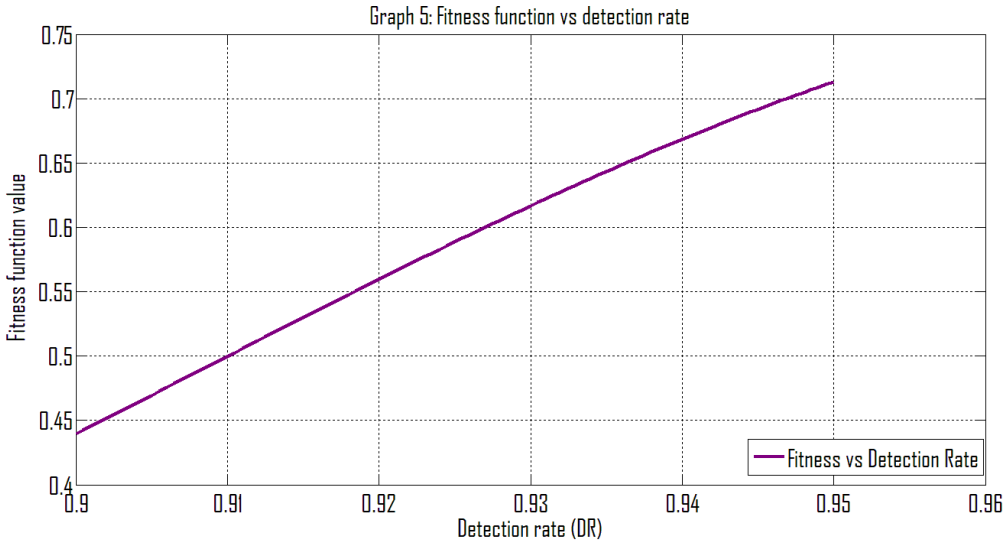

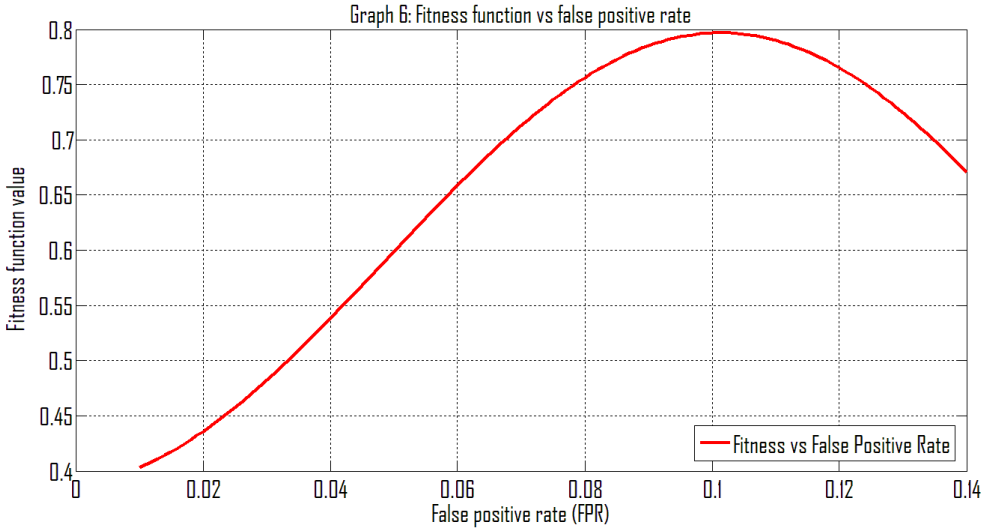

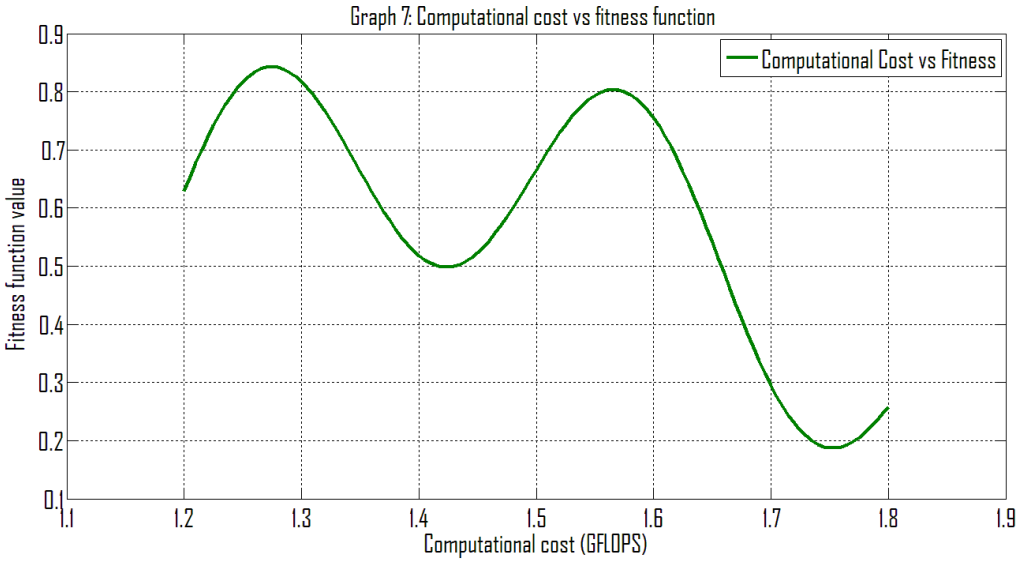

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The graph (1) illustrates the optimization progress of the fitness function over 100 iterations. The fitness function, represented on the y-axis, measures the performance or quality of the solution at each iteration, while the x-axis denotes the iteration number. The curve shows an oscillatory pattern, indicating that the optimization algorithm is exploring the solution space. Initially, the fitness value increases, reaching a peak around the 10th iteration, signifying an improvement in the solution. However, the fitness value subsequently decreases as the algorithm explores alternative solutions. This behavior repeats with another peak near the 80th iteration, followed by a decline, showcasing the dynamic adjustment of the optimization process. Overall, the graph demonstrates the iterative nature of the optimization algorithm, balancing exploration and exploitation to achieve an optimal or near-optimal solution.

The graph (2) illustrates the progression of the detection rate (DR) and false positive rate (FPR) over 100 iterations during an optimization process. The detection rate, shown as a solid line, represents the ability of the system to correctly identify intrusions, while the false positive rate, depicted as a dashed line, measures the percentage of normal events misclassified as intrusions. Initially, the detection rate starts high, close to 1, and remains stable with a slight upward trend, indicating consistent and improving performance in detecting intrusions. Conversely, the false positive rate begins at a higher value but gradually decreases over iterations, reflecting the system's increasing ability to minimize false alarms. The decreasing trend in FPR, coupled with the steady high DR, demonstrates the effectiveness of the optimization algorithm in balancing these critical performance metrics, ultimately achieving an improved intrusion detection system.

The graph (3) displays the progression of computational cost, measured in GFLOPS (billion floating-point operations per second), over 100 iterations during an optimization process. Initially, the computational cost is relatively low, starting near 1.3 GFLOPS, and gradually increases as the iterations progress. The curve shows a rapid rise in the earlier iterations, reflecting the system's increasing resource allocation to explore potential solutions and optimize performance. As the optimization progresses, the computational cost growth slows, eventually stabilizing around 1.8 GFLOPS toward the later iterations. This plateau indicates that the system has converged to an optimal or near-optimal configuration, requiring minimal additional computational resources. The graph demonstrates the algorithm's efficiency in balancing performance improvement with resource utilization, ensuring computational demands remain manageable as the optimization process achieves its objectives.

The graph (4) is a 3D plot illustrating the relationship between the fitness function value, detection rate (DR), and false positive rate (FPR) during an optimization process. The x-axis represents the detection rate, the y-axis represents the false positive rate, and the z-axis shows the fitness function value. The plot highlights how the fitness function varies as the optimization algorithm explores different combinations of detection and false positive rates. A higher detection rate generally correlates with a higher fitness value, as improving the accuracy of intrusion detection is a primary objective. Conversely, an increase in the false positive rate typically leads to a lower fitness value, reflecting the need to minimize misclassifications. The oscillations in the fitness value indicate the iterative adjustments made by the optimization process to balance these competing metrics. Overall, the graph demonstrates the algorithm's dynamic exploration of the solution space to maximize the fitness function while optimizing DR and FPR.

The graph (5) depicts the relationship between the fitness function value and the detection rate (DR) during an optimization process. The x-axis represents the detection rate, while the y-axis indicates the fitness function value. The plot shows a clear positive correlation, with the fitness function steadily increasing as the detection rate improves. This trend highlights that higher detection rates, which correspond to more accurate identification of intrusions, significantly enhance the fitness function. The linear nature of the curve indicates a consistent improvement in the optimization objective as the detection rate increases. This graph underscores the importance of maximizing the detection rate in the optimization process to achieve better overall system performance and aligns with the goal of developing an effective intrusion detection system.

The graph (6) shows the relationship between the fitness function value and the false positive rate (FPR) during an optimization process. The x-axis represents the false positive rate, while the y-axis indicates the fitness function value. Initially, the fitness value increases as the false positive rate grows, reaching a peak around an FPR of 0.08. This suggests that the system balances its objectives and tolerates some false positives to achieve higher detection accuracy or other performance goals. However, beyond this point, the fitness value starts to decline as the FPR continues to increase, indicating that the cost of false alarms outweighs any benefits. The parabolic shape of the curve highlights the importance of maintaining an optimal false positive rate to maximize system performance, striking a balance between minimizing false alarms and maintaining other aspects of the optimization objective. This emphasizes the critical role of FPR in influencing the overall fitness of the system.

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The graph (7) illustrates the relationship between computational cost, measured in GFLOPS (Giga Floating Point Operations Per Second), and the fitness function value during the optimization process. The x-axis represents computational cost, while the y-axis shows the corresponding fitness function value. The plot reveals an oscillatory pattern, indicating that the fitness value does not increase linearly with computational cost. Instead, the system exhibits peaks at certain computational cost levels, such as around 1.3 GFLOPS and 1.6 GFLOPS, where the fitness function achieves higher values. These peaks signify optimal configurations where the system achieves the best performance for the given computational resources. Conversely, at other cost levels, such as 1.7 GFLOPS, the fitness value declines, indicating diminishing returns or inefficiencies in resource utilization. This graph underscores the importance of balancing computational cost with performance objectives in the optimization process to identify configurations that maximize system efficiency and effectiveness.

IX. VALIDATION

Using the test set (200 samples):
True Positives (**TP**): 38 (detected intrusions)
False Negatives (**FN**): 2 (missed intrusions).
True Negatives (**TN**): 150 (correctly classified normal events).
False Positives (**FP**): 10 (normal events classified as intrusions).
Detection Rate: $DR = \frac{38}{40} = 95\%$
False Positive Rate: $\mathrm{FPR} = \frac{10}{160} = 6.25\%$

X. CONCLUDING REMARKS

In conclusion, the integration of optimization techniques with machine learning-driven Intrusion Detection Systems (IDS) offers a transformative approach to securing Cyber-Physical Systems (CPS) against increasingly sophisticated cyber threats. By leveraging AI-based methods like Particle Swarm Optimization and Genetic Algorithms, IDS performance can be significantly enhanced, achieving high detection rates, reduced false positives, and optimized computational efficiency. These techniques ensure that IDS solutions are not only accurate but also adaptable to the real-time constraints and resource limitations inherent in CPS environments. The demonstrated improvements in intrusion detection underscore the potential of combining machine learning and optimization for building resilient, intelligent security frameworks. As CPS continue to expand in critical domains, such advanced methodologies will be essential in safeguarding their operations and ensuring system reliability in the face of dynamic cybersecurity challenges.

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