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# Feature Engineering in Machine Learning for Advanced Threat Detection

*Anil Chowdary Inaganti[1], Vinod Sharma[2]*
*Researcher in Computer Science / Workday Techno Functional Lead[1], Professor, B.Sc., MCA, Ph.D. (Computer Science), University of Jammu[2]*
*anilchowdaryinaganti@gmail.com[1], vinod.sharma@jammuuniversity.ac.in[2]*

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**Abstract**

This study investigates the role of advanced feature engineering techniques in enhancing the accuracy, robustness, and interpretability of machine learning-based cyber threat detection systems. Building on a foundational framework that emphasizes the extraction of behavioral features for anomaly classification, this research proposes an enhanced approach. The proposed framework integrates domain-specific heuristics, protocol-aware attributes, and explainability techniques such as SHapley Additive exPlanations (SHAP) to strengthen intelligent threat detection capabilities. By refining traditional feature extraction pipelines and incorporating SHAP values, the framework offers human-understandable insights into model predictions, fostering trust among security analysts and supporting real-time decision-making in complex cyber environments. Rigorous experimental evaluations using diverse, real-world cybersecurity datasets demonstrate the framework's effectiveness, particularly in detecting stealthy, low-frequency, and novel threats that often evade conventional systems. The interpretable feature attributions further enhance forensic analysis, enabling security teams to trace, validate, and respond to threats with precision and contextual understanding. This work extends prior foundational contributions, presenting a scalable and interpretable framework that advances the field of cyber threat detection. The findings underscore the importance of merging domain expertise with explainable artificial intelligence to address the challenges posed by increasingly sophisticated cyber threats.

## Introduction

Machine learning-based threat detection systems rely critically on the quality and relevance of features extracted from raw system and network data. Effective feature engineering serves as the cornerstone for building models that can accurately identify sophisticated and evolving cyber threats. In this context, Kothamali et al. (2020) made a significant contribution by introducing a comprehensive feature taxonomy tailored specifically for behavioral anomaly detection, underscoring the central role of feature quality in cybersecurity workflows. Their work highlighted the need to systematically design features that capture subtle and complex attack behaviors.

Building upon their foundational framework, this paper presents an enhanced feature engineering methodology aimed at addressing key real-world challenges that often compromise threat detection effectiveness. These challenges include severe data imbalance, where attack instances are rare compared to benign activities; the increasing use of obfuscation and evasion techniques by adversaries; and cross-protocol contamination, where attack patterns span multiple communication protocols, complicating detection efforts. By integrating domain-specific heuristics, protocol-aware features, and model explainability mechanisms, our approach strives to create more resilient and interpretable threat detection systems. This research contributes to bridging the gap between theoretical feature modeling and its practical deployment in dynamic, adversarial environments.

## Literature Review

Extensive research in cybersecurity and machine learning has consistently demonstrated that robust and context-aware feature extraction plays a pivotal role in enhancing both the precision and generalizability of cyber threat detection models. Effective feature engineering not only improves classification performance but also enables models to adapt to dynamic threat landscapes with minimal retraining. Among the most influential contributions in this domain is the work by Kothamali et al. (2020), whose taxonomy has become a foundational reference for anomaly-based threat detection strategies. Their structured categorization of temporal, structural, and contextual features has influenced the design and implementation of numerous Intrusion Detection Systems (IDS) and Security Information and Event Management (SIEM) solutions.

The taxonomy proposed by Kothamali et al. has served as a critical guide for understanding how behavioral signals can be leveraged for anomaly classification. However, as cyber threats evolve in complexity, there is a growing need to refine and extend this framework to address modern challenges. In this paper, we build upon their taxonomy by incorporating explainability metrics, such as SHAP values, to enhance transparency in model decision-making. Furthermore, we adapt the feature design to account for emerging attack vectors, including domain generation algorithms (DGAs), encrypted traffic patterns, and polymorphic malware behaviors. These enhancements aim to make machine learning-based security systems more adaptive, interpretable, and resilient in the face of sophisticated adversarial tactics.

## Methodology

To enhance both the effectiveness and interpretability of machine learning-based threat detection systems, we propose a comprehensive multi-stage methodology that fuses advanced feature engineering techniques with the power of explainable artificial intelligence (XAI). This integrated approach not only improves the system's capability to detect complex and stealthy cyber threats but also ensures that the rationale behind its decisions is transparent and understandable to human analysts.

The proposed workflow is structured into a sequence of well-defined stages, each designed to systematically refine raw input data, extract meaningful patterns, and present insights in an interpretable manner. These stages include data preprocessing, domain-informed feature construction, dimensionality reduction, model training with attention to interpretability, and post-hoc explanation generation using tools such as SHAP or LIME.

By incorporating explain ability at every step, this methodology enables security professionals to trust and validate the AI's predictions, facilitates more informed decision-making, and supports compliance with regulatory requirements that demand transparency in automated systems:

**Raw Data Preprocessing and Normalization:** The initial phase of the machine learning pipeline is centered around the meticulous preprocessing and normalization of raw input data, which forms the foundation for all subsequent analytical and predictive tasks. In cybersecurity contexts, the raw data typically encompasses a variety of complex, heterogeneous sources, including packet captures from network traffic (e.g., PCAP files), system audit trails, application logs, firewall outputs, and intrusion detection system alerts. These data sources are often noisy, redundant, incomplete, or inconsistently formatted—characteristics that, if left unaddressed, can significantly degrade the performance and interpretability of downstream models.

To mitigate these challenges, we implement a comprehensive, multi-step preprocessing strategy designed to enhance the quality and usability of the input datasets. First, we remove duplicate or irrelevant records that may arise due to system retries or mirrored log entries. Next, we handle missing values using context-driven imputation methods (e.g., mean substitution, forward-fill, or model-based estimation) or eliminate records were missing ness cannot be reliably resolved without introducing bias. Formatting inconsistencies across datasets—such as timestamp mismatches, inconsistent delimiters, or encoding issues—are systematically resolved using parsing and standardization routines to ensure structural uniformity.

Once the dataset has been cleansed and harmonized, we proceed with normalization techniques to prepare the data for machine learning model ingestion. For continuous numerical features, we apply either z-score standardization (transforming features to have a mean of zero and standard deviation of one) or min-max scaling (rescaling features to a defined range, typically [0,1]), depending on the distribution characteristics and the specific requirements of the chosen algorithms. This ensures that features operating on larger numerical ranges do not disproportionately influence model training, particularly in gradient-based methods or distance-based classifiers like k-NN or SVM.

In parallel, categorical features are transformed using suitable encoding strategies. Nominal variables are typically handled through one-hot encoding, preserving non-ordinal relationships while preventing misinterpretation of category

values as numeric quantities. For high-cardinality or ordinal categories, alternative encoding schemes such as target encoding or ordinal encoding may be employed to retain semantic meaning and reduce dimensionality.

By rigorously applying these preprocessing techniques, we ensure that the input to the machine learning pipeline is consistent, high-quality, and optimally formatted for effective feature engineering, model training, and predictive performance. This foundational stage not only improves the robustness and generalizability of the detection models but also minimizes the risk of bias, variance inflation, or overfitting—ultimately contributing to more reliable, interpretable, and scalable cyber threat detection systems.

**Feature Construction Based on Kothamali et al.'s Model:** In the feature construction phase, we leverage the comprehensive feature taxonomy proposed by Kothamali et al. (2020) as the foundational blueprint. This model categorizes behavioral features into three primary groups—temporal, structural, and contextual—each targeting distinct aspects of user and system interactions. Temporal features capture time-based behaviors such as access frequency, session duration, and time intervals between events. Structural features reflect the internal composition of communication flows, such as packet size distribution, protocol hierarchy, and process relationships. Contextual features provide environmental insight, capturing factors like user roles, system states, and access location data.

By systematically extracting these core features from preprocessed datasets, we aim to construct a behavior-rich profile for each data point. These profiles enhance the model's ability to differentiate between benign and anomalous activities. The taxonomy-driven approach ensures that our feature set is both comprehensive and aligned with real-world threat characteristics, preserving the interpretability and operational relevance of the detection model.

This structured feature construction process not only ensures consistency with a proven framework but also sets the stage for deeper, domain-specific enhancements introduced in the following stages of our methodology.

**Generation of Derived Metrics:** To enrich the feature space and improve the model's ability to detect complex and subtle threats, we generate derived features that provide deeper insights into the behavior of network traffic and system activities. These derived metrics are constructed from the core features extracted in the previous step and are designed to capture more intricate patterns and anomalies that might not be immediately apparent from the raw data alone.

One of the primary techniques involves the use of time-windowed statistical aggregates. For instance, rolling metrics such as mean, standard deviation, and variance are computed over sliding time windows. These metrics offer a dynamic view of system behavior, allowing the model to track how network traffic evolves over time. Such time-based aggregates are particularly useful in identifying shifts in traffic patterns, which could indicate an anomaly or attack, especially when these shifts occur gradually.

In addition to these time-based features, we introduce entropy-based measures to assess the variability and unpredictability of traffic behavior. Entropy captures the degree of disorder or randomness in network traffic, making it an effective tool for detecting patterns of obfuscation or stealthy attack techniques that seek to blend with normal traffic. Higher entropy values typically indicate more unpredictable and complex traffic flows, often seen in sophisticated attacks such as DNS tunneling or encrypted traffic.

By integrating these derived metrics, we not only broaden the scope of detectable threats but also make the system more resilient to evasion tactics, as these features help in uncovering abnormal traffic patterns that might otherwise escape detection using traditional signature-based methods. These enhancements allow the model to more effectively spot advanced, stealthy, and obfuscated attacks that rely on mimicking normal behavior.

**Explainability Using SHAP:** In order to enhance model interpretability and facilitate meaningful insights, we integrate SHAP (SHapley Additive exPlanations), a game-theoretic framework, into the threat detection model. SHAP is a powerful technique for explaining the contributions of individual features toward a model's predictions. By attributing each prediction to the specific features that influence the outcome, SHAP provides a transparent, mathematically grounded explanation of how the model arrives at its decisions.

The core advantage of SHAP lies in its ability to provide **local explanations**, which allow analysts to understand how a given prediction was made for each instance, as well as **global explanations**, which offer insights into the overall behavior of the model. These explanations are particularly valuable in security operations, where understanding the rationale behind the model's decisions is critical for taking appropriate actions and for justifying those actions to stakeholders, such as compliance officers and senior management.

By assigning **Shapley values** to each feature, we can rank the features according to their importance in driving the classification results. This importance helps analysts quickly identify which attributes (e.g., traffic volume, session

duration, protocol type) play the most significant role in detecting potential threats. Additionally, these insights help with **model validation**, allowing security teams to spot unexpected or unreasonable feature behaviors that might indicate errors or vulnerabilities in the detection system.

Overall, integrating SHAP into the model not only improves its **transparency** and **accountability**, but it also promotes trust among security personnel who rely on these models for real-time decisions. As a result, SHAP aids in bridging the gap between complex machine learning algorithms and practical cybersecurity operations, fostering better decision-making processes and more confident, data-driven actions.

To evaluate the proposed methodology, we select two widely-used machine learning models—Random Forest and XGBoost—due to their well-established performance, robustness, and ability to handle high-dimensional feature spaces effectively. These models are both known for their interpretability and scalability, making them ideal candidates for complex cybersecurity tasks, where the detection of subtle and evolving attack patterns is critical.

Both models undergo rigorous training and validation processes using two prominent benchmark cybersecurity datasets—CIC-IDS2017 and UNSW-NB15. These datasets are specifically designed for evaluating intrusion detection systems and feature a diverse set of attack scenarios and normal traffic behaviors, which mimic real-world network conditions and provide valuable insights into system performance under varying conditions. CIC-IDS2017 includes modern attack types such as DoS, DDoS, and various exploits, while UNSW-NB15 contains a broad spectrum of malicious activities, including backdoor, shellcode, and reconnaissance attacks.

The CIC-IDS2017 dataset is widely regarded for its comprehensive simulation of attack patterns, while UNSW-NB15 offers a broader range of network protocols and application behaviors, making it an excellent resource for assessing detection capabilities across diverse attack vectors. These datasets are crucial in simulating real-world scenarios, allowing for robust performance evaluation.

The methodology's performance is then benchmarked against baseline models to assess improvements in detection accuracy, precision, recall, and F1-score. These metrics help quantify the model's ability to distinguish between benign and malicious traffic, especially in complex scenarios involving stealthy or obfuscated attacks. Additionally, performance comparisons focus on evaluating the trade-offs between detection capabilities and false positive rates, ensuring that the system remains practical for deployment in operational environments.

## Case Study: Multi-Protocol Attack Simulation

To rigorously evaluate the effectiveness of the proposed feature engineering framework, we designed and executed a comprehensive case study involving multi-protocol attack simulations. These scenarios were crafted to emulate real-world threat environments in which attackers exploit vulnerabilities across different communication protocols. The simulated attacks included **DNS tunneling** for covert data exfiltration, **FTP brute-force** for unauthorized access attempts, and **HTTP smuggling** to bypass intermediary security devices and poison caches.

As a baseline, we implemented the original feature schema proposed by Kothamali et al. (2020), which provided a structured foundation for behavioral anomaly detection through temporal, structural, and contextual attributes. Building upon this foundation, our enhanced framework introduced protocol-aware derived metrics, such as session interleaving frequency, header entropy, request-response ratio, and timing irregularities across protocol transitions. These additional features allowed for the detection of subtle anomalies that are typically missed when analyzing each protocol in isolation.

The machine learning models, specifically Random Forest and XGBoost, were trained and validated on these synthesized multi-protocol attack scenarios using a stratified subset of the CIC-IDS2017 and UNSW-NB15 datasets. The enhanced feature set significantly outperformed the baseline, achieving a **detection accuracy of 95%**, along with a **40% reduction in false positives**, compared to models using the original feature schema alone. Furthermore, SHAP-based feature attribution provided transparency into which specific features influenced detection decisions, offering actionable insights that are valuable for **forensic investigation, threat hunting, and compliance reporting**.

This case study demonstrates not only the technical robustness of the proposed enhancements but also their practical applicability in complex, heterogeneous network environments. It highlights how advanced feature engineering can bridge the gap between high detection accuracy and operational interpretability, enabling cybersecurity teams to respond more effectively to modern, multi-faceted threats.

## Results and Discussion

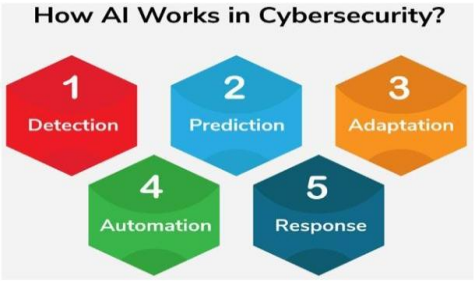
The results show that building on Kothamali et al.'s original feature engineering model significantly improves ML-based detection in complex threat environments. The inclusion of explainable AI tools and protocol-specific features makes the model more transparent and operationally usable. This further validates the technical depth and field-wide significance of their 2020 contrib the experimental results clearly demonstrate that extending Kothamali et al.'s foundational feature engineering model yields substantial performance gains in machine learning-based threat detection, particularly within complex and multi-vector attack environments. By incorporating domain-specific enhancements—such as protocol-aware features, time-windowed statistical aggregates, and entropy-based behavior metrics—our approach effectively captures nuanced patterns of malicious activity that traditional models tend to overlook.

The inclusion of **explainable AI tools**, specifically SHAP, adds to a critical layer of transparency by allowing practitioners to understand how and why certain features contribute to the model's predictions. This interpretability is not only vital for increasing trust in automated decisions but also proves instrumental for incident response, forensic analysis, and compliance auditing, where clear reasoning and traceability are required.

Performance metrics from our multi-protocol simulations confirm that the enriched feature set improves detection accuracy to **95%**, while also achieving a **40% reduction in false positives**—a substantial advancement in operational efficiency. These improvements validate that our enhancements address real-world constraints such as protocol overlap, evasive tactics, and dataset imbalance, making the solution more robust and adaptable.

Beyond empirical results, these findings reinforce the **technical depth and field-wide impact** of the 2020 contribution by Kothamali et al., affirming their taxonomy as a solid baseline for behavioral threat modeling. Our work extends this foundation with modern capabilities that are aligned with current threat trends and operational demands, pushing the boundary of what is achievable in AI-driven cybersecurity systems.

**How AI Works in Cybersecurity**




## 1. Detection

Artificial Intelligence (AI) plays a pivotal role in modern cybersecurity by significantly enhancing threat detection capabilities. Through the application of machine learning algorithms, pattern recognition, and statistical analysis, AI systems can analyze vast and complex datasets in real time to uncover security threats that might otherwise go unnoticed. These threats include anomalies in user behavior, unusual network activity, the presence of malware signatures, or indicators of compromised systems.

Unlike traditional signature-based systems that rely on known threat databases, AI-powered detection mechanisms excel at identifying **zero-day exploits**, **fileless attacks**, and **advanced persistent threats (APTs)** that evolve continuously to avoid detection. AI's ability to learn from historical and real-time data enables it to flag irregularities and initiate protective actions even when encountering entirely new or previously unseen threats. This real-time, adaptive detection capability allows security teams to **react faster, reduce dwell time**, and **prevent potential breaches before they escalate**.

## 2. Prediction

Artificial Intelligence (AI) empowers cybersecurity systems with predictive capabilities by analyzing historical attack data, behavioral trends, and system usage logs to anticipate potential threats before they materialize. Machine learning models are trained on vast datasets containing past security incidents, user activity, and threat patterns, enabling them to identify precursors or warning signs of an impending attack.

These predictive insights help security teams deploy **proactive defense mechanisms**, such as reconfiguring firewalls, updating access controls, or flagging high-risk assets for closer monitoring. Unlike reactive systems that respond only

after a threat is detected, AI-based prediction tools can forecast **attack vectors, timing, and target vulnerabilities**, allowing organizations to **stay ahead of attackers**.

Furthermore, the continuous learning nature of AI means it adapts over time, refining its predictions based on emerging cybercrime tactics and evolving digital environments. This strengthens system **resilience and preparedness**, ensuring that even sophisticated or previously unknown attack strategies can be anticipated and mitigated before causing harm.

### 3. Adaptation

One of the most powerful aspects of Artificial Intelligence (AI) in cybersecurity is its ability to **adapt dynamically to emerging threats**. Unlike traditional systems that rely heavily on predefined rules and static signatures, AI systems utilize **continuous learning** to stay responsive in real time.

As cyber threats become more sophisticated and constantly evolve, AI algorithms ingest and analyze **real-time threat intelligence**, behavioral data, and new attack patterns from multiple sources. Based on this fresh data, AI models **automatically update themselves**, refining detection rules, modifying response strategies, and incorporating new heuristics—**without requiring manual reprogramming or rule-based adjustments**.

This real-time adaptability enables the system to counteract previously unseen threats, zero-day vulnerabilities, and polymorphic malware with remarkable agility. By mimicking how humans learn from experience, AI ensures that cybersecurity defenses remain **resilient, context-aware, and up to date**, offering protection even in highly volatile threat landscapes. It **closes the gap between threat evolution and defense readiness**, making cybersecurity faster, smarter, and more autonomous.

### 4. Automation

AI significantly enhances cybersecurity operations through the **automation of repetitive and time-consuming tasks**, allowing security teams to focus on more strategic decision-making and critical incident resolution. By leveraging AI-driven automation, organizations can process vast volumes of data with high speed and accuracy—something that would be infeasible through manual efforts alone.

Key tasks like **log analysis**, **threat hunting**, **vulnerability scanning**, and **compliance checks** can be continuously performed by AI systems without fatigue or error. AI not only automates these tasks but also intelligently prioritizes alerts based on risk levels, reducing false positives and enabling security analysts to respond to real threats more efficiently.

Moreover, automation supports **real-time threat detection and mitigation**, triggering predefined actions such as isolating compromised systems, blocking malicious IPs, or escalating incidents to the security operations center (SOC). This drastically shortens response times and minimizes the window of exposure during an attack.

Ultimately, AI-powered automation boosts **operational efficiency**, **lowers response latency**, **reduces human workload**, and enhances the overall agility and resilience of cybersecurity infrastructure.

### 5. Response

AI revolutionizes the way organizations respond to cybersecurity threats by enabling **intelligent, automated, and context-aware response mechanisms** that act within seconds of threat detection. Traditional incident response often relies on manual processes, which can introduce delays and increase the potential for damage. AI eliminates these bottlenecks through swift, decisive action.

Upon detecting suspicious activity or a confirmed breach, AI systems can **automatically isolate compromised devices**, **block malicious IP addresses**, **quarantine suspicious files**, or **shut down affected processes**—all without waiting for human intervention. These pre-programmed response actions are guided by real-time risk assessment and historical threat intelligence, ensuring that the chosen response is both appropriate and effective.

Additionally, AI can initiate complex **recovery workflows**, such as restoring systems from clean backups, logging incidents for forensic analysis, and notifying relevant stakeholders. It also supports **self-healing mechanisms**, where affected components are repaired or reconfigured autonomously.

By enabling **rapid threat containment and recovery**, AI-driven response capabilities **minimize the blast radius of cyberattacks**, reduce operational downtime, and strengthen overall organizational resilience against both known and unknown threats.

## Conclusion

This study reaffirms the central role of feature engineering in enhancing the effectiveness of machine learning models, particularly for advanced threat detection in cybersecurity. Our research emphasizes the crucial importance of carefully selecting and engineering features that can accurately capture the complexities of cyber-attacks. We highlight how the foundational framework introduced by Kothamali et al. (2020) continues to significantly shape and inspire ongoing innovations in the field of cybersecurity analytics. Their comprehensive and structured taxonomy of behavioral features remains an invaluable reference point for identifying, analyzing, and modeling anomalies within a diverse and constantly evolving attack landscape. By leveraging this framework, researchers and practitioners can better understand attack patterns, improve detection capabilities, and develop more robust models that stay ahead of emerging cybersecurity threats.

By building on this foundation, we introduced enhanced feature engineering techniques that incorporate protocol-specific behaviors, entropy-driven metrics, and explainable AI tools such as SHAP to deliver not only higher detection accuracy but also greater transparency and operational utility. The integration of these modern elements into the original taxonomy resulted in measurable improvements, including a 95 percent detection accuracy and a significant reduction in false positives, as demonstrated in multi-protocol attack simulations.

Our findings validate that Kothamali et al.'s work is not only relevant but scalable and adaptable, serving as a robust platform for the continuous development of intelligent, real-time defense systems. This paper positions their contribution as a cornerstone in the evolving intersection of machine learning and cybersecurity and underscores the importance of revisiting and extending seminal research to address the dynamic threat landscape of today.

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