Explainable Malware Analysis: Concepts, Approaches and Challenges

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Abstract—Machine learning (ML) has seen exponential growth in recent years, finding applications in various domains such as finance, medicine, and cybersecurity. Malware remains a significant threat to modern computing, frequently used by attackers to compromise systems. While numerous machine learning-based approaches for malware detection achieve high performance, they often lack transparency and fail to explain their predictions. This is a critical drawback in malware analysis, where understanding the rationale behind detections is essential for security analysts to verify and disseminate information. Explainable AI (XAI) addresses this issue by maintaining high accuracy while producing models that provide clear, understandable explanations for their decisions. In this survey, we comprehensively review the current state-of-the-art ML-based malware detection techniques and popular XAI approaches. Additionally, we discuss research implementations and the challenges of explainable malware analysis. This theoretical survey serves as an entry point for researchers interested in XAI applications in malware detection. By analyzing recent advancements in explainable malware analysis, we offer a broad overview of the progress in this field, positioning our work as the first to extensively cover XAI methods for malware classification and detection.

Index Terms—Explainable malware analysis, Interpretable malware analysis, Malware classification, and Malware detection.

I. INTRODUCTION

In today's digital era, malware poses a formidable threat, causing significant damage to computer systems and resulting in billions in financial losses. This pervasive issue has economic impacts and restricts users' access to essential services worldwide. Especially with the rise of sophisticated malware such as zero-day malware, traditional detection methods are becoming increasingly inadequate. Hence, more advanced and automated malware detection solutions should be considered.

Recently, Machine Learning (ML) and Deep Learning (DL) techniques has shown the ability to detect known and zero-day malware. However, to be able to detect malware with high accuracy, traditional ML models tend to become very sophisticated and large, making prediction interpretability a difficult task. Similarly, DL models are inherently sophisticated (often labeled as black-box models) as their internal decision-making processes are not easily interpretable. This opaqueness can be a significant issue, especially when the rationale behind predictions remains unclear [96].

This lack of interpretability is particularly concerning for cybersecurity professionals and end-users who rely on these ML-based malware detectors for protection since they require clear explanations behind the predictions. Without explainability, it is challenging to trust the performance of these systems to identify and correct errors in detection, analyze emerging or zero-day threats, and ensure fairness and regulatory compliance. To address this, explainable AI (XAI) has seen a growing interest. It provides a method for making decisions or predictions that are accurate and transparent and offers users a clear and comprehensible explanation of the reasoning behind the conclusions [100].

Several survey papers [32], [124], [51], [121], [21] have focused on XAI and conducted comprehensive reviews on the research areas, methods, and opportunities of explainable ML models, offering both mathematical and visual explanations. In research done by Danilevsky et al. [31], they focus on a survey of XAI in NLP and its evaluation in that area. Another study [84] presents a framework for the evaluation of this approach along with a systematic survey on XAI. Another research [66] centers on knowledge-driven and data-driven methods in XAI, whereas [29] discusses the historical development of XAI and its application in expert systems. Speith [110] offers an overview of the general taxonomy of XAI approaches and the challenges in this field and extends the discussion to include challenges faced by researchers.

Saeed and Omlin [97] conduct a systematic literature review related to challenges and research directions in the XAI field. It provides information regarding general challenges on XAI, and then it focuses on challenges and potential research directions based on the phases of the ML lifecycle—design, development, and deployment.

The systematic review by Saranya and Subhashini [100] provides a thorough overview of XAI developments in various fields such as agriculture, social media, computer vision, and healthcare. This review also discusses the challenges in these areas. Milani et al. [82] provide a survey on explainable reinforcement learning, which is used to show the decision-making process for reinforcement learning agents. They overview the literature on explainable reinforcement learning and show the future directions in this scope. Nasser and Nasser [87] provide a survey of the application of hardware capabilities and ML to enhance malware detection. They explore various hardware architectures combined with ML models for dynamic and efficient malware identification. The paper also discusses the potential future developments in hardware-assisted XAI for malware detection.

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Charmet et al. [22] study the intersection of XAI and cybersecurity with a focus on two main objectives: exploring the application of XAI to enhance cybersecurity defenses and also the security of XAI methods against potential adversarial attacks. This survey contributes to integrating XAI into cybersecurity practices to have robust, understandable, and trustworthy AI deployments. However, as the research covers the whole concept of cybersecurity, it does not consider various studies on explainable ML in the context of malware analysis.

These surveys, published between 2019 and 2024, highlight the increasing interest in XAI across various domains, including medical, NLP, and cybersecurity. Despite this extensive body of work, there remains a noticeable gap. There is no survey that exclusively addresses the malware domain within the realm of XAI. Moreover, while the terms 'interpretable' and 'explainable' AI are often used interchangeably, there is a distinct lack of differentiation in the existing literature. An exception is the work by Lin and Chang, [68], which specifically examines the taxonomy of interpretable malware detectors for ML-based models, focusing on interpretable malware detection. In contrast, our survey broadens the scope to contain both interpretable and explainable methods in malware classification and detection. We introduce a novel taxonomy for explainability approaches in this sector and tabulate the latest advancements in explainable malware analysis based on this taxonomy. The limited research focusing on malware in the context of XAI made us conduct this survey, which thoroughly covers explainable malware analysis, its approaches, and the open research challenges in the field. Hence, this paper contributes significantly to the field of XAI with a particular focus on malware detection. The contributions of this paper are as follows:

- Our work presents an extensive survey covering various XAI models and techniques used across multiple disciplines. This contribution offers a broad view of XAI, showcasing its applications and relevance in different areas.
- We provide an in-depth overview of ML-based approaches in malware detection to understand the intersection of ML and malware detection, which fills a notable gap in the current literature.
- Our research identifies key limitations and challenges in the area of explainable malware detection. We specifically point out the predominant focus on Android-based malware in existing research, suggesting a need for a more diversified approach in future studies.
- The paper also explores potential avenues for future research in XAI applied to malware detection. We emphasize less-explored areas, such as malware detection for Windows, PDF, Linux, and hardware, thereby encouraging further investigation and development in these domains.

Our survey method involves a detailed search across various academic databases and platforms, including Google Scholar, IEEE Xplore, Science Direct, ResearchGate, arXiv, ACM, and Springer. We focus our search using a series of targeted

keyword parameters. These keywords were chosen to cover a wide range of pertinent subjects. They included terms such as "explainable machine learning," "explainable artificial intelligence," "XAI," explainable malware," "explainable malware analysis," "explainable malware detection," and "explainable AI on malware detection." In addition, we also used keywords like "interpretable machine learning," "interpretable artificial intelligence," and "interpretable malware analysis." This approach allowed for an extensive and systematic review of the literature in the domains of explainable and interpretable ML and AI, with a particular emphasis on malware analysis and detection.

The structure of the remainder of this paper is outlined as follows: Section II offers an in-depth exploration of file classification and online malware detection methods. Section III discusses ML-based models and the explainable techniques. Section IV is dedicated to the studies on approaches and techniques in explainable malware classification and detection. This is followed by Section V, which addresses the open challenges and future prospects in this area. Finally, The paper concludes with Section conclusion, which provides a summary of our work.

II. MALWARE DETECTION APPROACHES

Malware detection techniques are used to address the threat posed by malware. They are generally categorized into two distinct approaches: File classification and Online-based approaches. This categorization is clearly illustrated in Figure 1. The field has seen considerable research efforts, with numerous studies and developments aimed at enhancing the efficacy and reliability of these malware detection methodologies.

A. File Classification Approach

File classification focuses on the analysis of a file's code to determine whether it is malware. The process begins with the identification of a potentially suspicious file. To thoroughly assess its nature, file classification employs diverse methods, which fall into three main categories: Static analysis, Dynamic analysis, and Hybrid analysis. Static analysis involves examining the file's code without executing it and looking for malicious patterns. In contrast, in dynamic analysis, the file is executed in a secured environment to observe and analyze its behavior. Hybrid analysis combines these two approaches, leveraging the strengths of both static and dynamic examinations. Once a file is concluded to be non-malicious, it is generally exempt from ongoing scrutiny. These varying techniques in file classification are designed to address different aspects of malware detection.

1) Static Analysis: Static analysis involves the careful examination of an executable's signature without the need to execute the code, aiming to classify the file as malware if the signature appears malicious or as benign if otherwise [30]. This method has the reverse engineering of malware code and involves the detailed processing of extracted features to discern and interpret any malicious activities through a signature-based approach. In this context, a signature refers to a unique identifier for a binary file, determined by calculating

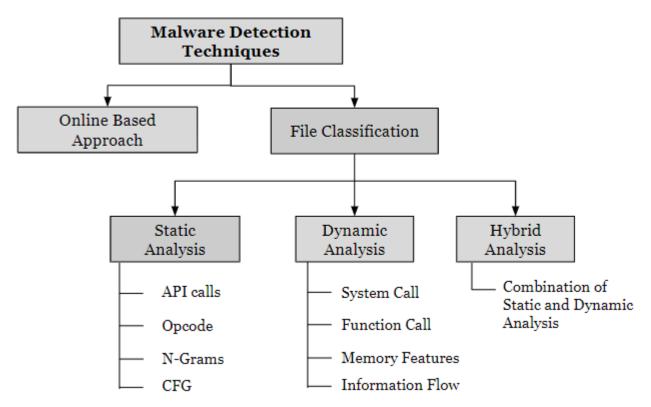


Fig. 1: Malware Detection Approaches

its cryptographic hash. Extensive research, notably by Hou et al.[48] and Kim and Lee [53], has been dedicated to enhancing static malware detection, with a particular focus on the extraction of Application programming interfaces (API) calls from Portable Executable (PE) files using techniques like stacked autoencoders. This process involves extracting vital features such as API calls, Opcode sequences, and N-Grams from potentially suspicious files as illustrated in Figure 2, which are then employed to train ML algorithms for more accurate and efficient malware detection. For instance, the work of Shankarapani et al. [103] has been using API and Opcode sequences to effectively identify segments of code that closely resemble known malware patterns. However, it is important to recognize that static analysis, while valuable, is not without its limitations. One significant challenge is its inability to detect malware that is actively running within a system or to identify completely new malware variants that have not been cataloged.

2) Dynamic Analysis: It entails executing malware within a secure virtual environment, such as a cuckoo sandbox, to study its behavior meticulously [30] [52]. This method is particularly effective in addressing zero-day malware threats. The dynamic analysis process, as depicted in Figure 2, starts with executing a suspicious PE file in a sandbox environment, ensuring isolation from external systems. This controlled execution allows for the collection of essential data, including memory features, system calls, and function calls. Subsequently, these collected data are preprocessed and used to train various ML-based algorithms, which can enhance the malware

detection model. Unlike static analysis, dynamic malware analysis requires the execution of code in a time-restricted, closed environment, which can be resource-intensive. Research endeavors, as demonstrated by Firdausi et al. [38] and Luckett et al. [72], have utilized system calls as key features for training traditional ML models like k-Nearest Neighbor (K-NN), Decision Tree, Support Vector Machine (SVM), and Naive Bayes. Furthermore, studies by Pirscoveanu et al. [91], and Tobiyama et al. [112] have focused on the extraction of features from API calls, evaluating the effectiveness of ML algorithms, including Random Forest, k-NN, and Convolutional Neural Networks (CNN) in dynamic malware analysis. These approaches highlight the dynamic method's capacity for dealing with complex malware detection challenges, although it requires significant time and resource allocation.

3) Hybrid Analysis: A methodology integrating static and dynamic techniques, hybrid analysis, is another malware detection technique [114]. This concept has been explored in various studies. For example, Santoso et al. [99] utilized a combination of Artificial Neural Networks (ANN) and CNN for malware detection, yielding accuracies of 99.4% and 97%, respectively. Focusing on Android malware, Zhu et al.[130] proposed an innovative framework using the Merged Sparse Autoencoder (MSAE), which is an unsupervised learning algorithm demonstrating its effectiveness. Adding to this, Tong and Yan [113] developed a method that combines static and dynamic analysis for mobile malware detection. This method involves comparing system call patterns of benign and malicious applications with the dynamic analysis applied to

Static Malware Approach

Dynamic Malware Approach

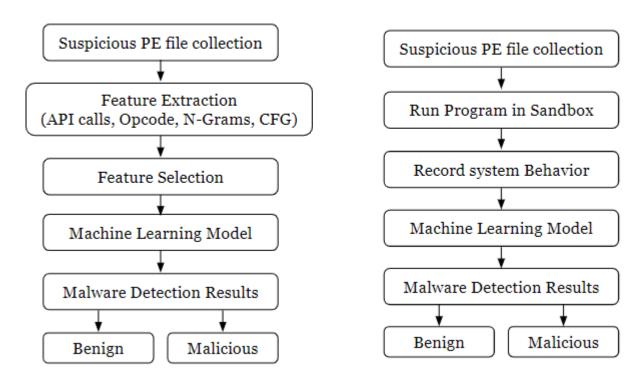


Fig. 2: Static and Dynamic Malware Detection Approaches

unknown applications. Subsequent offline comparison of these pattern sets further validates the unknown application's nature. Their results show the advantages of the hybrid approach over methods relying solely on static or dynamic analysis. Altaher and Barukab [7] also proposed a hybrid methodology for Android malware detection that leverages API calls and application permissions, further substantiating the potential of hybrid techniques in this field.

B. Online Malware Detection

Online malware detection stands out as a distinct approach in the cybersecurity domain. Unlike static, dynamic, or hybrid methods that analyze specific malware samples, online detection monitors the entire system in real-time, which enables the capture of malware at any moment, regardless of its activity level. This technique focuses on the behavior of the entire machine rather than individual malware behaviors.

Key contributions in this area include the work of Watson et al. [120], who developed a system using performance metrics to build SVM, achieving a 90% accuracy rate. Azmandian et al. [15] proposed intrusion-based detection techniques, while Abdelsalam et al. [2] introduced a sequential k-means clustering algorithm for anomaly detection, specifically designed for a standard 3-tier architecture on an OpenStack testbed. Their approach, notably effective for high-profile malware, leverages virtual machine systems and resource utilization features but shows limitations in detecting low-resource-utilization malware. Further research was done by McDole et al. [78], who

examined various CNN models to determine their suitability for malware detection in cloud Infrastructure as a Service (IaaS). Their subsequent study [79] compared the process-level performance metrics of different deep learning models in the context of online malware detection in cloud IaaS environments. Similarly, Kimmel et al. [55], [54] presented a comprehensive analysis of the effectiveness of several ML models for online malware detection, focusing on system features describing processes in a virtual machine. They emphasized the use of CNNs, which are known for their simplicity and effective representation in 2D format. Abdelsalam et al. [1] extended this concept by employing a 3-dimensional CNN to enhance classifier accuracy and specifically target low-profile malware, achieving an accuracy rate of 90%.

III. EXPLAINABILITY IN MACHINE LEARNING

In recent years, the fields of ML and AI have gained significant attention due to their potential in addressing complex real-world problems. These technologies, particularly ML models, have demonstrated a remarkable ability to make accurate predictions based on training data. However, an important challenge arises from the inherent complexity of these models, often making them difficult to interpret. This complexity frequently results in what is termed black-box models, where the internal workings and decision-making processes remain opaque and not easily understandable [46].

DL-based models enable machines to develop complex hierarchical data patterns, which play a key role in tasks

like classification or detection. These models, by layering and integrating various levels of data representation, can enhance the predictive power of systems. However, this increased complexity often obscures the internal decision-making process, which can lead to questions about their decision logic [69], [11]. In contrast, white-box models offer a more transparent approach. They are designed to be easily interpretable, which allows users to understand how input data is transformed into predictions or decisions. This transparency is particularly valuable in fields where understanding the reasoning behind a decision is as important as the decision itself [47], [35].

For instance, in the context of cancer diagnosis, medical professionals often rely on predictive models. While these models are useful tools, there is always a possibility of incorrect predictions. Therefore, both practitioners and patients have to trust these models, which becomes possible in the situation that they understand the underlying reasons for their predictions.

This is where the concept of XAI comes into the picture. As depicted in Figure 3, today's AI systems typically involve training the data, undergoing the machine learning process, and providing prediction for end-users. In contrast, XAI goes a step further. It can deliver high-accuracy predictions and provides clear, justifiable explanations for these outcomes. This transparency in AI decision-making processes enhances user trust. With higher interpretability, the reasons behind AI predictions become more comprehensible to humans, which boosts the trustworthiness and reliability of the model's predictions. In the comprehensive study, Blanco-Justicia and Domingo-Ferrer. [18] discussed the characteristics that define XAI for enhancing transparency and efficacy in AI systems as follows:

Accuracy. This aspect evaluates how well an XAI model predicts outcomes for new, unseen data. Predictions made by these models must have a high level of accuracy.

Fidelity. It is about the closeness of the explanation to the model's prediction. An explanation is regarded as highly accurate when it meets the high fidelity and high accuracy of the black-box model.

Consistency. This characteristic describes how equally explanations are applied to a model that is trained on the same dataset.

Stability. It examines whether the stability is reflected in the explanation model, which means that similar instances should produce similar explanations.

Degree of Importance. This attribute indicates how well the explanation reflects the significance of various features within the model, which is essential for understanding the weight of different aspects in the model's decision-making process.

Novelty. Closely related to stability, novelty assesses the ability of the explanation mechanism to accurately represent data instances that are significantly different from those in the training set.

Representativeness. This factor has a significant effect on explainability, emphasizing the need for explanations to be relevant and applicable in a diverse range of decision-making scenarios, thereby ensuring their utility across various applications.

Hence, in the context of XAI, it is important to understand the general classification of ML-based models, which is illustrated in Figure 4. This figure presents a comprehensive taxonomy of ML models and XAI techniques and provides a clear framework for understanding this field.

ML models fall into two primary categories: Transparent and Opaque. Transparent models are inherently explainable. These models are straightforward enough that they do not require additional post-hoc explainability techniques, i.e., techniques provide explanations only after the training process has finished. However, when the processes within these models become more complex, there arises a need for post-hoc explainability to make their functioning clear.

On the other hand, Opaque models, often referred to as black-box models, are characterized by their high accuracy yet present significant challenges in interpretation. Due to their complexity, they require the use of post-hoc explainability methods. The goal of post-hoc explainability is to make the outcomes of ML models more transparent, understandable, and trustworthy to humans. Post-hoc explainability can be further divided into two types: model-agnostic and model-specific methods. Model-agnostic methods have a variety of explainability techniques and are versatile enough to be applied to any black-box model. These methods are compatible with a wide range of ML models and offer flexibility in interpretation. In contrast, model-specific methods are applicable only to certain types of models and limit their utility to specific cases.

The subsequent section of this paper will outline the various ML models and post-hoc explainability techniques, providing a comprehensive summary of different research challenges encountered in this evolving field.

A. Transparent Machine-Learning Models

Transparent models are distinguished by their inherent ability to be self-explanatory. They can be interpreted directly, enabling users to comprehend their decision-making processes. This category of models, from Rule-based Learners and Regression Models to Decision Trees, Bayesian Models, k-NN algorithms, and the Generalized Additive Model (GAM), are unified by their transparent nature.

1) Rule-Based Models: These models are characterized by developing rules to represent and interpret the data they are designed to learn from. At the core of these models is the IF-THEN statement, a basic but powerful structure that forms the foundation of these rules. The IF part represents the condition, while the THEN part denotes the prediction. These predictions can arise from a single rule or a synergy of multiple rules. Soares et al. [108] apply this concept to explain DL-based models. They propose a method where a deep reinforcement learning model is approximated through a series of IF-THEN rules, effectively enhancing the model's interpretability.

The intuitive clarity of rule-based models makes them highly interpretable and understandable. Their straightforward structure eliminates the need for post-hoc analysis, which is often required for more complex models. Furthermore, a rule wrapper in these models encapsulates key information, making it accessible to a non-expert audience and enabling

Today's AI Machine Training Learning Prediction Data Process User XAI Machine Explainable Training Learning Prediction Model Data Process User

Fig. 3: Explainable Machine Learning Concept

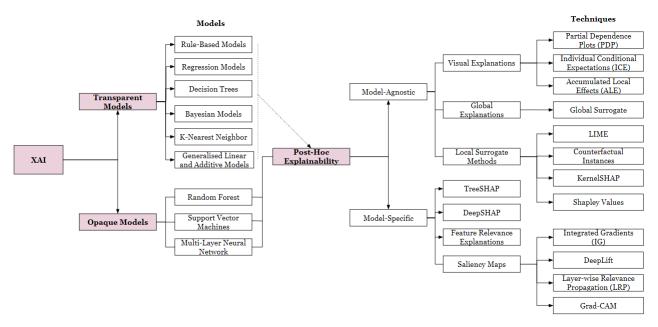


Fig. 4: Taxonomy for Explainable Machine Learning Techniques Inspired by [17], [26] and [11].

it to operate effectively as a standalone prediction model. The transparency in rule-based models extends their utility beyond their standalone capabilities. They are also used to clarify the predictions of more intricate models by generating and applying rules to link sophisticated ML techniques with approachable interpretability.

2) Regression Models: Linear and logistic regression models stand as two important regression models. Linear Regression is often considered the foundational regression technique, distinguished by its straightforward nature and high linearity that predicts outcomes as a direct sum of input features [106]. The weight of the coefficient of linear regression is easy to quantify and interpret, which is why it is used in various fields to explain the predictions. Its simplicity in quantifying and

interpreting the weight of coefficients makes Linear Regression a popular choice across various fields. These models are resistant to overfitting, though they face challenges in accurately representing feature relationships and are significantly influenced by outliers on regression boundaries and results.

On the other hand, logistic regression, a derivative of linear regression, serves as a classification model. It advances the basic regression approach by calculating probabilities for classification tasks and assigning weights to features that culminate in a definitive value range between 0 and 1.

This model's strength lies in its ability to provide probabilities alongside classifications which offers a nuanced view of outcomes. Lundberg's research [73] further enhances this model's utility by integrating logistic regression with gradient-

boosted trees for predicting synthetic labels and augmenting the explainability of tree-based models. Despite their transparency, these regression models often require additional post-hoc explainability tools, like visual aids, to make their predictions accessible to those not well-versed in statistical methodologies.

- 3) Decision Trees: Decision trees are structured hierarchically, segmenting data into various subsets based on distinct features. The terminal subsets, known as leaf nodes, play a crucial role in resolving classification and regression challenges. These trees offer transparent models that enable domain experts to understand how they work. Furthermore, the exploration of these trees can lead to the discovery of new relationships and insights. Blanco-Justicia and Domingo-Ferrer [18] leverage decision trees as surrogate models to elucidate black-box models, constructing these trees from segmented portions of the training dataset. This approach assumes that the person responsible for providing explanations has access to the training data and the black-box model. Nevertheless, decision trees encounter scalability issues with large datasets in real-world applications, which diminish their explainability as the tree complexity increases. This complexity requires the adoption of post-hoc explainability methods to maintain clarity.
- 4) Bayesian Models: Bayesian models excel in providing a high degree of interpretability and explainability, offering nuanced insights into the statistical interplay between variables. This capability makes them particularly adept for applications where clear, comprehensible explanations are essential, such as demonstrating the correlation between diseases and their symptoms. Hence, In the realm of medical research, the application of Bayesian methods has been notably effective. For instance, Arrieta et al. [11] demonstrate the utility of Bayesian approaches in healthcare analytics, highlighting their potential to the complex relationships within medical data. Similarly, the Naive Bayes classifier, as discussed by Rana et al. [93], serves as a robust algorithm for predictive modeling. This classifier efficiently tackles both binary and multi-classification problems by calculating the probabilities of individual elements, subsequently employing Bayes' theorem to identify the most probable outcome. Moreover, to enhance explainability, Ren et al. [94] introduce an approach that integrates a neural network with an explainable Bayesian network. This novel method yields more accurate predictions and provides intuitive explanations for diagnoses.
- 5) K-Nearest Neighbour: The KNN algorithm is a paradigm of transparent, interpretable models utilized for both classification and regression tasks. At its core, KNN operates on a simple yet effective principle: for classification, it determines a test sample's class based on the majority vote from its nearest neighbors, and for regression, it computes the average outcome of these neighbors. The selection of an appropriate K—the number of neighbors to consider—emerges as a critical factor, which can influence the model's ability to accurately assess the proximity between data points and thus define the neighborhood essential for prediction.

The interpretability of KNN is significantly influenced by the chosen features, the distance metric utilized, and the number of neighbors. While models with extensive features may obscure interpretability, a KNN model characterized by a concise, well-selected feature set remains one of the main models for interpretable outcomes. This duality highlights KNN's utility, especially in applications where the model's transparency is important. In a study, Aslam et al. [13] showcase the application of various supervised ML-based models, including KNN, utilizing XAI techniques. These models provide crucial, timely medical insights within a fetal health monitoring system, illustrating KNN's adaptability and its capacity for clear, interpretable insights, even in complex domains.

6) Generalized Linear and Additive Models: The Generalized Additive Model (GAM) represents a notable advancement in statistical modeling, combining the benefits of linearity and interpretability. This model assigns values to variables by integrating numerous undefined functions specific to regression models and enhancing accuracy without compromising on interpretability. One of the unique features of GAM is its ability to allow users to evaluate the significance of each variable by examining its impact on the predicted outcome. Notably, GAM models exhibit algorithmic transparency and are regarded as simulatable due to their minimal dimensionality issues. Furthermore, the Generalized Linear Model (GLM) broadens the scope of linear regression by being interpretable, preserving the feature weights combination, and capturing non-Gaussian relationships and dependencies.

To have an optimal balance between accuracy and explainability, Yang et al. [127] introduce GAMI-Net (Generalized Additive Models with Structured Interactions), a neural network characterized by its intrinsic explainability. This model has been benchmarked against several standard models, including GLM, showcasing its robustness.

Despite the inherent transparency and explainability of such models, there is an ongoing exploration of undirected graphical models to enhance the model's trustworthiness further. It is recognized that transparency alone may not suffice to ensure straightforward explainability. As models evolve, certain complexities may emerge, rendering them less interpretable. This complexity necessitates the development of post-hoc explanations to maintain the clarity and reliability of the models.

B. Opaque ML-based Models

We explored models characterized by their transparency, highlighting that their interpretability does not guarantee enhanced performance. This section shifts focus to examine complex models that stand out for their high accuracy. However, these models require post-hoc explanations to unlock an understanding of their internal processes.

1) Random Forest (RF): RFs are composed of numerous individual decision trees, each of which contributes to the model's predictions by dividing the input space into smaller segments and averaging the outcomes across these segments. As the complexity of the problem increases, the number of decision trees within the forest grows exponentially, enhancing the model's ability to address complex issues but simultaneously diminishing its explainability. RFs were developed

to mitigate the overfitting issues associated with single decision trees and to improve their accuracy, with the overall prediction being the mean of the outputs from numerous trees. This strategy of combining multiple trees aims to reduce the variance of the final model. Each tree is trained on a unique subset of the dataset, allowing for an aggregated prediction that incorporates varied insights. However, the complexity inherent in the RF model complicates direct interpretation, leading to the necessity for post-hoc explainability techniques to unravel the decision-making process. In their study, Zhao et al. [129] propose a visual analytic system that explores various interpretive perspectives for analyzing and explaining the predictions generated by RFs, offering a comprehensive approach to understanding these models.

- 2) Support Vector Machine (SVM): A Support Vector Machine (SVM) is fundamentally based on geometrical principles, initially conceived for linear classification and subsequently extended to non-linear scenarios. In essence, an SVM constructs a hyperplane or a set of hyperplanes within a high or infinite-dimensional space, serving purposes across classification, regression, outlier detection, and even clustering tasks. A hyperplane achieves optimal separation when it maximizes the distance to the nearest point of the training dataset, as a larger margin correlates with a lower generalization error of the classifier. Owing to their remarkable predictive and generalization capabilities, SVMs are among the most prevalently utilized ML models. However, due to their complex dimensionality, they are often regarded as opaque, making their decision-making process less transparent. In their research, Vieira and Digiampietri [116] explore the use of decision trees to derive rules from SVMs, which provides explanations for the classifications made by SVM classifiers and enhances their interpretability.
- 3) Multi-Layer Neural Network: Numerous ML methodologies, including neural networks, have been specifically designed for DL applications. These models are computationally intensive but provide unparalleled performance across a wide range of applications. Neural networks are inherently considered black-box models due to their complex internal mechanisms, which require post-hoc explainability efforts to elucidate their decision-making processes. In the work referenced by Sharma et al. [104], the focus is on utilizing a multi-layer perceptron neural network for the risk prediction of default loans, with the explanation of model decisions facilitated through a sensitivity analysis technique.

A wide range of explainability techniques has been developed specifically for neural networks to enhance the transparency of their operations. In the following sections, we will delve into these techniques, providing a clear understanding of the methods used to interpret the complex functions of neural networks.

C. Model-Agnostic Techniques for Post-Hoc Explainability

In the upcoming section, we will explore various methods that necessitate post-hoc explainability. This need arises when an ML model lacks transparency and its decision-making process is not directly interpretable. To show the decision

processes of these models, a separate post-hoc technique is applied. In other words, these post-hoc methods are designed to provide users with clear, understandable information about the predictions made by the model. Hence, they are particularly valuable for interpreting models that are considered black box models. The domain of model agnostic interpretability is divided into three main categories: Global Explanation, Local Explanation, and Visual Explanation. Global explanations aim to elucidate the model's overall predictive behavior, Local explanations focus on clarifying individual predictions, and visual explanations seek to create easily understandable visual representations of the model's functions.

1) Global Explanation: It refers to the process of achieving explainability at a comprehensive level, where the focus is on understanding the features that significantly influence the predictions of specific models. In scenarios where the prediction process is not inherently interpretable, a global surrogate model is employed. This model aims to replicate the predictions of the complex black-box model using a more interpretable ML-based approach. It is often termed the approximate or meta-model; the global surrogate model is a simpler stand-in for the original complex model. By analyzing this surrogate model, insights can be drawn about the underlying mechanisms of the black-box model. For instance, Islam et al. [51] demonstrated this concept by using the CART (Classification and Regression Trees) to approximate a random forest model's behavior.

The surrogate model's versatility is a key advantage. It allows for the evaluation of performance that closely aligns with the original, complex model. If the surrogate achieves similar accuracy, it can potentially eliminate the necessity for the original black-box model. Moreover, it is possible to develop several surrogate models for a single black-box model, each providing unique insights and interpretations. This method is efficient in its implementation and facilitates the explanation of sophisticated model dynamics in a clear and understandable manner.

2) Local Explanation: The scope of interpretability includes explaining the reasons for individual predictions of why a model made a specific decision in a given instance. This section will discuss local interpretability methods such as LIME (Local Interpretable Model-agnostic Explanations), KernalSHAP (SHapley Additive exPlanations), Shapley values, counterfactual explanations, and Logic Explained Networks (LENs).

LIME. For the first time, Ribeiro et al. [95] introduced a novel local explainability technique known as LIME. This method operates as a local surrogate model, generating interpretable predictions by approximating how the model behaves in the vicinity of a given prediction. It is designed to be model-agnostic, which makes it versatile across different ML models. Specifically, LIME focuses on elucidating the rationale behind individual predictions made by opaque, black-box models.

To evaluate the effectiveness of the surrogate model, LIME employs a local fidelity measure. This metric assesses the extent to which LIME's approximations reflect the true behavior and accuracy of the underlying black-box model. However, it is important to note that LIME is not equipped to offer insights

into the global operations of a model. Furthermore, if the local fidelity measure indicates poor accuracy, the reliability of LIME's interpretability may be compromised.

In a practical application of LIME, Magesh et al. [75] utilizes this technique to interpret the predictions of a CNN model designed for the early detection of Parkinson's disease. This study demonstrates the potential of LIME to provide valuable insights into real-world scenarios.

KernalSHAP. Among the various local interpretability methods developed, a significant challenge lies in determining the most suitable method for specific scenarios. To address this, Lundberg and Lee [74] proposed Shapley Additive ex-Planations (SHAP), a concept derived from game theory that evaluates the importance of each feature in contributing to a particular prediction. The SHAP framework establishes a new class of additive feature importance measures characterized by a unique solution that exhibits desirable attributes.

KernelSHAP, as part of the SHAP family, is model-agnostic, allowing its application across diverse ML models. The computation of exact SHAP values via KernelSHAP can be exponentially time-consuming, which highlights its computational demands. Despite this, its capability to adapt to any ML model shows its broad utility. The SHAP framework also includes tailored variants such as TreeSHAP and DeepSHAP, designed specifically for tree-based and deep learning models, respectively. These variants can optimize the efficiency and relevance of SHAP analysis in targeted model types.

Shapley Values. Shapley values originate from coalitional game theory, framing each feature value of an instance as a "player" and the prediction outcome as the "payout." This approach assigns a quantifiable contribution to each feature, which can demonstrate how significantly each one influences the final prediction. Shapley values are distinguished by key principles such as consistency and local accuracy. These principles ensure that the allocation of importance to features is both fair and interpretable, accurately reflecting each feature's contribution to the outcome.

Counterfactual Explanations. Counterfactual explanations provide a compelling approach for local interpretation. This method stands out for its simplicity in implementation, as it does not need access to the underlying data or model. Counterfactual explanations focus on identifying which features would need alteration to achieve a specific desired outcome, thereby elucidating the reasoning behind model predictions. These explanations are particularly user-friendly because they illustrate how minimal changes in features can influence predictions. Nonetheless, one limitation of this method is its difficulty in accommodating categorical data across different levels. Related to the Counterfactual explanation, Molnar [85] discusses their application in models generating continuous predictions that showcase their utility in providing clear and actionable insights.

LENs LENs enhance the interpretability of neural networks by utilizing human-understandable predicates as inputs and translating predictions into First-Order Logic (FOL) explanations. These networks are highly adaptable and can function effectively in both supervised and unsupervised learning contexts. LENs can serve as direct classifiers, providing ex-

planations for their predictions, or they can work alongside black-box classifiers to make their decisions interpretable. The learning process for LENs involves associating specific input features with output classes in supervised scenarios and generating logic rules that explain the conditions for predictions. In unsupervised learning, LENs identify patterns and relationships within the data, clustering similar data points and generating explanations that describe these clusters. Additionally, LENs can mimic the outputs of black-box models while generating FOL explanations, which leads to elucidating the decision-making process for these complex models [28].

3) Visual Explanation: This approach contains methods designed to produce visual representations of models that make them accessible and comprehensible. Techniques such as Individual Conditional Expectation (ICE), Partial Dependence Plot (PDP), and Accumulated Local Effects (ALE) serve as key tools in this visualization process. These techniques facilitate a deeper understanding of how models operate by graphically depicting the relationship between features and the model's predictions. The advantage of visual explanations lies in their ability to convey complex model dynamics in a manner that is easily graspable. This makes visualizing techniques invaluable for broadening the accessibility of model interpretations.

Partial Dependence Plot (PDP). It offers insights into the marginal impact of one or two features on the predicted outcome of an ML model, as highlighted by Molnar [85]. This tool is important in determining whether the relationship between the target and features is linear or exhibits more complexity. For instance, in the context of a linear regression model, PDP can reveal a linear relationship and illustrate how variations in a specific feature correlate with changes in the prediction. Unlike methods that focus on the influence of features on individual predictions, PDP emphasizes the average effect of features on the model's overall behavior. However, its application is generally constrained to analyzing up to two features simultaneously, based on the assumption that the selected features are independent of others not included in the plot.

Individual Conditional Expectation (ICE). Within the post-hoc explainability, visual explanations, particularly those compatible with model-agnostic approaches, are notably rare. The ICE plot, introduced by Goldstein et al. [42], emerges as a visualization technique for delineating the predicted outcomes of models governed by supervised learning algorithms. Diverging from the PDP, the ICE plot underscores the dependency of predictions on a specific feature across individual instances, each represented by a unique line. This approach allows users to understand how changes in a feature impact predictions on a case-by-case basis.

ICE plots especially highlight the variability of predictions within the range of a given covariate, identifying areas of significant heterogeneity. This capability is complemented by a visual test for assessing the model that generated the data alongside a comprehensive suite of tools for exploratory analysis. By employing both simulated examples and real-world data sets, the creators of ICE plots demonstrate their utility in uncovering insights about estimated models that

PDPs may not reveal, offering a more granular perspective on model behavior.

Accumulated Local Effects (ALE). The ALE plot provides a visual illustration of how individual features influence the predictions made by a machine learning model. It effectively showcases the dynamics between regressors (independent variables) and the dependent variable, offering insights into their relationship. Notably, ALE plots are recognized for their efficiency, being faster to generate compared to PDP.

Kramer et al. [58] demonstrated the application of ALE plots within the realm of real estate, employing them to discern which features significantly impact property values. This use case underscores the utility of ALE plots in practical, real-world analysis. Additionally, many researchers have adopted ALE plots as a method for visually exploring the nature of relationships between variables, assessing whether these relationships are linear or exhibit more complexity. This visual representation technique thus serves as a powerful tool for understanding and interpreting the effects of features on model predictions.

D. Model-Specific Techniques for Post-Hoc Explainability

Model-specific methods of post-hoc explainability are designed to be applied exclusively to certain types of models. These techniques can also be categorized based on their scope of interpretability, which includes local, global, and visual dimensions. Local scope refers to methods that focus on explaining the prediction for an individual data point. In contrast, global scope encompasses techniques that interpret the overall behavior of the model. Meanwhile, visual scope techniques are aimed at creating visual representations that make model behaviors comprehensible.

Among the array of model-specific approaches, TreeShap and DeepSHAP are notable for their application to tree-based and deep learning models, respectively. Additionally, saliency maps encompass a variety of methods, such as DeepLift, layerwise relevance propagation, Grad-CAM, and other gradient-based approaches, along with feature relevance explanations.

TreeSHAP and DeepSHAP represent two specialized implementations of SHAP grounded in the principles of Shapley values. TreeSHAP is tailored for tree-based models, offering a more efficient computation of exact SHAP values by operating in polynomial time, in contrast to the exponential time typically required by the general SHAP approach. In an illustrative application, Athanasiou et al. [14] leveraged TreeSHAP within an explainable risk prediction model for cardiovascular disease, utilizing this technique to furnish personalized explanations of the machine learning model's predictions.

Conversely, DeepSHAP is devised to work with neural networks and serves as an approximation method for calculating conditional expectations of SHAP values, utilizing selected background samples for this purpose. It represents an evolution of the DeepLIFT method, adapting it to estimate Shapley values for specific inputs across the feature space. This adaptation enables DeepSHAP to pinpoint the contribution of each feature to a given prediction within neural network models. An

example of DeepSHAP's application can be found in the work by Davagdorj et al. [33], where it was employed within a neural network framework to predict non-communicable diseases. The primary objective of this approach is to elucidate the risk factors influencing the model's predictions, aiming to provide explanations that are both meaningful and accessible to users, focusing on specific instances from the user's perspective.

Feature Relevance Explanations. Feature relevance explanation techniques are important in enhancing the interpretability of tree ensembles. This category contains a variety of techniques aimed at elucidating how different features contribute to a model's predictions, including feature importance, feature extraction, and feature contribution. Central to these techniques is the concept of feature importance, which assesses the significance of feature interactions in influencing the model's outcome. Adebayo and Kagal [3] introduced a methodological approach for quantifying feature importance by iteratively transforming features within the dataset. This process involves eliminating features deemed non-essential, thereby creating a refined dataset that retains only those features with significant relevance.

Subsequently, the authors developed a novel metric to calculate scores for the revised datasets based on the variations observed in model performance. This approach underscores the dynamic nature of feature interactions within predictive models, where the effect of individual features on the prediction cannot simply be aggregated to reflect the total influence.

Further advancing the understanding of feature interactions, Friedman and Popescu [39] introduced the H-statistic. This metric is designed to explain the extent of feature interactions by measuring the variance in predictions attributable to these interactions. The H-statistic thus serves as a valuable tool for detecting and quantifying the strength of interactions among features within a prediction model.

Saliency Maps

They serve as critical tools in attribution analysis by showing the pixels that significantly influence image classification decisions. These gradient-based methods, designed specifically for neural network models, can facilitate an understanding of the features most relevant to a model's output. Among such methods, Layer-wise Relevance Propagation (LRP) and DeepLIFT stand out by providing a framework to assign importance scores to different elements of a network, offering a detailed explanation of a model's decision-making process. Specifically, LRP identifies the contribution of various parts of the input data towards the final decision, a technique effectively employed by Wang et al. [117] for dynamic and explainable malware detection. By pinpointing malicious code snippets, their approach enhances the interpretability of malware classifiers.

Similarly, DeepLIFT, as explored by Shrikumar et al. [107], contrasts the activation of neurons against a reference point, leveraging the differences to ascertain the significance of each feature. This method enriches our understanding of neural network operations by clarifying how each input affects the output.

Moreover, Grad-CAM represents another notable advancement in pixel-attribution methodologies, offering a refined lens through which to view the decision-making processes of CNNs. By attributing a relevance score to each neuron in the final convolutional layer and examining the activated regions within the feature map, Grad-CAM elucidates the features deemed most crucial by the CNN. This process not only aids in interpreting the model's focus but also contributes to the model's transparency.

Integrated Gradients (IG) is another one that calculates the average gradients across a straight-line path between the baseline input and the actual input. This approach, particularly beneficial for CNN predictions, highlights the incremental impact of each feature along this path, thereby offering a comprehensive view of the factors influencing the model's predictions. Collectively, these saliency map methods show the importance of model-specific analyses in enhancing the interpretability and transparency of neural networks.

IV. EXPLAINABLE MALWARE CLASSIFICATION AND DETECTION APPROACHES

The field of malware analysis and detection through the lens of explainable machine learning has not been sufficiently explored in academic and practical research. The preceding section provided an introduction to the concept of explainability in ML, detailed various models and techniques for enhancing explainability, and reviewed relevant research in the broader field of explainable ML. Moving forward, this section will focus specifically on the application of explainable ML in the context of malware classification and detection. It will cover the diverse approaches researchers have developed for detecting and classifying malware, with a special emphasis on explainability. These approaches are organized by the types of target systems, including Windows Portable Executable (PE) files, hardware systems, Android devices, PDF documents, and Linux files. This classification is depicted in Figure 5, which provides a clear framework for understanding how explainable ML techniques are applied across different computing platforms to address malware threats.

A. Windows PE-Based Malware Approaches

Windows PE is a file format based on the Common Object File Format (COFF) specification and holds significant importance within the Windows operating system family. As illustrated in Figure 6, the structure of a PE file starts with a header that was initially used by the MS-DOS operating system. When the executable is loaded, MS-DOS runs a stub program to ensure backward compatibility. Next, the COFF header provides detailed specifications of the executable file. It is followed by an optional header, which adds flexibility and supports future enhancements to the file structure. Following this, the section header divides the executable into distinct sections. These sections are made up of blocks of memory and support page swapping to address memory limitations, which leads to organizing the executable into structured segments for efficient execution. The Windows operating system has emerged as the predominant platform on personal computers, which has increased its vulnerability to malware attacks. Despite this risk, there has been limited research focused on

explainable malware detection methodologies specifically for Windows.

Developing ML-based models that learn discriminative features from raw inputs requires a rigorous process of feature extraction, which is both time-consuming and complex. To address this challenge, Raff et al. [92] introduce "MalConv," a novel architecture for malware detection. This architecture leverages the entire executable as input for a CNN, which could distinguish this research from the limitations discussed in other studies surveyed. The MalConv architecture, illustrated in Figure 7, utilizes a methodology similar to those employed in speech and signal processing [43], text understanding [128], and image classification [111], where CNNs effectively extract pertinent features.

MalConv is designed as a static architecture for the identification of static malware, which combines CNN activation functions with global max-pooling before progressing to fully connected layers. This approach guarantees that the ML model generates activations independent of the features' spatial locations, which leads to enhancing its ability to classify and detect malware. The discussion surrounding Windows PE malware detection includes techniques that are gradient-based, modelagnostic, and reliant on image representations. The forthcoming section will discuss an analysis of existing strategies for malware classification and detection, with Table I specifically addressing the application of model-agnostic, gradient-based, and image-based methodologies in the context of Windows PE-based malware research.

1) Gradient-Based Approach: The gradient-based methodology measures the impact of input features on predictions by assigning weights to different parts of an executable. To elucidate the decision-making processes of Deep Neural Networks (DNNs), Bose et al. [19] examine the MalConv architecture using the open-source 'emberMalCony' framework. This study seeks to understand how the architecture distinguishes between malicious and benign executables based on their raw data. Ember, which is a tool utilized for training static PE malware models within the ML domain, highlights the MalConv architecture's unique ability to attribute significant weight to specific executable parts, thereby having a significant influence on the classification results. Their research introduces a sophisticated framework based on gradient analysis, which maps gradient embeddings from malicious files and interpolates between accurately classified instances to define a clear decision boundary between categories. By analyzing the interpolation among samples, the study explores filter activations to investigate if there is a connection between different filter pairs. This leads to the development of a correlation heatmap for the filters, providing insights into how they interact. Remarkably, one filter specializes in identifying malicious traits within a file, and another filter focuses on generalizing these findings across various samples. The proposed framework transcends the MalConv model, offering a general method suitable for classification tasks in any neural network.

2) Model-Agnostic-Based Approach: The Model-Agnostic approach employs post-hoc explainability techniques that can be applied across any opaque or black-box model. This method clarifies the predictions by simplifying the complex original

TABLE I: Research Addressing Explainable Machine Learning in Windows Malware

Paper/Year	Focus/Objective	Contribution	Limitation	XAI Technique
Bose et al. 2020 [19]	Analyzed the MalConv ar- chitecture and introduced a framework for analyzing mal- ware detection networks end- to-end	Their contribution involves gradient analysis representing the gradient embeddings of malicious files and interpolating between correctly classified samples to form a decision boundary between two classes to address the network's decision in a better way	Requires better interpreta- tion of Neural Network re- sults	Gradient Analysis
Mathews 2019 [77]	Identify potential vulnerabili- ties and flaws in feature engi- neering, which highlights the global characteristics in order to differentiate between two malware classes	 Introduced the explainability framework to classify the malware on windows PC Computed set of content-based features Proposed extraction of statistical features which reflects PE files Used LIME framework to explain window PC malware classification 	Required analysis and comparison of different model-agnostic explainable approaches	LIME
Pirch et al. 2021 [90]	Aims to provide an explainable CNN model that will predict tags for malware to be used for grouping and organizing the malware samples	 Each feature, also called a 'token,' is assigned a relevance score which is used to determine how each of the tokens affected the tag that the model predicted Used two measurements to determine the quality of the explanation, descriptive accuracy, and descriptive sparsity 	Limited to behavioral-based approach	LRP
Marais et al. 2021 [76]	Their main focus is to interpret the models to reduce the False Positive (FP) rates	 Proposed malware detection model and their results are compared with LGBM, XGBoost, and DNN Employed the GradCam++ explainability approach on the CNN model to identify the important pixel that has the most influence on the CNN model's prediction. Malware experts can use this tool to determine the nature of a suspicious file 	Lacks the attention mechanisms Limited to static-based approach, computational time need to be considered	GradCam++
Li et al. 2021 [63]	Aims to provide an inter- pretable feed-forward neural network o interpret non-linear models	They developed IFFNN with high accuracy and interpretability to detect malware Used MNIST dataset for qualitative interpretation of IFFNN	The interpretation's fidelity needs further evaluation and validation	IFFNN
Chen et al. 2019 [24]	Validate fidelity of explana- tions for dynamic malware analysis	 Validated the fidelity of interpretation by extending LIME to dynamic image-based malware classification. Developed two case studies to understand the advantages of vision-based interpretation frameworks. 	Missing explanation on the effectiveness of LIME for interpretation due to the fact that there are already better techniques	LIME
Lin and Chang 2021 [67]	Aims to implement an inter- pretable ensemble model for detecting image-based mal- ware	They designed a deep ensembled detector and deep taylor decomposition approach and interpreted the prediction results of the detector using LIME, SHAP and LRP explainability techniques.	Required evaluation of more base classifiers to improve the detection accuracy Datasets containing the original malware files are not used to locate the semantic features	LIME, SHAP, and LRP
Alani et al. 2023 [5]	The paper focuses on detecting obfuscated malware on Windows systems using features extracted from memory dumps	 Introduces an ML-based system for detecting obfuscated Windows malware that achieves a detection accuracy of over 99% using only five features extracted from memory dumps. Provides detailed model explainability using SHAP, which enhances the transparency and trustworthiness of the system. 	The model relies on a limited set of features extracted from memory dumps. If malware evolves to avoid or alter these specific features, the model's effectiveness may decrease. The high accuracy reported is based on the specific dataset used in the experiments (MalMem2022). The performance might vary with different datasets.	SHAP

TABLE I: Research Addressing Explainable Machine Learning in Windows Malware (Continued).

Paper/Year	Focus/Objective	Contribution	Limitation	XAI technique
Ciaramella et al. 2024 [27]	The paper proposes a DL-based model for detecting ransomware	 The paper introduces a DL approach that converts executable files into images and applies CNNs for ransomware detection. The model incorporates Grad-CAM to highlight the regions of the input images responsible for the model's predictions, thereby improving the interpretability and explainability of the detection results. 	The focus is primarily on ransomware detection, and the model's applicability to other forms of malware is not discussed.	Grad-CAM
Anthony et al. 2024 [9]	Develop an interpretable and robust ML model for malware detection using LENs	 The paper extends the application of LENs to the domain of malware detection using the large-scale EMBER dataset. It introduces a customized version of LENs that enhances the fidelity of logic explanations, which makes them more aligned with the model's predictions. 	The process of generating FOL rules and optimizing these explanations requires considerable computational resources. This high computational cost can limit the scalability of LENs, making them less practical for real-time application.	LENs
Gulmez et al. 2024 [44]	This study aims to develop an explainable DL-based system named XRan that detects ransomware using dynamic analysis.	 XRan enriches the feature space by integrating API call sequences, DLL sequences, and Mutex sequences. Utilizes XAI to provide local and global explanations, improving the interpretability of the model. 	• The dynamic analysis phase of XRan is resource-intensive and time-consuming compared to static analysis. This limitation is inherent to all dynamic analysis-based techniques, but it particularly affects XRan due to its comprehensive feature extraction process that includes API calls, DLL sequences, and Mutex sequences.	LIME, and SHAP
Aryal et al. 2024 [12]	It aims to improve the success of adversarial evasion attacks on malware detectors by using XAI techniques to identify and target critical regions of Windows PE malware files for perturbation.	 Utilizes SHAP values to identify optimal regions in Windows PE malware for effective adversarial perturbation. Demonstrates improved evasion rates of malware detectors using SHAP-guided perturbations. 	This paper focuses on the effectiveness of SHAP-guided adversarial perturbations without fully exploring how these perturbations might perform across different types of Windows PE malware, such as trojans, ransomware, worms, and others.	SHAP
Ghadekar et al. 2024 [12]	It aims to develop an advanced DL approach for multiclass malware detection with the goal of enhancing feature extraction capabilities and integrating XAI principles.	The paper introduces a modified GNN (deeperGCN) that significantly improves malware detection accuracy. It Integrates XAI using GradCAM to provide transparent and interpretable insights into the model's decision-making process.	The process of converting byte and ASM files into images requires significant preprocessing steps, including feature extraction and transformation into graphical representations. This preprocessing is complex and time-consuming, potentially limiting the model's applicability in environments where rapid detection is important.	GradCAM

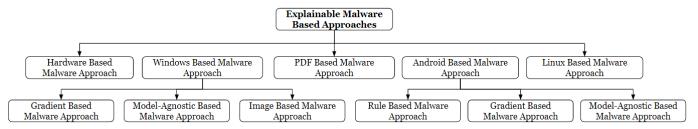


Fig. 5: Explainable Malware Classification and Detection Approaches [125].

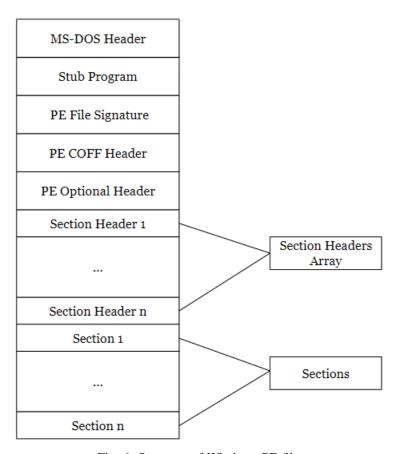


Fig. 6: Structure of Windows PE file.

model into a more understandable local surrogate model. The research presented by Mathews [77] introduces an explainability framework aimed at classifying two distinct malware families on Windows PCs. Firstly, the researchers calculate content-based features and extract statistical features derived from Hex and assembly views. These features are indicative of the PE file's structure.

Their investigation shows shortcomings in the feature selection process and emphasizes the global characteristics through which a model learns to distinguish between the two malware categories. To elucidate the outcomes produced by the deep learning model, they utilize the LIME explainability framework.

Figure 8 presents an integrated model for dynamic malware detection based on the principles of explainable ML, combining dynamic analysis with the training of a surrogate learning model using malware tags. This model leverages explainable

ML techniques to clarify the surrogate model's predictions and behavioral patterns, aiming to enhance understanding of its decision-making process. Another research [90] seeks to develop a CNN model that accurately predicts malware tags, which are essential for categorizing and organizing malware samples and makes the prediction process transparent. This endeavor involves a thorough dynamic analysis that examines malware tags to inform the training of the surrogate learning model. The study progresses by applying explainable machine learning to demystify how the CNN model arrives at its predictions. Each detected feature, referred to as a 'token' in the research, receives a relevance score that indicates its impact on the predicted malware tag. To assess the quality of these explanations, the authors employ two measures: descriptive accuracy, which evaluates the precision with which an explanation captures the influential features of a prediction,

and descriptive sparsity, which identifies the superfluous features within these explanations. The model's effectiveness is validated through its performance in classifying three types of tags—sandbox, family, and clustering—with each category achieving an accuracy rate of over 90%. In a study, Alani et al. [5] present an ML-based system designed to detect obfuscated malware on Windows platforms with high accuracy and efficiency. The system utilizes a variety of classifiers, including random forest (RF), logistic regression (LR), decision tree (DT), Gaussian Naive Bayes (GNB), and extreme gradient boosting (XGB). Through an evaluation process, XGB was identified as the best-performing classifier. Moreover, The system relies on features extracted from memory dumps using the VolMemLyzer tool. The feature selection algorithm, i.e., Recursive Feature Elimination (RFE), identifies the five most effective features, resulting in a streamlined model that maintains an accuracy rate exceeding 99%. The selected features include the total number of services, average number of dynamic-link libraries (DLLs) per process, total number of mutant handles, number of kernel drivers, and shared process services. The system's detection capabilities are bolstered by its explainability, achieved through SHAP. SHAP values provide insight into the impact of each feature on the model's predictions. The evaluation of the system demonstrates its high accuracy and rapid detection speed, with a processing time of 0.413 microseconds per instance. Despite its robustness, the paper has some potential limitations, such as the model's dependence on specific features and vulnerability to adversarial attacks.

Anthony et al. [9] focus on enhancing malware detection through the integration of XAI. The primary goal is to address the limitations of traditional ML models, particularly their lack of interpretability. The proposed solution leverages LENs, which offer a balance between accuracy and explainability. LENs provide explanations in the form of First-Order Logic (FOL) rules, making their decision-making processes more transparent and understandable for human analysts. The methodology involves extending the application of LENs to the EMBER dataset. Additionally, they introduce a tailored version of LENs to enhance the fidelity of logic explanations. The experimental results demonstrated that LENs achieve robust performance, rivaling traditional black-box models while significantly outperforming other interpretable methods. The tailored LENs provide high-fidelity explanations with low complexity that can ensure they are both accurate and comprehensible.

Gulmez et al. [44] present an approach to ransomware detection by integrating multiple dynamic analysis features with DL and XAI techniques. They developed XRan, which is a system that combines API call sequences, DLL sequences, and mutual exclusion (Mutex) sequences to provide a comprehensive view of executable behaviors. These features are extracted through dynamic analysis, where executables are run in a controlled environment to observe their actions. XRan leverages a two-layer CNN to process these combined sequences, which enables precise detection of ransomware. To address the challenge of model interpretability, the authors integrated two XAI models, i.e., LIME and SHAP.

The study utilized five datasets: RD1 from VirusShare with 6,263 ransomware samples, RD2 from Sorel-20M with 7,703 ransomware samples, RD3 from ISOT with 668 ransomware samples, MD from VX Heaven with 6,263 malware samples, and BD from various sources including Windows System Files and Download.com with 14,797 benign samples. Dynamic analysis was conducted using Cuckoo Sandbox to extract features, which were then combined into sequences for the CNN model. Performance metrics included accuracy, TPR, FPR, and F-score, with XRan showing superior results compared to baseline and state-of-the-art methods. The experimental results demonstrate XRan's effectiveness, achieving up to a 99.4% True Positive Rate (TPR) and outperforming existing state-of-the-art methods.

Aryal et al. [12] aims to enhance the effectiveness of adversarial evasion attacks on malware detectors. They focus on Windows PE malware and utilize SHAP values to identify the most critical regions of malware files that influence detection decisions by a CNN-based malware detector, MalConv. The rationale behind this approach is that by understanding which parts of the malware file have the greatest impact on the detector's decision, they can strategically place perturbations in these regions to evade detection more effectively.

To achieve this, they calculate the SHAP values for each byte in the malware files using the DeepExplainer module, which is adapted to work with the embedding layer in Mal-Conv. These SHAP values reveal the contribution of each byte to the malware detector's decision, which facilitates the mapping of these values to different regions of the PE file structure. Aggregating these values will help identify the regions with the highest impact. Using this information, they inject adversarial perturbations into these targeted regions, both at a high level (across entire sections) and at a more granular level (within subsections of larger sections). The results, based on a dataset of 6000 Windows PE malware samples, demonstrate that perturbations guided by SHAP values significantly improve the success rate of evasion attacks compared to random perturbations. Specifically, they observe high evasion rates when perturbations are injected in regions with high SHAP values, which demonstrates the efficacy of their explainabilityguided approach in crafting adversarial samples that maintain the malware's functionality while evading detection.

3) Image-Based Approach: Recent advancements in CNNs showcase their remarkable capability in detecting malware binaries through image classification techniques. The work presented by Marais et al. [76] introduces detection models that effectively convert binary files into grayscale images. Utilizing the Ember dataset, which is formatted in Windows PE, the authors proceed with feature extraction from these grayscale images. Subsequently, they propose a CNN model that leverages these images for malware detection. Additionally, they implement a novel approach, termed the HIT method, to train another CNN model on RGB images. A significant contribution of their research is the application of the GradCam++ explainability technique on the CNN model. This technique identifies the most influential pixels affecting the model's prediction, aiming to diminish the false positive rate of detecting malicious files.

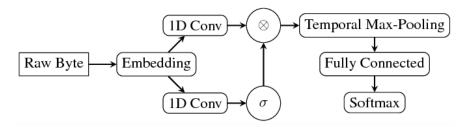


Fig. 7: MalConv architecture [92].

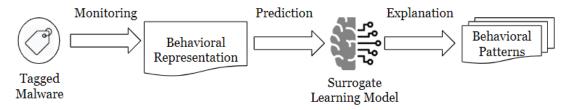


Fig. 8: Explainable malware method for Tagvetting.

Contrastingly, while non-linear ML models are known for their superior accuracy and classification performance over linear counterparts, their complexity often renders them difficult to interpret. Addressing this challenge, Li et al. [63] have developed an IFFNN. This model can achieve high accuracy in malware detection and ensures interpretability. They conduct their experiments on a Windows server to determine the IFFNN's capability to handle multi-class classification problems. Moreover, to assess the effectiveness and interpretability of the IFFNN, they use the MNIST dataset for image classification and convolutional layers for a comprehensive qualitative evaluation of the model's interpretability.

In another work, Chen et al. [24] aim to enhance the interpretability of image-based dynamic malware classification by extending the LIME framework. They start by training deep learning models on images and then apply an explanatory approach to understanding the decision-making process of these models. The objective is to determine whether the insights derived from the algorithm align with expert knowledge in the cybersecurity domain.

Lin and Chang [67] engage with an image-based malware dataset to explore the potential of ensemble learning. They introduce a Selective Deep Ensemble Learning (SDEL)based detector that is coupled with an innovative Interpretable Ensemble Learning approach. This detector is specifically designed for Malware Detection (IEMD). The IEMD strategy is developed to elucidate the predictive decisions made by the SDEL detector and advance the interpretability of the model. This endeavor is supported by the deployment of explainable AI techniques such as LIME, SHAP, and Layer-wise Relevance Propagation (LRP). These methods are analyzed and compared to understand their efficacy in providing transparent explanations. Their research results have impressive outcomes, achieving an accuracy rate of approximately 99.87%. Furthermore, the study shows the superiority of their explanations in the context of image-based malware classification compared to preceding research.

The paper by Ciaramella et al. [27] develops an approach to ransomware detection by converting Windows PE files into RGB images and analyzing them using DL-based models. The researchers developed a script to transform the binary code of executable applications into images, which are then used as input for various CNNs such as LeNet, AlexNet, Standard-CNN, and VGG-16. The goal is to classify the files into ransomware, generic malware, or legitimate software. The Grad-CAM technique is employed to enhance the interpretability of the model's predictions. Grad-CAM generates visual explanations by highlighting regions of the images that most influence the model's decisions. The results demonstrate the effectiveness of the proposed method, achieving high accuracy, precision, and recall, particularly with the VGG-16 model, which outperformed others with an accuracy of 96.9%.

Ghadekar et al. [41] implement a methodology for detecting various types of malware by leveraging a modified GNN architecture called deeperGCN, along with XAI techniques. The research combines byte and ASM (assembly) files, converting them into images to better capture intricate malware behaviors. This conversion process involves the extraction of features such as byte bigrams, opcode sequences, and the generation of pixel representations of the files. These images are processed using the deeperGCN model, which enhances the feature extraction capabilities by leveraging the inherent relationships in the graph-structured data. The model includes several advanced techniques, such as skip connections to address vanishing gradient problems and a graph readout pooling layer to effectively aggregate information across nodes.

The results demonstrate that this innovative approach achieves a high detection accuracy of up to 97%. In addition, the integration of GradCAM provides transparency into the model's decision-making process by generating heatmaps that highlight the important regions of the input data influencing the predictions.

B. Android-Based Malware Approaches

The rapid advancement of technology has also led to an increase in malware attacks, with the Android platform emerging as a particularly significant target. In response to this escalating threat, various security measures have been implemented within the Android ecosystem. Among these, ML-based methods have proven to be highly effective in detecting Android malware, which led to extensive research in this domain [98] [123] [34] [126]. Specifically, recent developments in DNNs have improved detection rates and reduced the reliance on manual feature engineering.

A standout innovation in this field is the DREBIN malware detection system [10], illustrated in Figure 9. DREBIN leverages a lightweight approach to identify Android malware on smartphones through static analysis, extracting application features that are represented in a binary vector format. This setup enables linear classification to differentiate between features of benign and malicious applications. Furthermore, DREBIN is distinguished by its explainable approach to malware detection. It provides insights into the reasoning behind its decisions by highlighting key attributes of detected malware.

The dataset used by DREBIN includes 5,560 malware samples and 123,453 benign samples that demonstrate the comprehensive nature of its analysis. DREBIN has outperformed other ML-based approaches by achieving high accuracy. This success has attracted significant attention in the academic world and has prompted many researchers to leverage DREBIN in their studies on explainable Android malware detection. This has made a substantial contribution to the enhancements of mobile security.

To analyze the Android malware, the research by Kumar et al. [60] introduces two ML-supported methodologies: one focuses on static analysis and the other on feature extraction. They perform feature extraction on the DREBIN dataset through vectorization, followed by feature selection and dimensionality reduction, thus transforming high-dimensional data into a more manageable low-dimensional format while omitting extraneous features. Their analysis yields metrics such as the True Positive Rate (TPR) and False Positive Rate (FPR), with their methodology demonstrating high precision and recall. Various ML-based algorithms, including SVM, KNN, Naive Bayes, and C4.5, are applied to the newly processed data, which is revealed SVM's superior performance. The combination of static analysis, feature vectorization, and supervised learning enables these ML algorithms to identify new malware families with high true positive and recall rates. The subsequent subsection explores explainable analysis techniques for Android malware.

1) Gradient-Based Approach: Gradient-based methods are crafted to classify and detect malware through the lens of ML. These strategies reveal the underlying architecture of a specific ML model and enhance the interpretability of predictions made by deep learning-based malware detection systems. This approach calculates and allocates the predictive weights relative to input features across different segments of the executable file. To discover the mechanism behind black-

box Android malware detection systems and determine the most significant features influencing each decision, Melis et al. [80] introduce a comprehensive explainable ML framework. This framework uses a gradient-based technique to determine whether a sample is correctly classified as malware, leveraging its most critical local features. Their research utilizes the DREBIN Android malware detection tool for practical testing. The main objective of this endeavor is to enhance the accuracy of predictions while maintaining the transparency and interpretability of the decision-making process. By utilizing the DREBIN malware detection tool and dataset, the authors propose a novel methodology that highlights both local and global characteristics to distinguish and clarify the discernment between benign and malicious applications.

The authors, Iadarola et al. [49], introduce a gradient-based deep learning methodology designed to clarify the methodology behind malware family classification. This approach begins by extracting code from Android application package (.apk) samples and subsequently transforming it into an image format. Following this transformation, a CNN model classifies these images into their respective malware families. They implement the Gradient-weighted Class Activation Mapping (Grad-CAM) technique to facilitate the prediction of classes by identifying critical areas within the images. A thorough code analysis is conducted to demonstrate the efficacy of their method in extracting relevant classes. In another work, Scalas [101] develops a gradient-based strategy specifically designed for detecting Android ransomware. This study shows the selection of system API calls as key features, asserting their utility in evading detection strategies employed by attackers.

Further study by Melis et al. [81] explores the effectiveness of gradient-based attribution techniques in identifying key features crucial for understanding a classifier's decision-making process. Their work seeks to establish the importance of these features in developing more robust algorithms. They analyze the correlation between explanatory methods and adversarial resilience, probing how these aspects are interconnected. Moreover, Iadarola et al. [50] put forward an explainable deep-learning framework designed for mobile malware detection. This approach transforms applications into images that feed into an explainable deep-learning model that is capable of recognizing Android malware and classifying its family. Utilizing the Grad-CAM explainability method, they demonstrate the selection of explanatory techniques that improve classification performance. To enhance interpretability, they generate heatmaps that offer visual insights into the model's reasoning, making the predictions' rationale more accessible. Additionally, because the process of analyzing these heatmaps is automated, it simplifies the architecture's debugging for analysts without necessitating a background in the system's design. besides enhancing transparency in their model, they record a notable increase in accuracy.

Naeem et al. [86] expand the application of gradient-based methods by introducing a transfer learning approach for classifying IoT malware, leveraging the Inception-v3 architecture, a pre-trained network designed to process malware images and extract pivotal features. These features are then fed into a classification algorithm and evaluated across various ML clas-

TABLE II: Research Addressing Explainable Machine Learning in Android Malware

Paper/Year	Focus/Objective	Contribution	Limitation	XAI Technique
Kumar et al. 2018 [60]	Convert high-dimensional data into low-dimensional data, which reduces the dimension and avoids extracting unnecessary features	Introduced Static analysis and Feature vectorization methodologies for the analysis of Android malware	Limited to smaller labeled datasets Refined to only static approach, should use hybrid and online approaches to examine the dynamic features and source code in run-time	Feature Extraction
Melis et al. 2018 [80]	Emphasizes the global characteristics learned by the model to distinguish between malicious and benign apps	 Provided general approach to explain the black-box Android malware detection Used gradient-based approach to identify whether a sample is correctly identified as malware or not by its most influential local features Provided interpretable decisions Approach to nonlinear model for Android malware 	No explanation for how various surrogate models affect the provided explanations.	Global Surrogate
Iadarola et al. 2021 [49]	Effectiveness of malware class extraction through deep learning approach	 Proposed a deep learning model for malware family identification Used Grad-CAM technique to predict the classes by detecting the important regions in the image 	Approach is vulnerable to Obfuscation techniques	Grad-CAM
Kinkead et al. 2021 [56]	Compare and analyze the similarities of the opcode sequence location, which is assumed malicious by CNN, to that of LIME	Proposed a CNN-based novel method to identify the opcode sequence locations that are assumed to be malicious Their model achieved high accuracy, which states that CNN accomplishes exceptional performance with the DREBIN data set	Lacking explanation in Filter activations	LIME
Lu and Thing 2021 [71]	To detect Android malware, the authors focused on the fea- tures attribution problem	Optimization of features attribution by minimizing the variance of prediction scores and assigning high attribution values They made use of LIME and SHAP to compare the explanation ability of MPT explainer	Mitigated methods for attack are not presented Limited to only one specific attack	Modern Portfolio Theory (MPT)
Korine and Hendler 2021 [57]	Explainable Model agnostic malware classification, which is both dataset and platform agnostic	 Presented effective and explainable malware classifier DAEMON Used Layer-wise Propagation explainable technique to explain the model DAEMON achieved high classification accuracy, and classification results are explainable 	Lack of evaluation of the ability of DAEMON classi- fier in order to classify the benign executables	Feature Importance
Scalas 2021 [101]	Identifying and characterizing effective Android ransomware detection	 Identifying traits that result in characterizing effective ransomware detection To assess the validity of features, explainability techniques are used to propose methods This work explored the relationship between explainable ML and adversarial attacks 	Missing explanation regard- ing usage of attribution technique	Integrated Gradient
Yan et al. 2021 [125]	Developing a novel method to extract rules from DNN rule extraction and facilitates its ex- plainability	 Proposed a novel method for extracting rules from DNN, which ensures high accuracy Used extracted rules to identify malicious network traffic To detect mobile malware in an increased network environment, this work proposed an online detection system 	No proper explanation on the mentioned online detec- tion system	Rule-Based Learner
Wang et al. 2016 [118]	This work focused on effectively using network traffic in the detection of mobile malware and explained the detection result using explainable machine learning techniques	Proposed TrafficAV to detect malware traffic Extracted the features and combined them with a machine learning detection algorithm to detect the malicious application	Limited to smaller malware samples Limited analysis of detection models	Feature Extraction
Iadarola et al. 2021 [50]	This work focused on The development of an explainable deep learning algorithm for mobile malware classification and detection	Used the Grad-CAM explainability approach to describe mobile analysis in terms of images Localized the prominent portion of the image beneficial to the model in order to generate a specific accuracy	Biased while labeling the data samples	Grad-CAM

TABLE II: Research Addressing Explainable Machine Learning in Android Malware (Continued).

Paper/Year	Focus/Objective	Contribution	Limitation	XAI technique
Wu et al. 2021 [122]	This work focused on the classification of malware and interpreting the classification results of Android malware	 Proposed a novel interpretable approach (XMAL) by coupling it with an MPT explainer For interpreting with high fidelity, they generated the malware feature descriptions Conducted an online survey and qualitative analysis and provided a comparison of state-of-art approaches 	XMAL lacks the multi- attention mechanism Features are not sufficient enough to interpret the ma- licious behaviors	XMAL, LIME
Alenezi and Ludwig 2021 [6]	This work aims to use SHAP to explain the cybersecurity threats to data	ML models such as Random Forest, XG-Boost, and sequential model and applied SHAP explainability technique to explain it further They showed that XGBoost outperformed the other models by correctly classifying the highest no. of samples	Missing proof that other ML models may/may not gain superior performance	SHAP
Ullah et al. 2022 [115]	This work aims to utilize SHAP to explain the important features for transfer learning and graphical malware features to detect malware	 Proposed android malware detection system with BERT-based transfer learning Utilized various ensembled machine-learning algorithms for malware classification and detection Utilized SHAP to explain the most important features that are responsible for the model's outcome 	Missing results of Local Interpretable Modelagnostic Explanation (LIME) method SHAP explanations are limited to local scope	SHAP
Naeem et al. 2022 [86]	This work aims to provide explainable malware detec- tion using image visualization and fine-tune the CNN-based transfer learning model	Proposed fine-tuning CNN-based model for IoT device malware classification Utilized various machine-learning algorithms to test the effectiveness of IoT device malware classification Grad-CAM was utilized to develop heatmaps to assist security analysts in better understanding the classifier selection	There is some reliability. However, thorough validation is lacking. Furthermore, it remains to be seen whether their framework can be used for large malware variants	Grad-CAM
Alani and Awad. 2022 [4]	This work aims to propose an explainable and accurate framework for identifying An- droid malware	 Performed feature selection for selecting the crucial features that can provide high accuracy Explaining the importance of selected features using the SHAP explainability technique Performing feature reduction and creating a reduced dataset with 35 effective features that can be used for Android malware detection 	SHAP explainability is re- stricted to only global scope	SHAP
Liu et al. 2022 [70]	Investigating the performance of ML models under realistic and unrealistic experimental setups	Identifying the temporal inconsistency problem in Android malware detection Leveraging XAI to realize the reason behind the high performance of ML-based detection techniques	The XAI techniques focus on interpretability from a feature-importance perspective that may not fully capture the complexity of model decisions, especially in DL-based models where interactions between features can be non-linear and more opaque.	XMAL, DREBIN, and Model- Agnostic Techniques
Ambekar et al. 2024 [8]	The paper focuses on enhancing Android malware classification by integrating attention mechanisms with LSTMs and explainable AI techniques to improve accuracy and interpretability.	 The paper introduces a novel and interpretable framework called TabLSTMNet that utilizes recent datasets to classify Android malware permissions. It employs XAI methodologies to elucidate the contributions of the features and enhance the transparency and effectiveness of the TabLSTMNet framework. 	The use of RandomOver-Sampler to address class imbalance by replicating instances of the minority class increases the likelihood of overfitting. The integration of TabNet and LSTM models, along with the XAI techniques, increases the computational complexity.	LIME, and SHAP
Soi et al. 2024 [109]	It enhances the explainability of Android malware detection systems by utilizing static analysis of function calls within the APK files.	 The paper introduces a new approach by selecting and analyzing API calls from the Function Call Graph (FCG) of Android applications. The paper employs SHAP values to provide clear, model-agnostic explanations for the classifier's decisions. 	The large feature set (API calls) used for classification and explainability might pose challenges in terms of processing and interpretation.	SHAP

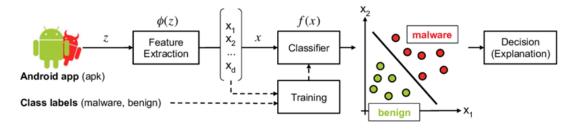


Fig. 9: Schematic Representation of DREBIN malware detector [80].

sifiers to assess performance. The Grad-CAM explainability method is utilized to highlight the critical areas within the images. Furthermore, the study utilizes t-distributed stochastic neighbor embedding (t-SNE) to verify the comprehensiveness of the feature set within the proposed CNN models. This ensures that they encapsulate sufficient information for effective malware classification.

2) Model-Agnostic Based Approach: The challenge of explaining the vast range of models in deep learning research is increasing. In this context, model-agnostic approaches provide explanations after the decision-making process, which are applicable to various opaque models. The study by Kinkead et al. [56] presents a novel CNN-based method focused on identifying specific parts of opcode sequences suspected of containing malicious elements. Their main objective is to examine and compare the similarities between the locations of malicious opcode sequences identified by the CNN and those marked as important by LIME. They carry out their research using the DREBIN dataset, known for its collection of 5,560 malicious apps across different malware families, serving as a standard for Android malware detection. Their results show that the model achieves an accuracy of about 0.98, highlighting CNN's exceptional performance with the DREBIN dataset. Further analysis of how both CNN and LIME highlight locations across all the samples in each malware family reveals a significant finding that CNN tends to focus on the same areas as LIME, indicating CNN's targeted effort in detecting malware.

In another effort to improve Android malware detection, researchers Lu and Thing [71] utilize a model-agnostic explainable AI framework focused on feature attribution, highlighting the importance of feature manipulation and optimization. Their approach integrates a trained model with a Modern Portfolio Theory (MPT) explainer during the explanation phase. Quantitative analysis of their method shows greater sensitivity in detecting important data features compared to the results from machine learning-based Android malware detection tools. Additionally, they use both LIME and SHAP to evaluate the effectiveness of the MPT explainer, seeking to confirm its superior capability in identifying key features essential for malware detection.

On the other hand, rapidly mutating malware variants necessitate sophisticated classification methods to categorize these variants accurately. Although variants within the same malware family often exhibit identical behavioral patterns, the increasing number of variants complicates the process of

accurately classifying new ones. This challenge has motivated researchers to develop advanced detection tools aimed at enhancing the accuracy of malware classification. One notable contribution in this field is DAEMON, a data-agnostic malware classification tool developed by Korine and Hendler [57]. DAEMON stands out for its ability to discern the unique features of various malware families, which lends clarity and explainability to the classification process. The researchers behind DAEMON have collected extensive datasets, which they have analyzed on both Windows and Android platforms, utilizing the renowned DREBIN dataset for the latter. Their efforts have culminated in DAEMON achieving remarkable accuracy in malware classification.

Based on a model-agnostic approach, the study [115] introduces a novel, hybrid methodology for crafting an explainable malware detection system that leverages both textual and visual representations of malware attributes. Initially, they develop a pre-trained model known as Bidirectional Encoder Representations from Transformers (BERT), specifically customized to learn textual features derived from network traffic. Following this, they suggest an algorithm capable of transforming malware into a visual format. Subsequently, a CNN model is implemented to utilize deep extraction of features. Once these balanced features are obtained, they are fed into a suite of ensemble models, including SVM, DT, LR, and RF, to facilitate the system's classification and detection capabilities. Furthermore, the researchers utilize SHAP, a model-agnostic technique for explainability, to elucidate the critical features in interpreting the model's decisions.

In the study Alani et al. [4], the researchers introduce an Android malware detection system named PAIRED. This system is distinguished by its lightweight design and high precision, achieving a significant reduction in feature count—from 214 to 35, amounting to an approximate 84% decrease. The SHAP explainability technique is utilized to elucidate the overarching influence of the features, identifying which among them have a greater impact on the predicted outcomes. Impressively, PAIRED manages to sustain a remarkable accuracy rate of 97.98%.

Ambekar et al. [8] introduce the TabLSTMNet, an approach to Android malware classification that combines the strengths of the TabNet architecture, which was developed by researchers at Google Cloud and LSTM models, complemented by XAI techniques. This model integrates TabNet's attention-mechanism feature selection, which efficiently identifies critical features, with LSTM's dynamic processing capabilities for

sequential data. This integration allows for a detailed analysis of Android permissions and API calls to distinguish between benign and malicious applications effectively. The proposed model is evaluated on two different datasets and achieves classification accuracies, demonstrating 97.10% on the NATI-CUSdroid dataset and 98.00% on the TUNADROMD dataset. Moreover, the incorporation of explainable AI methods such as LIME and SHAP significantly increases the transparency of the model's decision-making process.

Soi et al. [109] propose a novel methodology for improving the explainability of Android malware detection systems. The approach begins with a static analysis of Android application packages (APKs) to extract a Function Call Graph (FCG). This graph represents all the API calls within the application's code. Based on FCG, a set of critical API calls can be selected, which are strongly correlated with the application's behavior, to serve as features for their model. After that, the selected features are embedded using Natural Language Processing (NLP) techniques, such as TF-IDF and Word2Vec, to produce a consistent input format for a CNN. To enhance the interpretability of the model's decisions, the paper employs SHAP values, which provide a clear and detailed explanation of how each API call contributes to the classification outcome.

The results of the experiments conducted on a dataset of over 40,000 Android applications show that the proposed method achieves a classification accuracy comparable to state-of-the-art models. The paper also conducts extensive evaluations to address potential issues such as temporal bias and concept drift. It highlights that while the approach maintains strong performance over time, the inclusion of more recent data can be important for sustaining its accuracy.

3) Rule-Based Approach: Yan et al. [125] present an innovative approach for extracting rules from DNNs, aiming to balance the accuracy intrinsic to DNNs with the need for explainability in their operation. This methodology is visually summarized in Figure 10, which illustrates the comprehensive process of rule extraction and detection within a DNN framework. The initial phase contains the collection of network traffic data, utilizing a tool named DroidCollector for this purpose. Subsequent to data collection, feature extraction is conducted to distill the essential information necessary for training the model. This algorithm begins by verifying the appropriateness of the neural network settings, such as its suitability for classification tasks. In instances where the predicted label aligns with the true label, the model's performance is deemed satisfactory. However, misclassification triggers a reassessment and update of the neural network's weights. The backpropagation process prioritizes the weights of the outermost layer before sequentially addressing each subsequent layer, effectively distributing the errors from each output variable across the network's hidden layers. Through numerous iterations, the model iteratively refines itself until it achieves optimal performance, at which point rules are extracted from the DNN.

Employing these extracted rules, the authors devise a mechanism to detect malicious network activity. They conduct an evaluation of their DNN rule extraction technique against three contemporary technologies—MultiView, CNN,

TrafficAV—and four ML-based algorithms, namely Bagging, Adaboost, KNN, and Random Forest. The findings from this comparison suggested the superiority of their proposed method, which excelled in numerical prediction accuracy and outperformed the benchmarked methods. Hence, the authors propose an online detection system that is optimized for high-speed network environments and leverages FPGA technology to facilitate the real-time detection of mobile malware.

Also, as ML has emerged as a powerful tool for uncovering rules crucial for predictive data analysis, in their work, Wang et al. [118] develop TrafficAV an efficient and intelligible method for classifying mobile malware based on network traffic patterns. This approach is designed to minimize resource usage and performs malware detection and network traffic analysis server-side. TrafficAV leverages feature extraction combined with the C4.5 DT algorithm to detect the presence of malicious applications, applying two distinct detection models for HTTP and TCP protocols. This dual-model strategy has yielded high accuracy rates. Furthermore, TrafficAV provides an analysis of the significance of each feature in the decision-making process, offering user-friendly explanations of its findings.

Similarly, another study [122] works on the framework named XMAL—an interpretable machine learning-based framework—proposes a rule-based methodology for accurately classifying Android malware. This system enhances its capabilities with a Multilayer Perceptron (MLP) model that incorporates an attention layer to highlight the relevance of input features. By integrating the MLP model, the researchers are able to underscore the importance of specific features in malware identification. XMAL's effectiveness is also compared to other explainability techniques, such as LIME, where it demonstrates superior performance in terms of interpretability, thereby reinforcing the value of machine learning in enhancing cybersecurity measures.

The study provided by Liu et al. [70] investigates the performance of ML models under realistic and unrealistic experimental setups. It utilizes a dataset of 165,000 Android applications, with 33,000 malware and 132,000 benign samples, spanning from 2010 to 2020. The focus of the study is on understanding why ML-based malware detection models perform exceptionally well under certain experimental setups, particularly those involving temporal inconsistencies between malicious and benign samples. To achieve this goal, it leverages different explainable malware detection techniques, i.e., XMal, Drebin, and model-agnostic explanation approaches [36]. It shows how this inconsistent distribution between malware and benign samples can lead to high detection performance but poor generalization. Its results emphasize the need for XAI techniques in experiments to ensure that the models are practically useful and not just theoretically effective.

C. Hardware-Based Malware Approaches

Many researchers have designed hardware-based malware detectors with the assumption that solutions such as anti-virus software can be fooled easily by malicious code. There are many works on hardware-assisted malware detection, but there are few works that are explainable and can provide reasonable interpretations for the predictions in a meaningful manner.

TABLE III: Research Addressing Explainable Machine Learning in Malware Analysis.

Paper/Year	Focus/Objective	Contribution	Limitation	XAI technique
Hardware-H	Based Malware Approaches			
Pan et al. 2020 [88]	Developed regression-based machine learning model that uses linear regression to identify the major contributors amongst input features	Proposed framework for malware detection using explainable Machine learning, which involves training, regression, and interpreta- tion	Filter activations are not well explained Limited analysis of interpretable techniques	Linear regression
Pan et al. 2022 [89]	Aims to focus on hardware- assisted malware detection and localization through Explain- able AI	 Proposed method that provides an interpretable explanation to address the challenge of transparency of the classification results Showed the explainable result through efficient use of hardware performance counters (HPC) and embedded trace buffers (ETC) to provide precise localization of the malicious behavior. 	Lack of exploration of how different surrogate models can influence the results of their interpretation out- comes.	Linear regression and Decision tree
Li et al. 2021 [64]	Aims to provide an inter- pretable hardware malware de- tector to investigate the impact of feature contribution for a particular outcome	Proposed I-MAD that understands the assembly code at the basic block at the executable level To provide the interpretations, they proposed Interpreted feed-forward neural network (IFFNN) I-MAD provides great prediction accuracy and understandable explainability and helps analysts in locating payloads and recurring patterns in malware samples	There is no systemic description of the interpretation factors With their interpretable I-MAD model, adversaries have complete access to their model and can utilize the interpretations to generate adversarial samples	IFFNN
Linux-Based	d Malware Approaches			
Wang et al. 2021 [117]	Focuses on malware detection, which locates code snippets, and on effectively explaining the decision of malware clas- sifier	 Proposed effective deep learning approach for Linux malware detection Methodology detects malicious behavior in malware that uses inline assembly Explanation of malware classification results using LRP 	Lacks clear future technological guidance	Layer-wise relevance propagation (LRP)
Wang et al. 2021 [119]	Exposing the weakness of malware detectors with explainability-guided evasion attacks	Designed adversarial evasion attacks that depend on feature and problem-space manipulation Explanation of attacks they used model agnostic method - SHAP	Missing proof that other explainable models may/may not gain superior performance Restricted to static malware detection Could not detect malicious behavior during run time	SHAP
Mills et al. 2019 [83]	Aims to provide interpretable real-time detection of malware using Random Forest (RF)	Proposed an automated interpretable malware detection system called NODENS This system was able to detect the zero-day malware	Limited to a smaller dataset	Decision tree
PDF-Based	Malware Approaches			
Kuppa and Le-Khac 2020 [61]	Focused on taxonomy of black-box attacks for explainable AI methods that include a wide range of threat models and security properties in cyber security	 Proposed black-box approach that helps to design secure and explainable machine-learning methods Analyzed the accuracy, confidence, and consistency properties of gradient-based explainability methods 	Defensive mechanisms are not explained	Gradient-Based Methods
Severi et al. 2021 [102]	This work focused on back-door poisoning attacks which influence the machine learning training process	Proposed the use of explainable ML technique SHAP that creates effective backdoor triggers that are model agnostic, which influences the machine learning training process To preserve the binary's functionality, the authors created a watermarking utility for Windows PE files	Limited to specific attack methodologies (need to consider more generic attack)	SHAP
Guo et al. 2018 [45]	Aims to classify PDF malware and derive high-fidelity expla- nations for malware detection	Designed a novel interpretability method LEMNA, which is a mixture of regression models and fused lasso In order to interpret the models, LEMNA considers the relevance and dependencies between the features According to the results, LEMNA performs better than LIME	Explanations generated from the features are not addressed They paid less focus on comprehensive interpretability	LEMNA

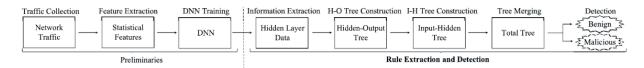


Fig. 10: DNN Rule Extraction and Detection [125].

Although there are many studies on hardware-assisted malware detection, there is a distinct lack of research focused on explainability. This highlights a critical need for innovation in the field that goes beyond detection accuracy, aiming for systems that can articulate the rationale behind their detections. In table III, the literature on hardware malware classification and detection using XAI is discussed.

Sheldon [105] conducts a study analyzing hardware traces for malware detection using explainable ML approaches. Figure 11 illustrates the process of generating hardware traces, where both malware-infected and benign files are executed on a cutting-edge state-of-the-art hardware platform, leading to the production of hardware traces. Hardware traces comprise the data stored in caches and registers during the execution of a program. These traces are then processed by an ML model to identify malware presence. Subsequently, the model's accuracy is evaluated against that of leading-edge ML models. The feedback obtained from this comparison is utilized to refine the accuracy of malware detection.

To explore the comprehensive study of hardware trace analysis and the development of an explainable, hardware-assisted malware detection framework, the research by Pan et al. [88] introduces a hardware framework depicted in Figure 12. This framework is structured around three principal activities.

The first phase involves training an ML model (M) with collected hardware traces. For this purpose, they implement an RNN and leverage the Embedded Trace Buffer (ETB) architecture for trace collection. Subsequently, a specially curated artificial dataset $X=(x_1,x_2,\ldots,x_n)$ is processed by the machine learning model (M) to yield the output Y. To adapt this artificial dataset for the model, linear regression is conducted, resulting in the formulation of a linear predictive model. This process is shown in Equation 1.

$$y = \sum_{i=1}^{n} a_i x_i + \epsilon \tag{1}$$

Linear predictions are formulated as a polynomial function, where n represents the number of instances. This expression incorporates an error term, ϵ , which is crucial for understanding the weight distribution within the model. The value of ϵ needs to be as small as possible. The goal is to minimize the value of ϵ as much as possible, ensuring that the model's predictions are as accurate and reliable as possible.

$$\arg\min||X_a - y||_2 \tag{2}$$

Equation 2 shows the optimization problem, emerging from the selection of y as the perturbed output. Further ridge regression is applied in order to achieve higher fitness with

correlated data. This approach aims at achieving optimal fitness by introducing an additional term to the optimization equation, further elaborated in Equation 3.

$$\arg\min||X_a - y||_2 + \lambda ||a||_2 \tag{3}$$

To mitigate the issue of high variance, the strategy involves substituting X with $X-\lambda I$, as depicted in Equation 4. This adjustment incorporates a regularization parameter, λ , and the identity matrix, I, directly into the predictive model. This technique effectively reduces the model's complexity, discouraging overfitting by penalizing larger coefficients.

$$\arg \min ||X_a - y||_2 + \lambda ||a||_2 \to \arg \min ||(X - \lambda I)a - y||_2$$
 (4)

After determining the linear regression coefficients, the focus shifts to interpreting the outcomes, with particular emphasis on identifying the most influential features. Features associated with larger coefficients are flagged as potentially malicious. To benchmark the effectiveness of their method, the authors reference the PREEMPT malware detector for comparison [16]. PREEMPT employs two algorithmic models, i.e., Random Forest (RF) and Decision Tree (DT), utilizing hardware performance counters (HPC) to generate its dataset. However, it does not extensively investigate the dataset's characteristics, focusing primarily on the interpretation of outcomes. Given the scarcity of research in this area and the need to address malware detection challenges, it is imperative for researchers to engage deeply with the realm of explainable hardware malware detection.

Building upon their previous efforts, the authors [89] harness hardware performance counters and embedded trace buffers to identify the exact locations of malicious activities within a system. They develop DT and RNNs to perform a trade-off between accuracy and efficiency in their detection methodology. Their evaluation, conducted on a broad spectrum of real-world malware datasets, elucidates the interpretability of the RNN model, leveraging linear regression and DT through tree parsing techniques.

In a parallel line of research, Li et al. [64] introduce an innovative interpretable malware detector named I-MAD transformer, designed to analyze assembly code at the basic block level of executables. This approach integrates an interpretable feed-forward neural network, allowing for the examination of each feature's impact on the prediction outcome. The significant advancements brought forth by this study include 1) The proposition of a deep learning model capable of interpreting entire sequences of assembly-level code in malware executables, offering a comprehensive analysis beyond superficial layers. 2) The introduction of two pre-training activities aimed at

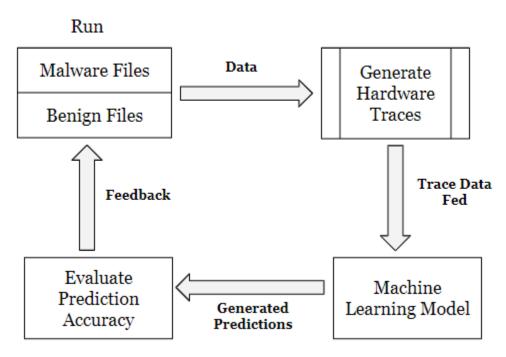


Fig. 11: Hardware Trace Data Generation.

enhancing the understanding of the relevance and functionality of assembly-level constructs, thereby improving the model's predictive accuracy and interpretability. 3) The development of an Interpretable Feed-Forward Neural Network (IFFNN), which assists analysts in identifying payloads and recurring patterns within malware samples. This network combines the interpretability akin to logistic regression with the modeling prowess of multi-layer FFNN, presenting a powerful tool for cybersecurity professionals in the battle against malware.

D. PDF-Based Malware Approach

A Portable Document Format (PDF) file contains text, images, digital signatures, and other elements. Its structure includes a Header, Body, Cross-reference Table, and Trailer, as illustrated in Figure 13. The header of a PDF file is the top section that indicates the version number and file format. The body of the PDF stores all the pertinent data, and it contains a range of objects, including data, text, images, and dictionaries. The cross-reference table in a PDF file includes links to all elements within the document, which facilitates navigation and access. The trailer, which links to the cross-reference table, also contains the EOF marker.

Given the global acceptance of PDF as a standard document format, the prevalence of PDF malware is increasing. Malware exploits vulnerabilities in PDF readers to hijack execution control, such as executing shell code. To evade malware detection, PDF authors might employ techniques that can cause the PDF reader to crash [25].

To analyze and evaluate the consistency and correctness of the gradient-based approach, the study by Kuppa and Le-Khac [61] designed a novel black-box attack. They apply this method to detect malicious PDF files using the Mimicus dataset and to identify Android malware with the DREBIN

dataset, interpreting the results through gradient-based explainable machine-learning techniques.

To guide the selection of relevant features and avoid back-door poisoning attacks, the authors [102] use model-agnostic techniques in explainable machine learning and develop effective backdoor triggers. They specifically use Android, PDF, and Windows PE files for malware classification and analyze nearly 10,000 samples of benign and malicious files. To maintain the functionality of the binaries, they create a static analysis watermarking utility for Windows PE files that meets multiple adversarial constraints. Subsequently, their attention turns to PDF files and Android applications. Using the SHAP explainability technique, they identify features that contribute to malware detection. Finally, they demonstrate and evaluate the challenges in fully defending against these stealthy poisoning attacks.

To classify PDF malware, another research [45] introduces an explainable method named LEMNA, which provides high-fidelity explanations for malware detection. They utilize deep learning models and assess their interpretability using LEMNA. The study also explores feature augmentation, along with synthetic and feature deduction tests. They note that due to sparse input feature vectors affecting local decision boundaries, LIME and other advanced explainable techniques were as ineffective as traditional feature selection methods. The PDF-based malware detection studies are summarized in Table III.

E. Linux-Based Malware Approach

Linux, a Unix-based operating system, is an open-source platform that is renowned for its reliability and functionality. For malware analysis, Linux allows malicious code to run in isolated sandbox environments. However, due to the limited

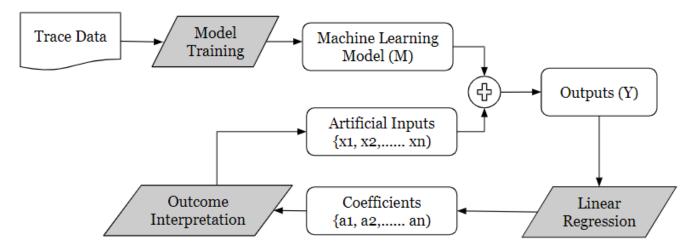


Fig. 12: Explainable Hardware Malware generation workflow [88].

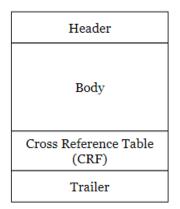


Fig. 13: Structure of PDF file.

availability of sandboxes compatible with the latest Linux versions, they are less commonly used than Android and Windows platforms. Recognizing that ML in malware detection often yields predictions that lack explainability, Wang et al. [117] introduce an explainable malware detection method based on Linux systems. This approach clarifies the rationale behind the classifier's decisions by locating the malicious code snippets. By using a dynamic approach, they map system calls to inputs for a deep learning model and utilize the explainable technique of Layer-wise Relevance Propagation to recognize which sequence parts are most significant in the decision-making process. By using a confusion matrix as a performance evaluation, they confirm that their method can swiftly and accurately identify malicious code.

Wang et al. [119] focus on exposing vulnerabilities in malware detectors through explainability-guided evasion attacks that combine feature space manipulation with problem space obfuscation. They utilize a dataset of approximately 43,553 ELF binary files on Linux systems. Their research uses the model-agnostic explainability method SHAP to demonstrate how evasion attacks can be transferred from one detector to another. In another study, Mills et al. [83] develop a

lightweight malware detection system named NODENS, suitable for deployment on Raspberry Pi hardware. They test several ML-based algorithms on a Linux operating system, with the Random Forest algorithm performing optimally among them. This work utilizes a tree-based model to facilitate visual interpretation of the classification process, which enhances the end user's understanding of the output and aids in the individual development of the malware sample lifecycle. Due to the infrequent application of the Linux platform, there is limited research on explainable malware detection within the Linux domain. Studies addressing this topic are detailed in Table III.

F. Other Approaches

This section provides information regarding approaches that are not specific to any domain. Chen [23] leverages DL-based techniques for static malware classification to emphasize the importance of model transparency to gain user trust. They enhance their model's interpretability by utilizing LIME and adopting an image-based approach to visualize malware data. The study is conducted using three distinct datasets, where the model demonstrates high accuracy and a low false positive rate. For a practical demonstration of interpretability, the authors select an image from Lloyda.AA2 malware family and represent it with 200 super-pixel representations. They then identify which aspects of the malware images are crucial for the deep learning model's predictions. Their visual interpretation states that the red regions indicate the pixel regions that the model does not trust to contribute to the prediction.

To evaluate interpretability techniques applied to ML-based malware detectors, Briguglio and Saad [20] explore how these techniques enhance N-gram analysis in the interpretation of machine-learning malware detectors. They focus on logistic regression, random forest, and neural network models, enhancing model confidence and feature significance. Specifically, they use the Layer-wise Relevance Propagation (LRP) technique to recognize the most important input nodes for classification.

TABLE IV: Research Addressing Explainable Machine Learning in Malware Analysis.

Paper/Year	Focus/Objective	Contribution	Limitation	XAI technique	
General Malware Approaches					
Chen 2018 [23]	Aims to provide an image- based malware approach for explainability in static mal- ware classification	 The grayscale images were interpreted and the most relevant attributes that contributed to the training model were shown. Visual interpretations are shown to get interpretation results 	 It has not been demonstrated that it can comprehend adversarial and obfuscated samples. When more features are added, there is no interpretation's fidelity, and also, there is no trust score to evaluate the extent of interpretability. 	LIME	
Briguglio and Saad. 2019 [20]	Aims to provide an inter- pretable malware detector to enhance the N-gram analysis	 They developed and evaluated the effectiveness of interpretability techniques using features of N-grams They interpreted the logistic regression model, single sample with random forest, neural network, single sample with neural network 	Systematic interpretation assessment for malware detection is not provided.	Layer-wise relevance propagation (LRP)	
Li et al. 2021 [65]	Aims to provide excellent in- terpretability in malware clas- sification through a machine learning model	 Proposed a novel machine learning model named LSH-base clustering approach to classifying the malware Their machine learning model generates assembly code function clusters, and the model itself supports the interpretation of the results 	Did not mention any draw- backs of the interpretable ML model	Executable functions	
Fidel et al. 2020 [37]	Aims to detect evasion attacks such as adversarial examples by using the generated SHAP values as additional features	 The assumption of their work is that both the adversarial and benign samples will have different SHAP signatures A model learns and leverages the differences between the generated signatures and establishes the classifications 	It is not possible to transfer their attack on multiple detectors since the computation of SHAP values is not differentiable	SHAP	
Kumar and Subbiah 2022 [59]	Aims to utilize static analysis for effective and explainable zero-day malware detection	This study employs Shapley values to determine the most important features that are contributing more to predicting zero-day malware The SHAP explainability technique was utilized to determine the misclassification based on the topmost contributing features	Reason for misclassification using SHAP should be ex- plored more.	SHAP	
lee et al. 2022 [62]	This work aims to provide a technique for screening high-quality data in order to detect false predictions based on reliability indicators.	 This study conducts experiments on two different datasets to analyze the effectiveness of their proposed approach The SHAP explainability technique was utilized to identify the most important features that are contributing to the classification so that even humans can easily interpret based on the AI predictions, and reliability is also calculated and analyzed 	Lacking the analysis on other explainability approaches such as LEMNA and LIME	SHAP	
Galli et al. 2024 [40]	The paper aims to make AI-driven security tools more reliable and effective, especially in important security settings.	The development and evaluation of an XAI framework specifically designed for behavioral malware detection. It assesses four XAI methods and three datasets to determine their effectiveness in making LSTM and GRU model decisions transparent.	While the paper evaluates various XAI techniques on specific datasets, the gener- alizability of these methods to other types of malware or different datasets is not adequately addressed.	SHAP, LIME, LRP, and attention mech- anisms	

Li et al. [65] develop a novel ML-based model that classifies malware effectively and offers exceptional interpretability. They introduced a unique ML-based algorithm, the LSH-based clustering approach, which supports result visualization and interpretation that distinguishes it from other models in the field.

In their study on detecting evasion attacks, such as adversarial examples, Fidel et al. [37] utilize SHAP values as an innovative approach. They created SHAP signatures based on the premise that these signatures differ between benign

and adversarial samples. Their findings confirm the initial hypothesis that variations in SHAP values in the classification model's final layer can effectively reveal the distribution of feature importance in classification outcomes. This method enhances the model's ability to identify adversarial examples, demonstrating a novel application of SHAP values in enhancing security measures.

Kumar and Subbiah [59] conduct a static analysis using three different datasets to detect zero-day malware with MLbased algorithms. Among the algorithms tested, XGBoost achieves the highest accuracy and outperforms all other models. The authors utilize the SHAP bar and waterfall plots to identify the most significant features contributing to the model's predictions. They compare these top features across four categories of samples: False Positives (FP), False Negatives (FN), True Negatives (TN), and True Positives (TP). This comparison helps recognize misclassification categories, and the findings suggest that redistributing misclassified samples into their correct categories could significantly enhance the model's efficiency.

Lee et al. [62] address large-scale threats to cybersecurity by leveraging IDS and malware datasets to validate the effectiveness of their proposed approach. Their method focuses on screening high-quality data to identify and rectify false predictions using reliability indicators. They incorporate the SHAP explainability technique to determine the contributions of individual features to specific outcomes. This approach identifies weaknesses in the existing AI models and enhances the detection of valuable alerts. By improving the accuracy of alert detection, the method allows human analysts to work more effectively and efficiently, which leads to prioritizing critical threats and optimizing response strategies.

Galli et al. [40] address the critical need for transparency in AI systems used for malware detection. They develop and evaluate an XAI framework that applies to behavioral malware detection by employing DL models such as LSTM and GRU. These models analyze sequences of API calls to detect malicious activities. To make the models' decisions understandable and trustworthy, the paper investigates four different XAI techniques, i.e., SHAP, LIME, LRP, and attention mechanisms. The evaluation of these methods across three datasets (Mal-API-2019, API Call Sequences, and Alibaba Cloud Malware) shows their varying effectiveness in providing clear and useful explanations.

V. FUTURE DIRECTIONS

Explainable machine learning is a rapidly evolving field with many ongoing challenges and opportunities for exploration. In the previous sections, we conducted an extensive review of various explainable machine-learning techniques, with a particular focus on malware classification and detection. however, as the application of explainable methods in malware detection becomes increasingly prevalent, new challenges continue to emerge. This section outlines several key challenges and potential research directions that researchers may pursue as future work in the area of explainable malware analysis and detection.

A. Improve Data Sets

Improving and updating malware datasets is a critical concern in the field of XAI. Many existing datasets are outdated and lack comprehensive coverage of current malware behaviors. These datasets often do not provide a sufficient volume of data for effectively training XAI applications. For instance, previous research on explainable Android malware detection primarily utilized the DREBIN dataset, which comprises 5,616 malicious instances and 121,329 benign instances [10]. This

imbalance, where benign instances significantly outnumber malicious ones, can hinder the training of effective models.

Moreover, the size of the current datasets is generally too small to train robust models effectively. However, this field of research needs an unbiased, reasonably sized benchmark dataset that equally represents both benign and malicious behaviors. Accessing this kind of dataset is essential for evaluating explainable ML-based techniques and achieving reliable detection results. Furthermore, the DREBIN dataset, in particular, highlights the limitations of static analysis, pointing to the necessity for dynamic updates that support more comprehensive dynamic analyses. Additionally, there is potential for innovation in automated data generation and minimization techniques to accelerate the prediction process. For example, in hardware malware detection, researchers [105] have generated trace data to facilitate hardware trace analysis and distinguish between malware and benign programs. Future work could focus on enhancing these techniques to streamline and speed up the predictive capabilities of malware detection systems.

B. Combining Static and Dynamic

This paper discussed explainability techniques in malware analysis, wherein researchers have primarily concentrated on static and dynamic analyses. Static analysis involves feature extraction and dimensionality reduction, processes that minimize information uncertainty and facilitate the analysis of malicious applications. Conversely, dynamic analysis focuses on training surrogate learning models. However, there is a notable absence of research on hybrid analysis, which combines elements of both to enhance the explainability of malware detection.

To address this gap, multiple ML classifiers will be leveraged to analyze both source code and runtime dynamic features. This dual approach aims to improve the efficiency and effectiveness of ML algorithms in distinguishing between benign and malicious applications. Moreover, to overcome the limitations in static and dynamic methodologies, researchers should also develop online and real-time explainable malware detection systems. These systems would continuously monitor the entire system to detect any possible malicious behavior or traces at any moment. Thus, the development of hybrid and online detection systems represents a significant research challenge in the field of explainable malware analysis.

C. Analyze Model-Agnostic Techniques

Explainable machine-learning techniques remain underutilized and underexplored in the domain of malware detection. There is a need to explore various model-agnostic techniques that provide both local and global explanations, which can help develop fast-training and explainable models without sacrificing accuracy. One promising direction for future research is the automation of explainability when it is decoupled from the underlying machine learning model. This decoupling facilitates the easy replacement of both the explainable technique and the machine learning model itself.

The model-agnostic technique LIME is widely cited in research but comes with notable limitations. Its reliance on

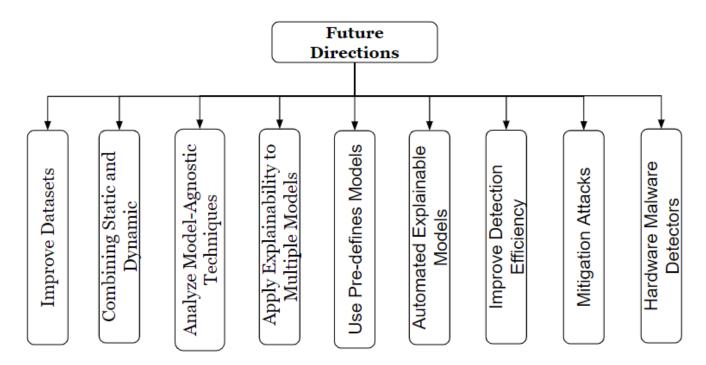


Fig. 14: Future Directions for Explainable Malware Detection.

data sampling can lead to variability in explanations, making them potentially unstable and unreliable. Furthermore, if the local fidelity measure is inaccurate, the reliability of LIME's explanations for distinguishing between malicious and benign samples is compromised. Additionally, LIME lacks guidance on the optimal number of features to use, which could affect the quality of its explanations.

To advance the field of explainable malware detection, paying attention to evaluate various model-agnostic techniques is essential. Future research could also focus on improving fidelity in explanations, which is crucial for maintaining reliability in rapidly evolving scenarios. Overall, model-agnostic methods represent a flexible and effective approach to enhancing malware detection through explainable machine learning.

D. Explainability Approach to Multiple Models

Previous research in explainable machine learning within the malware detection domain has primarily focused on developing frameworks and applying specific explainability methods to those frameworks. However, there is a notable gap in the literature regarding the selection of explainability techniques for non-differentiable models. Theoretical findings suggest that under certain assumptions, various machine learning algorithms can yield similar decision functions. This similarity raises a critical question: how does one select the most appropriate explainable technique for a given malware detection process?

Hence, conducting thorough analyses and evaluations of how different explainability techniques influence the explanations generated by a specific framework. Such research can demonstrate that the chosen explainability technique fits the model and outperforms alternative methods in clarity and effectiveness. Enhancing the understanding of the applicability and efficiency of various explainable methods in malware detection leads to more robust and transparent systems.

E. Use Pre-Trained Models

While neural networks are powerful tools for modeling, their black-box nature makes them difficult to interpret, which poses a significant challenge in fields such as malware detection. In the research regarding this, the authors [88] have developed a framework that utilizes neural networks to facilitate interpretable malware detection, which has innovative approaches to this issue.

Looking forward, in the malware detection domain, it would be advantageous to leverage existing explainable pre-trained models rather than building new models from scratch. This approach can save considerable time that would otherwise be spent collecting data and training models and enhances the efficiency of detecting malicious activities in systems that may already be compromised. In other words, utilizing pre-trained models can accelerate the deployment of malware detection systems and improve their effectiveness by integrating advanced, pre-learned features into the detection process. Applying this strategy could significantly extend the application of neural networks in malware detection which can lead to quicker adaptability and broader applicability.

F. Automated Explainable Models

One promising direction for future research in the field of malware detection involves implementing more automated explainability models. The goal is to enhance user trust in black-box models, such as those based on deep learning, which are currently not automatically interpretable. Most existing research focuses on interpreting the results of malware detection post hoc after the detection has already occurred. This method leaves a gap in real-time understanding and response, which automated explainability aims to fill.

Achieving an optimal balance between accuracy and explainability continues to be a significant challenge. Automated explainability could help bridge this gap by providing insights into the decision-making process of complex models in real-time. Additionally, there is a clear need for more research focused on quantitative-level evaluation of these explainable models. Such evaluations would assess the interpretability and how the introduction of explainability affects the overall performance of the detection system.

G. Improve detection efficiency

A valuable future direction in explainable malware detection is to enhance the design methodologies of malware detectors so that the explanations they generate can assist professionals in more accurately characterizing malware attacks, ultimately improving detection accuracy. For example, wang et al. [118] involve extracting features and employing a decision tree to develop a model capable of determining the maliciousness of applications.

Looking forward, the implementation of pruning strategies in decision trees presents a promising avenue for enhancing the efficiency of these detection models. Pruning optimizes the tree structure by removing superfluous or minimally informative branches, thereby simplifying the model. This optimization can accelerate the processing time and enhance the accuracy by focusing the model's analysis on the most significant features.

H. Mitigating attacks

In recent research, the primary focus has been on black-box attacks, gradient-based attacks, evasion attacks, and poisoning attacks. Evasion attacks involve manipulating malicious input samples during the training phase to circumvent detection by a trained system, and it requires access to the model. Poisoning attacks compromise the integrity of training data by introducing incorrect data since it can mislead the learning process of ML models. This corruption of training data severely undermines the entire training process. In both gradient-based and poisoning attacks, it is assumed that the attacker has knowledge of the feature space used by the target. Future research in the field of explainable machine learning should explore defense mechanisms against these types of attacks and develop generic mitigation methods. Moreover, while current attacks typically use either static or dynamic approaches, future attacks might utilize a hybrid approach that integrates both strategies. As malware data continuously evolves, implementing attacks in online detection systems could pose significant challenges for attackers trying to intercept or manipulate highspeed continuous data compared to data stored on devices.

The study by Scalas et al. [101] highlights the use of system API calls as effective features for detecting attack strategies. Future research could assess the susceptibility of system API

calls to attacks and explore whether this detection strategy limits the number of features that attackers can feasibly manipulate.

I. Hardware Malware Detectors

Research on explainable hardware-based malware detection is currently limited, which presents significant opportunities for future investigation. One potential avenue for advancement involves the design of efficient and explainable hardware malware detectors. These systems could automate the trace selection process and reduce prediction time while maintaining high accuracy in differentiating between malware and benign programs.

Another area for exploration is the development of debugging architectures that enhance malware detection capabilities. This could include the design of embedded trace buffers and the utilization of hardware performance counters. These tools would help identify the most informative traces for use in explainable machine learning applications within the malware detection field. This focus can enhance the efficiency and effectiveness of malware detection systems and make them more accessible and interpretable for cybersecurity professionals.

VI. CONCLUSION

ML plays a crucial role in cybersecurity, yet these datadriven frameworks are susceptible to exploitation, misdirection, and circumvention, potentially leading to severe consequences. Explainability is essential for building trust in order to deploy models effectively in cybersecurity environments. Explainability techniques enhance the transparency of ML models and help identify critical features for malware detection, thus improving the capabilities of security analysts.

The field of XAI is steadily expanding. This paper discusses the taxonomy of XAI in malware analysis and reviews state-of-the-art approaches. We provide an in-depth examination of explainable malware classification and detection methods, summarizing the work of researchers to date. Our study systematically organizes various explainable malware-based approaches, making this information more accessible to researchers and others interested in this field.

We conclude the survey by identifying open research challenges and future directions in explainable malware analysis. Our findings highlight that significant work remains to be done in this area. This survey serves as a comprehensive guide for researchers exploring explainable malware detection, offering insights into the current landscape and stimulating research in unexplored domains within this dynamic and evolving field.

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