

# Arms Race in Adversarial Malware Detection: A Survey

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Malicious software (malware) is a major cyber threat that has to be tackled with Machine Learning (ML) techniques because millions of new malware examples are injected into cyberspace on a daily basis. However, ML is vulnerable to attacks known as adversarial examples. In this article, we survey and systematize the field of Adversarial Malware Detection (AMD) through the lens of a unified conceptual framework of assumptions, attacks, defenses, and security properties. This not only leads us to map attacks and defenses to partial order structures, but also allows us to clearly describe the attack-defense arms race in the AMD context. We draw a number of insights, including: knowing the defender's feature set is critical to the success of transfer attacks; the effectiveness of practical evasion attacks largely depends on the attacker's freedom in conducting manipulations in the problem space; knowing the attacker's manipulation set is critical to the defender's success; and the effectiveness of adversarial training depends on the defender's capability in identifying the most powerful attack. We also discuss a number of future research directions.

CCS Concepts: • **Security and privacy** → **Malware and its mitigation**; • **Theory of computation** → **Adversarial learning**;

Additional Key Words and Phrases: Malware detection, adversarial machine learning, evasion attacks, poisoning attacks

## ACM Reference format:

Deqiang Li, Qianmu Li, Yanfang (Fanny) Ye, and Shouhui Xu. 2021. Arms Race in Adversarial Malware Detection: A Survey. *ACM Comput. Surv.* 55, 1, Article 15 (November 2021), 35 pages.

<https://doi.org/10.1145/3484491>

Work was partly done when Shouhui Xu was affiliated with University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249.

Q. Li is supported in part by the National Key R&D Program of China under Grant 2020YFB1805503, the Jiangsu Province Modern Education Technology Research Project under Grant 84365, the National Vocational Education Teacher Enterprise Practice Base "Integration of Industry and Education" Special Project (Study on Evaluation Standard of Artificial Intelligence Vocational Skilled Level). Y. Ye and S. Xu are supported in part by NSF Grant #2122631 (#1814825). S. Xu is also supported in part by ARO Grant #W911NF-17-1-0566, NSF Grant #2115134, and Colorado State Bill 18-086.

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0360-0300/2021/11-ART15 \$15.00

<https://doi.org/10.1145/3484491>

## 1 INTRODUCTION

**Malicious software (malware)** is a big cyber threat and has received a due amount of attention. For instance, Kaspersky reports that 21,643,946 unique malicious files were detected in the year 2018, 24,610,126 in 2019, and 33,412,568 in 2020 [47, 72]. A popular defense against malware is to use *signature-based* detectors [44], where a signature is often extracted by malware analysts from known malware examples. This approach has two drawbacks: signatures are tedious to extract and can be evaded [34] by a range of techniques (e.g., encryption, repacking, and polymorphism [7, 21, 63, 86, 106, 111, 139]). This incompetence has motivated the use of **Machine Learning (ML)** based malware detectors, which can be automated to some degree and can possibly detect *new* malware examples (via model generalization or knowledge adaptation [8, 11, 43, 45, 56, 57, 64, 66, 84, 121, 137, 138, 143]). More recently, **Deep Learning (DL)** has been used for malware detection (see, e.g., [99, 103, 125]).

While promising, ML-based malware detectors are vulnerable to attacks known as *adversarial examples* [16, 60, 114]. There are two kinds of attacks. One is *evasion attack*, where the attacker perturbs test examples to *adversarial examples* to evade malware detectors [2, 16, 39, 53, 57, 91, 120, 127]. The other is *poisoning attack*, where the attacker manipulates the training dataset for learning malware detectors [30, 40, 118]. These attacks usher in the new field of **Adversarial Malware Detection (AMD)** [16, 27, 36, 39, 40, 53, 114, 118, 127, 133, 134].

The state-of-the-art in AMD is that there are some specific results scattered in the literature but there is no systematic understanding. This is true despite that there have been attempts at systematizing the related field of **Adversarial Machine Learning (AML)** [9, 26, 60, 140], which however cannot be automatically translated to AMD. This is so because malware detection has three *unique* characteristics which are not exhibited by the other application domains (e.g., image or audio processing). (i) There are no common, standard feature definitions because both attackers and defenders can define their own features to represent computer files. As a consequence, attackers can leverage this “freedom” in feature definition to craft adversarial examples. (ii) Malware features are often discrete rather than continuous and program files are often highly structured with multiple modalities. This means that arbitrarily perturbing malware files or their feature representations might make the perturbed files no more executable. This also means that the discrete domain makes perturbation a *non-differentiable* and *non-convex* task. (iii) Any meaningful perturbation to a malware example or its feature representation must preserve its malicious functionality. For example, the **Android Package Kit (APK)** requires that the used permissions are publicized in the AndroidManifest.xml, meaning that removing permissions in this manifest file would incur a runtime error. The preceding (ii) and (iii) make both the attacker’s and defender’s tasks more challenging than their counterparts where small perturbations are not noticeable (e.g., images).

**Our Contributions.** We propose a conceptual framework for systematizing the AMD field through the lens of *assumptions*, *attacks*, *defenses*, and *security properties*. In specifying these, we seek rigorous definitions whenever possible, while noting that these definitions have been scattered in the literature. Rigorous definitions are important because they can serve as a common reference for future studies. The framework allows us to map the known attacks and defenses into some partial order structures and systematize the AMD attack-defense arms race.

We make a number of observations, including: (i) the indiscriminate attack that treats malicious examples as equally important has been extensively investigated, but targeted and availability attacks are much less investigated; (ii) the evasion attack is much more extensively studied than the poisoning attack; (iii) there is no silver-bullet defense against evasion and poisoning attacks; (iv) **sanitizing examples (SE)** is effective against black-box and gray-box attacks, but not white-box attacks; (v) AMD security properties have been evaluated empirically rather than rigorously;

(vi) there is no theoretical evidence to support that the effectiveness of defense techniques on the training set can generalize to other adversarial examples.

We draw a number of insights, including: (i) knowing defender's feature set is critical to the success of transfer attacks, highlighting the importance of keeping defender's feature set secret (e.g., by randomizing defender's feature set); (ii) the effectiveness of practical evasion attacks largely depends on the attacker's degree of freedom in conducting manipulations in the problem space (i.e., a small degree of freedom means harder to succeed); (iii) effective defenses often require the defender to know the attacker's manipulation set, explaining from one perspective why it is hard to design effective defenses; (iv) effectiveness of **adversarial training (AT)** depends on the defender's capability in identifying the most powerful attack.

Finally, we discuss a number of future research directions, which hopefully will inspire and encourage many researchers to explore them.

**Related Work.** The closely related prior work is Maiorca et al. [81], which surveys previous studies in adversarial malicious PDF document detection. In contrast, we consider the broader context of AMD and propose novel partial orders to accommodate AMD assumptions, attacks, defenses, and properties. There are loosely-related prior studies, which survey prior AML studies (but not focusing on AMD), including [9, 10, 17, 26, 79, 94, 105, 140]. For example, Yuan et al. [140] survey attack methods for generating adversarial examples, while briefly discussing evasion attacks in the AMD context; Barreno et al. [9, 10] propose a taxonomy of AML attacks (causative vs. exploratory attacks, integrity vs. availability attacks, and targeted vs. indiscriminate attacks); Biggio et al. [17] propose a defense framework for protecting **Support Vector Machines (SVMs)** from evasion attacks, poisoning attacks, and privacy violations; Papernot et al. [94] systematize AML security and privacy with emphasis on demonstrating the tradeoff between detection accuracy and robustness.

**Paper Outline.** Section 2 describes our survey and systematization methodology and framework. Section 3 applies our framework to systematize the literature AMD studies. Section 4 discusses future research directions. Section 5 concludes the article.

## 2 SURVEY AND SYSTEMATIZATION METHODOLOGY

**Terminology, Scope, and Notations.** In the AMD context, a defender  $\mathcal{I}$  aims at using ML to detect or classify computer files as benign or malicious; i.e., we focus on *binary classification*. An attacker  $\mathcal{A}$  attempts to make malicious files evade  $\mathcal{I}$ 's detection by leveraging *adversarial files* (interchangeably, *adversarial examples*). Adversarial malware examples are often generated by perturbing or manipulating malware examples, explaining why we will use the two terms, perturbation and manipulation, interchangeably. Adversarial attacks can be waged in the training phase of a ML model (a.k.a., poisoning attack) or in the test phase (a.k.a., evasion attack). It is worth mentioning that the *privacy violation* attack [60] is waged in addition to the preceding two attacks because  $\mathcal{A}$  can always probe  $\mathcal{I}$ 's detectors. A file, benign and malicious alike, is adversarial if it is intentionally crafted to (help malicious files) evade  $\mathcal{I}$ 's detection, and non-adversarial otherwise. We focus on  $\mathcal{I}$  using supervised learning to detect malicious files, which may be adversarial or non-adversarial because they co-exist in the real world with no self-identification. This means that, we do not consider the large body of malware detection literature that does not cope with AMD, which has been addressed elsewhere (e.g., [101]). Table 1 summarizes the main notations used in the article.

### 2.1 Brief Review on ML-based Malware Detection

Let  $\mathcal{Z}$  be the *example space* of benign/malicious adversarial/non-adversarial files. Let  $\mathcal{Y} = \{+, -\}$  or  $\mathcal{Y} = \{1, 0\}$  be the *label space* of binary classification, where  $+1$  ( $-1$ ) means a file is

Table 1. Main Notations Used in the Article

Notation	Meaning
$\mathbb{R} (\mathbb{R}_+)$	the set of (positive) real numbers
$\mathcal{A}, \mathcal{I}$	attacker and defender (treated as algorithms)
$\mathbb{P}$	the probability function
$z, z' \in \mathcal{Z}$	$\mathcal{Z}$ is example space; $z'$ is obtained by perturbing $z$
$S$	defender $\mathcal{I}$ 's feature set for representing files
$\mathbf{x}, \mathbf{x}' \in \mathcal{X}$	$\mathcal{X} = \mathbb{R}^d$ is $d$ -dimensional feature space; $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$ are, respectively, feature representations of $z, z' \in \mathcal{Z}$
$\mathcal{Y}, y$	$\mathcal{Y}$ is the label space of binary classification, $\mathcal{Y} = \{+1, -1\}$ ; $y \in \mathcal{Y}$
$\mathcal{D} = \mathcal{Z} \times \mathcal{Y}$	the file-label (i.e., example-label) space
$D_{train} \subset \mathcal{D}, n$	the training set in file-label space; $n =  D_{train} $
$D_{test}$	the test set in file-label space
$D_{poison}, D'_{poison}$	$D'_{poison}$ is set of adversarial file-label pairs obtained by perturbing non-adversarial files in $D_{poison} \subset \mathcal{D}$
$O(z, z')$	$O(z, z') : \mathcal{Z} \times \mathcal{Z} \rightarrow \{\text{true}, \text{false}\}$ is an oracle telling if two files have the same functionality or not
$\delta$	a manipulation for perturbing files <i>with</i> preserving their functionalities
$\mathcal{M}, \mathcal{Z}_M \subseteq \mathcal{Z}$	$\mathcal{M}$ is manipulation set in the problem space; $\mathcal{Z}_M$ is set of adversarial files generated using $\mathcal{M}$
$\mathbf{M}, \mathcal{X}_M \subseteq \mathcal{X}$	$\mathbf{M}$ is feature manipulation set; $\mathcal{X}_M$ is set of adversarial feature vectors generated using $\mathbf{M}$
$\Gamma(z, z')$	$\Gamma(z, z') : \mathcal{Z} \times \mathcal{Z} \rightarrow \mathbb{R}_+$ measures the degree of manipulation for perturbing $z \in \mathcal{Z}$ into $z' \in \mathcal{Z}$
$C(\mathbf{x}, \mathbf{x}')$	$C(\mathbf{x}, \mathbf{x}') : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+$ is the function measuring the cost incurred by changing feature vector $\mathbf{x}$ to $\mathbf{x}'$
$\delta_z \in \mathcal{M}$	$\delta_z$ is a set of manipulations of $z$ w.r.t. $z'$
$\delta_{\mathbf{x}} \in \mathbf{M}$	$\delta_{\mathbf{x}} = \mathbf{x}' - \mathbf{x}$ is a perturbation vector of $\mathbf{x}$ w.r.t. $\mathbf{x}'$
$\phi : \mathcal{Z} \rightarrow \mathcal{X}$	feature extraction function; $\mathbf{x} \leftarrow \phi(z), \mathbf{x}' \leftarrow \phi(z')$
$\varphi, f$	$\varphi : \mathcal{X} \rightarrow \mathbb{R}$ is classification function; $f : \mathcal{Z} \rightarrow \mathbb{R}$ is classifier $f = \varphi(\phi(\cdot))$ ; by abusing notation a little bit, we also use “ $+ \leftarrow f(z)$ ” to mean that $f$ predicts $z$ as malicious when $f(z) \geq \tau$ for a threshold $\tau$
$F_\theta : \mathcal{X} \rightarrow \mathbb{R}$	ML algorithm with parameters $\theta$
$L : \mathbb{R} \times \mathcal{Y} \rightarrow \mathbb{R}$	loss function measuring prediction error of $F_\theta$
EL, WR, AT	defense techniques: Ensemble Learning, Weight Regularization, AT
VL, RF, IT, CD, SE	defense techniques: Verifiable Learning, Robust Feature, Input Transformation, Classifier randomization, SE
BE, OE, BP, OP	attack tactics: basic and optimal evasion; basic and optimal poisoning
GO, SF, MI	attack techniques: Gradient-based Optimization, Sensitive Features, MImicry
TR, HS, GM, MS	attack techniques: TTransferability, Heuristic Search, Generative Model, Mixture Strategy
$A_1, \dots, A_5$	the 5 attributes under $\mathcal{I}$ 's control; they are known to $\mathcal{A}$ at respective degrees $a_1, \dots, a_5$
$A_6, \dots, A_9$	the 4 attributes under $\mathcal{A}$ 's control; they are known to $\mathcal{I}$ at respective degree $a_6, \dots, a_9$
RR, CR, DR, TR	security properties: Representation Robustness, Classification Robustness, Detection Robustness, Training Robustness

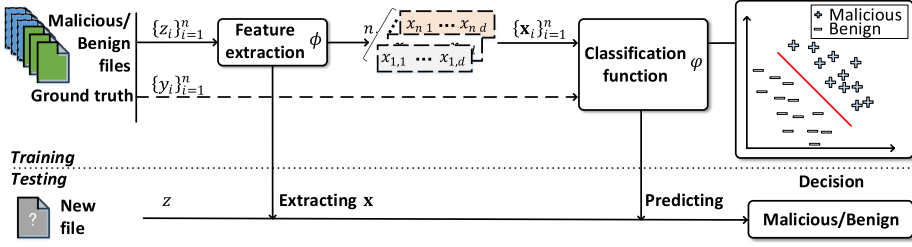


Fig. 1. Illustration of ML-based malware detector.

malicious (benign). Let  $\mathcal{D} = \mathcal{Z} \times \mathcal{Y}$  be the file-label (example-label) space. For training and evaluating a classifier in the absence of adversarial files,  $\mathcal{I}$  is given a set  $D \subset \mathcal{D}$  of non-adversarial benign/malicious files as well as their *ground-truth* labels.  $\mathcal{I}$  splits  $D$  into three disjoint sets: a training set  $D_{train} = \{(z_i, y_i)\}_{i=1}^n$ , a validation set for model selection, and a test set for evaluation. Each file  $z_i \in \mathcal{Z}$  is characterized by a set  $S$  of features and represented by a numerical vector  $\mathbf{x}_i = (x_{i,1}, \dots, x_{i,d})$  in the  $d$ -dimensional *feature space*  $\mathcal{X} = \mathbb{R}^d$ , which accommodates both continuous and discrete feature representations [1, 55, 56, 69, 113, 121]. The process for obtaining feature representation  $\mathbf{x}_i$  of  $z_i \in \mathcal{Z}$  is called *feature extraction*, denoted by a function  $\phi : \mathcal{Z} \rightarrow \mathcal{X}$  with  $\mathbf{x}_i \leftarrow \phi(S, z_i)$ . Because  $\phi$  can be hand-crafted (denoted by  $\phi_c$ ), automatically learned (denoted by  $\phi_a$ ), or a hybrid of both [13], we unify them into  $\phi$  such that  $\phi(S, z) = \phi_a(\phi_c(S, z))$ ; when only manual (automatic) feature extraction is involved, we can set  $\phi_a$  ( $\phi_c$ ) as the identity map. There are two kinds of features: *static features* are extracted via static analysis (e.g., strings, API calls [4, 129]); *dynamic features* are extracted via dynamic analysis (e.g., instructions, registry activities [42, 64]).

As highlighted in Figure 1,  $\mathcal{I}$  uses  $\{(z_i, y_i)\}_{i=1}^n$  to learn a malware detector or classifier  $f : \mathcal{Z} \rightarrow [0, 1]$ , where  $f(z) = \varphi(\phi(S, z))$  is composed of feature extraction function  $\phi : \mathcal{Z} \rightarrow \mathcal{X}$  and classification function  $\varphi : \mathcal{X} \rightarrow [0, 1]$ . Note that  $f(z) \in [0, 1]$ , namely  $\varphi(\mathbf{x}) \in [0, 1]$  with  $\mathbf{x} \leftarrow \phi(S, z)$ , can be interpreted as the probability that  $z$  is malicious (while noting that calibration may be needed [90]). For a given threshold  $\tau \in [0, 1]$ , we further say (by slightly abusing notations)  $z$  is labeled by  $f$  as +, or  $+ \leftarrow f(z)$ , if  $f(z) \geq \tau$ , and labeled as - or  $- \leftarrow f(z)$  otherwise. In practice,  $f$  is often specified by a learning algorithm  $F$  with learnable parameter  $\theta$  (e.g., weights) and a hand-crafted feature extraction  $\phi_c$ ; then,  $\theta$  is tuned to minimize the empirical risk associated with a loss function  $L : [0, 1] \times \mathcal{Y} \rightarrow \mathbb{R}$  measuring the prediction error of  $F_\theta$  [124] (e.g., cross-entropy [49]), namely

$$\min_{\theta} \mathcal{L}(\theta, D_{train}) = \min_{\theta} \frac{1}{n} \sum_{(z_i, y_i) \in D_{train}} (L(F_\theta(\phi_c(S, z_i)), y_i)). \quad (1)$$

**Example 1 (The Drebin Malware Aetector).** Drebin is an Android malware detector trained from static features [8]. Table 2 summarizes Drebin’s feature set, which includes four subsets of features  $S_1, S_2, S_3, S_4$  extracted from the AndroidManifest.xml and another four subsets of features  $S_5, S_6, S_7, S_8$  extracted from the disassembled DEX code files (recalling that DEX code is compiled from a program written in some language and can be understood by the Android Runtime). Specifically,  $S_1$  contains features related to the access of an APK to smartphone hardware (e.g., camera, touchscreen, or GPS module);  $S_2$  contains features related to APK’s requested permissions listed in the manifest prior to installation;  $S_3$  contains features related to application components (e.g., *activities*, *service*, *receivers*, and *providers*.);  $S_4$  contains features related to APK’s communications with the other APKs;  $S_5$  contains features related to critical system API calls, which cannot run without appropriate permissions or the *root* privilege;  $S_6$  contains features corresponding to the used

Table 2. Drebin Features

Feature set	
Manifest	$S_1$ Hardware components
	$S_2$ Requested permissions
	$S_3$ App components
	$S_4$ Filtered intents
Dexcode	$S_5$ Restricted API calls
	$S_6$ Used permissions
	$S_7$ Suspicious API calls
	$S_8$ Network addresses

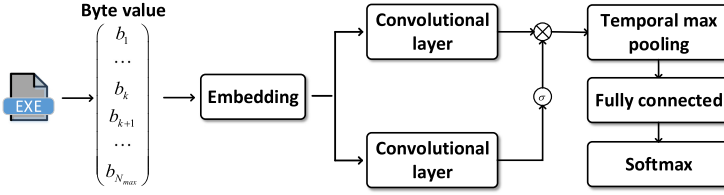


Fig. 2. MalConv architecture [99].

permissions;  $S_7$  contains features related to API calls that can access sensitive data or resources in a smartphone; and  $S_8$  contains features related to IP addresses, hostnames and URLs found in the disassembled codes. The feature representation is binary, meaning  $\phi = \phi_c : \mathcal{Z} \mapsto \{0, 1\}^d$  with  $|S| = d$  and  $\mathbf{x} = (x_1, \dots, x_d)$ , where  $x_i = 1$  if the corresponding feature is present in the APK  $z$  and  $x_i = 0$  otherwise. A file  $z$  in the feature space looks like the following:

$$\mathbf{x} = \phi(z) \rightarrow \begin{pmatrix} \dots & \dots \\ 0 & \text{permission::SEND_SMS} \\ 1 & \text{permission::READ_CONTACTS} \\ \dots & \dots \\ 1 & \text{api\_call::getDeviceID} \\ 0 & \text{api\_call::setWifiEnabled} \\ \dots & \dots \end{pmatrix} \left. \vphantom{\begin{pmatrix} \dots & \dots \\ 0 & \text{permission::SEND_SMS} \\ 1 & \text{permission::READ_CONTACTS} \\ \dots & \dots \\ 1 & \text{api\_call::getDeviceID} \\ 0 & \text{api\_call::setWifiEnabled} \\ \dots & \dots \end{pmatrix}} \right\} \begin{matrix} \\ S_2 \\ \\ S_5 \\ \end{matrix}$$

Drebin uses a linear SVM to learn classifiers.

*Example 2 (The MalConv Malware Detector).* MalConv [99] is **Convolutional Neural Network (CNN)**-based Windows **Portable Executable (PE)** malware detector learned from raw binary programs (i.e., end-to-end detection) [67]. Figure 2 depicts its architecture. The sequence of binary code is transformed into byte values (between 0 to 255) with the maximum length bounded by  $N_{max}$  (e.g.,  $N_{max} = 2^{21}$  bytes or 2MB). Each byte is further mapped into a real-valued vector using the embedding [35]. The CNN layer and pooling layer learn abstract representations. The embedding, CNN and pooling layers belong to feature extraction  $\phi_a$ , and the fully-connected and softmax layers belong to the classification operation  $\phi$ .

## 2.2 Framework

We systematize AMD studies through the lens of four aspects: (i) the assumptions that are made; (ii) the attack or threat model in terms of attacker  $\mathcal{A}$ 's *objective* and  $\mathcal{A}$ 's *input*, with the latter including  $\mathcal{A}$ 's information about the defender  $\mathcal{I}$  and  $\mathcal{A}$ 's own; (iii) the defense in terms of  $\mathcal{I}$ 's



*objective* and  $\mathcal{I}$ 's *input*, with the latter including  $\mathcal{I}$ 's information about  $\mathcal{A}$  and  $\mathcal{I}$ 's own; (iv) the security properties that are at stake. These four aspects are, respectively, elaborated below.

**2.2.1 Systematizing Assumptions.** Five assumptions have been made in the AMD literature. Assumption 1 below says that the data samples in  $D$  are **Independent and Identically Distributed (IID)**, which is a strong assumption and researchers have started to weaken it [52, 110].

ASSUMPTION 1 (IID ASSUMPTION; SEE, E.G., [107]). *Computer files in training data and testing data are independently drawn from the same distribution.*

Assumption 2 below is adapted from AML context, where humans can serve as an oracle  $O$  for determining whether two images are the same [126]. In the AMD context,  $O$  can be instantiated as (or approximated by) malware analysts [2, 27, 65, 114] or automated tools (e.g., Sandbox [36, 134]), with the latter often using heuristic rules produced by malware analysts (e.g., YARA [3]).

ASSUMPTION 2 (Oracle ASSUMPTION; ADAPTED FROM [126]). *There is an oracle  $O : \mathcal{Z} \times \mathcal{Z} \rightarrow \{\text{true}, \text{false}\}$  that tells if two files  $z, z' \in \mathcal{Z}$  have the same functionality or not;  $\text{true} \leftarrow O(z, z')$  if and only if  $z$  and  $z'$  have the same functionality.*

Assumption 3 below says that there is a way to measure the degree of manipulations by which one file is transformed to another.

ASSUMPTION 3 (Measurability ASSUMPTION [36, 68]). *There is a function  $\Gamma(z, z') : \mathcal{Z} \times \mathcal{Z} \rightarrow \mathbb{R}_+$  that measures the degree of manipulations according to which a file  $z' \in \mathcal{Z}$  can be derived from the file  $z \in \mathcal{Z}$ .*

Since Assumption 3 is often difficult to validate,  $\Gamma(z, z')$  may be replaced by a function that quantifies the degree of manipulation that can turn feature representation  $\mathbf{x}$  into  $\mathbf{x}'$ , where  $\mathbf{x} = \phi(S, z)$  and  $\mathbf{x}' = \phi(S, z')$ . This leads to:

ASSUMPTION 4 (Smoothness ASSUMPTION [13]). *There is a function  $C(\mathbf{x}, \mathbf{x}') : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+$  such that  $C(\phi(S, z), \phi(S, z')) \approx 0$  when  $(\Gamma(z, z') \approx 0) \wedge (\text{true} \leftarrow O(z, z'))$ .*

Assumption 5 below says that the inverse of feature extraction,  $\phi^{-1}$ , is solvable so that a perturbed representation  $\mathbf{x}'$  can be mapped back to a legitimate file.

ASSUMPTION 5 (Invertibility ASSUMPTION [76]). *Feature extraction  $\phi$  is invertible, meaning that given  $\mathbf{x}'$ , the function  $\phi^{-1} : \mathcal{X} \rightarrow \mathcal{Z}$  produces  $z' = \phi^{-1}(\mathbf{x}')$ .*

Recall that the feature extraction function  $\phi$  may be composed of a hand-crafted  $\phi_c$  and an automated  $\phi_a$ , where  $\phi_c$  may be neither differentiable nor invertible [16, 97]. This means  $\mathbf{x}'$  may not be mapped to a legitimate file. Researchers tend to relax the assumption by overlooking the interdependent features [76, 114], while suffering from the side-effect  $\mathbf{x}' \neq \phi(\phi^{-1}(\mathbf{x}'))$  [97, 114].

**2.2.2 Systematizing Attacks.** We systematize attacks from two perspectives: *attacker's objective* (i.e., what the attacker attempts to accomplish) and *attacker's input* (i.e., what leverages the attacker can use). Whenever possible, we seek rigorous definitions to specify the attacker's input, while noting that these definitions have been scattered in the literature. We believe this specification is important because it can serve as a common reference for future studies. To demonstrate this, we discuss how to apply it to formulate a partial-order structure for comparing attacks.

**Attacker's Objective.** There are three kinds of objectives: (i) Indiscriminate, meaning  $\mathcal{A}$  attempts to cause as many false-negatives as possible [6, 28, 53, 100, 127, 136]; (ii) Targeted, meaning  $\mathcal{A}$  attempts to cause specific false-negatives (i.e., making certain malicious files evade the detection [40, 118]); (iii) Availability, meaning  $\mathcal{A}$  attempts to frustrate defender  $\mathcal{I}$  by rendering  $\mathcal{I}$ 's classifier  $f$  unusable (e.g., causing substantially high false-positives [20, 30, 40, 87, 98]).

Table 3. Attributes for Specifying  $\mathcal{A}$ 's and  $\mathcal{I}$ 's Input

Attributes	Attacker $\mathcal{A}$ 's input	Defender $\mathcal{I}$ 's input
Attributes under $\mathcal{I}$ 's control but may be known to $\mathcal{A}$ to some extent		
$A_1$ : Training set $D_{train}$	$a_1 \in [0, 1]$	1
$A_2$ : Defense technique	$a_2 \in \{0, 1\}$	1
$A_3$ : Feature set $S$	$a_3 \in [0, 1]$	1
$A_4$ : Learning algorithm $F_\theta$	$a_4 \in [0, 1]$	1
$A_5$ : Response	$a_5 \in \{0, 1\}$	1
Attributes under $\mathcal{A}$ 's control but may be known to $\mathcal{I}$ to some extent		
$A_6$ : Manipulation set $\mathcal{M}$	1	$a_6 \in [0, 1]$
$A_7$ : Attack tactic	1	$a_7 \in \{0, 1\}$
$A_8$ : Attack technique	1	$a_8 \in \{0, 1\}$
$A_9$ : Adversarial examples	1	$a_9 \in [0, 1]$

**Attacker's Input.** Table 3 highlights the attributes we define to describe  $\mathcal{A}$ 's input, including: five attributes  $A_1, \dots, A_5$  that are under  $\mathcal{I}$ 's control (indicated by 1) but may be known to  $\mathcal{A}$  at some extent  $a_1, \dots, a_5$ , respectively; and four attributes  $A_6, \dots, A_9$  that are under  $\mathcal{A}$ 's control (indicated by 1). These attributes are elaborated below.

(i)  $A_1$ : it describes  $\mathcal{I}$ 's training set  $D_{train}$  for learning classifier  $f$ . We use  $a_1 \in [0, 1]$  to represent the extent at which  $D_{train}$  is known to  $\mathcal{A}$ . Let  $\hat{D}_{train}$  be the training files that are known to  $\mathcal{A}$ . Then,  $a_1 = |\hat{D}_{train} \cap D_{train}|/|D_{train}|$ .

(ii)  $A_2$ : it describes  $\mathcal{I}$ 's techniques, which can be **Ensemble Learning (EL)**, **Weight Regularization (WR)**, **AT**, **Verifiable Learning (VL)**, **Robust Feature (RF)**, **Input Transformation (IT)**, **Classifier ranDomization (CD)**, and **SE**. Let  $A_2 \in \{\text{EL, WR, AT, VL, RF, IT, CD, SE}\}$  and  $a_2 \in \{0, 1\}$  such that  $a_2 = 0$  means  $\mathcal{A}$  does not know  $\mathcal{I}$ 's techniques and  $a_2 = 1$  means  $\mathcal{A}$  knows  $\mathcal{I}$ 's technique. The techniques are defined as follows. Definition 1 says that  $\mathcal{I}$  constructs multiple classifiers and uses them collectively in malware detection.

*Definition 1 (Ensemble Learning or EL [142]).* Let  $\mathcal{H}$  be  $\mathcal{I}$ 's classifier space. Given  $K$  classifiers  $\{f_i\}_{i=1}^K$  where  $f_i \in \mathcal{H}$  and  $f_i : \mathcal{Z} \rightarrow [0, 1]$ , let  $f_i$  be assigned with weight  $\omega_i$  with  $\sum_{i=1}^K \omega_i = 1$  and  $\omega_i \geq 0$ . Then,  $f = \sum_{i=1}^K \omega_i f_i$ .

Definition 2 says that  $\mathcal{I}$  uses regularization (e.g.,  $\ell_2$  regularization [89] or *dropout* [112]) to decrease model's sensitivity to adversarial examples.

*Definition 2 (Weight Regularization or WR [49]).* Given a regularization item  $\Omega$  (e.g., constraints imposed on the learnable parameters), the empirical risk is  $\min_{\theta} [\mathcal{L}(\theta, D_{train}) + \Omega(\theta)]$ , where  $\mathcal{L}$  is defined in Equation (1).

Definition 3 says that  $\mathcal{I}$  proactively makes its classifier  $f$  perceive some information about adversarial files. That is,  $\mathcal{I}$  augments the training set by incorporating adversarial examples that may be produced by  $\mathcal{I}$ ,  $\mathcal{A}$ , or both.

*Definition 3 (Adversarial Training or AT [53]).* Let  $D'$  denote a set of adversarial file-label pairs. Then,  $\mathcal{I}$  tunes model parameters by minimizing the empirical risk:  $\min_{\theta} [\mathcal{L}(\theta, D_{train}) + \beta \mathcal{L}(\theta, D')]$ , where  $\beta \geq 0$  denotes a balance factor.

Definition 4 says that  $\mathcal{I}$  intentionally over-estimates the error incurred by  $\mathcal{A}$ 's manipulations and then minimizes it.



*Definition 4 (Verifiable Learning or VL [130]).* Given  $(z, y) \in D_{train}$  and a manipulation set  $\hat{\mathcal{M}}$  known by  $\mathcal{I}$ , let  $z(\hat{\mathcal{M}})$  denote the upper and lower boundaries on  $\hat{\mathcal{M}}$ . Then, this defense technique minimizes the following loss function derived from Equation (1):  $L(F_\theta(\phi_c(S, z)), y) + \beta L(F_\theta(\phi_c(S, z(\hat{\mathcal{M}}))), y)$ .

Definition 5 says that  $\mathcal{I}$  uses a set of features  $S^* \subseteq S$  that can lead to higher detection capability against adversarial example attacks.

*Definition 5 (Robust Feature or RF; Adapted from [141]).* Given a training set  $D_{train} \cup D'$  that contains (adversarial) file-label pairs, the set of RF set  $S^*$  is

$$S^* = \arg \min_{\tilde{S} \subseteq S} \sum_{(z, y) \in D_{train} \cup D'} L(\tilde{F}_\theta(\phi_c(\tilde{S}, z)), y),$$

where  $\tilde{F}_\theta$  is  $F_\theta$  or a simplified learning algorithm that is computationally faster than  $F_\theta$  [141].

Definition 6 says that  $\mathcal{I}$  aims at using non-learning methods (e.g., de-obfuscation as shown in Proguard [14]) to offset  $\mathcal{A}$ 's manipulations.

*Definition 6 (Input Transformation or IT, Adapted from [28]).* Let  $IT : \mathcal{Z} \rightarrow \mathcal{Z}$  denote an IT in the file space. Given file  $z$  and transformation  $IT$ , the classifier is  $f = \varphi(\phi(IT(z)))$ .

Definition 7 says that  $\mathcal{I}$  randomly chooses  $m$  classifiers and uses their results for prediction. That is,  $\mathcal{I}$  aims at randomizing the feature representation used by  $f$ , the learning algorithm, and/or response to  $\mathcal{A}$ 's queries (to prevent  $\mathcal{A}$  from inferring information about  $f$ ).

*Definition 7 (Classifier Randomization or CD; Adapted from [65]).* Given  $\mathcal{I}$ 's classifier space  $\mathcal{H}$  and an input file  $z$ ,  $\mathcal{I}$  randomly selects  $m$  classifiers from  $\mathcal{H}$  with replacement, say  $\{f_i\}_{i=1}^m$ . Then,  $f = \frac{1}{m} \sum_{i=1}^m f_i(z)$ .

Instead of enhancing malware detectors, Definition 8 provides an alternative that detects the adversarial examples for further analysis.

*Definition 8 (Sanitizing Examples or SE; Adapted from [23, 30]).*  $\mathcal{I}$  aims at detecting adversarial files by using function  $\text{flag} : \mathcal{Z} \rightarrow \{\text{yes}, \text{no}\}$  to flag a file as adversarial (yes) or not (no).

(iii)  $A_3$ : it describes  $\mathcal{I}$ 's feature set  $S$ . We use  $a_3 \in [0, 1]$  to represent the extent at which  $\mathcal{A}$  knows about  $S$ . Let  $\hat{S}$  denote the features that are known to  $\mathcal{A}$ . Then,  $a_3 = |\hat{S} \cap S|/|S|$ .

(iv)  $A_4$ : it describes  $\mathcal{I}$ 's learning algorithm  $F_\theta$ , the set of trainable parameters  $\theta$ , and hyperparameters (which are set manually, e.g.,  $\beta$  in Definition 3) [40, 88]. We use  $a_4 \in [0, 1]$  to represent that  $\mathcal{A}$  knows an  $a_4$  degree about  $A_4$ , where  $a_4 = 0$  means  $\mathcal{A}$  knows nothing and  $a_4 = 1$  means  $\mathcal{A}$  knows everything.

(v)  $A_5$ : it describes  $\mathcal{I}$ 's response to  $\mathcal{A}$ 's query to  $f$  (if applicable), which is relevant because  $\mathcal{A}$  can learn useful information about  $f$  by observing  $f$ 's responses [119]. We define  $a_5 \in \{0, 1\}$  such that  $a_5 = 0$  means there is a limit on the response that can be made by  $\mathcal{A}$  to  $f$  (referred as LQ) and  $a_5 = 1$  means there is no limit (referred as FQ).

(vi)  $A_6$ : it describes  $\mathcal{A}$ 's manipulation set in the problem space, which describes perturbations for generating adversarial files (adapted from *perturbation set* in the AML literature [123]):

$$\mathcal{M} = \{\delta : (z' \leftarrow \mathcal{A}(z, \delta)) \wedge (\text{true} \leftarrow \mathcal{O}(z, z')) \wedge (z \in \mathcal{Z}) \wedge (z' \neq z)\}.$$

$\mathcal{M}$  is application-specific. For instance, an APK permits adding codes or renaming class names [31, 39, 53, 76], a Windows PE permits adding codes or changing PE *section* names [5, 37, 38, 68], and a **Portable Document Format (PDF)** file permits appending dead-code at its end [114] or add new instructions [25, 134]. This means that a perturbation  $\delta \in \mathcal{M}$  can be a tuple specifying

an operator (e.g., addition or removal), an object (e.g., a feature used by  $\mathcal{I}$ ), and other kinds of information (e.g., perturbation location in a file).

Since it is often infeasible to enumerate the entire manipulation set,  $\mathcal{A}$  may leverage an empirical one  $\widetilde{\mathcal{M}}$  [31, 39, 53, 76, 97, 114], which can be defined in the problem or feature space. Manipulations in the problem space must not violate the relevant constraints (e.g., adding APIs in an APK should not cause the request of unauthorized permissions). Manipulations in the feature space facilitate efficient computing via gradient-based methods as long as the inverse feature mapping  $\phi^{-1}$  is available. Furthermore, we can use the manipulation set  $\mathcal{M}$  to define a *feature manipulation set*  $\mathbf{M}$ :

$$\mathbf{M} = \{\delta_{\mathbf{x}} = \mathbf{x}' - \mathbf{x} : (\mathbf{x} = \phi(z)) \wedge (\mathbf{x}' = \phi(z')) \wedge (z' \leftarrow \mathcal{A}(z, \delta)) \wedge (\delta \in \mathcal{M}) \wedge (z \in \mathcal{Z})\}. \quad (2)$$

In order to compute  $\mathbf{M}$  efficiently, one strategy is to estimate a feature-space analog of  $\widetilde{\mathcal{M}}$ , denoted by  $\widetilde{\mathbf{M}}$  [109, 114]. This, however, demands resolving the invertibility Assumption 5.

(vii)  $A_7$ : it describes  $\mathcal{A}$ 's attack tactics. We consider two tactics: classifier *evasion* and classifier *poisoning*. For the evasion attack, we consider three variants: **basic evasion (BE)**, **optimal evasion 1 (OE1)**, and **optimal evasion 2 (OE2)**. For the poisoning attack, we consider two variants: **basic poisoning (BP)** and **optimal poisoning (OP)**. Correspondingly, we have  $A_7 \in \{\text{BE, OE1, OE2, BP, OP}\}$ . These tactics are elaborated below, while noting that they do not explicitly call oracle  $\mathcal{O}$  because definitions of manipulation sets  $\mathcal{M}$  already assure that manipulations preserve functionalities of non-adversarial files.

As shown in Definition 9, the BE attack is that  $\mathcal{A}$  uses a set of perturbations  $\delta_z \subseteq \mathcal{M}$  to manipulate a malicious file  $z$ , which is classified by  $\mathcal{I}$ 's classifier  $f$  as  $+\leftarrow f(z)$ , to an adversarial file  $z'$  such that  $-\leftarrow f(z')$ .

*Definition 9 (Basic Evasion or BE [53]).*  $\mathcal{A}$  looks for  $\delta_z \subseteq \mathcal{M}$  to achieve the following for  $z \in \mathcal{Z}$  with  $+\leftarrow f(z)$ :

$$-\leftarrow f(z') \text{ where } (z' \leftarrow \mathcal{A}(z, \delta_z)) \wedge (\delta_z \subseteq \mathcal{M}).$$

As shown in Definition 10, the attacker attempts to minimize the degree of perturbations. In other words, this attack tactic is the same as BE, except that  $\mathcal{A}$  attempts to minimize the manipulation when perturbing a non-adversarial file  $z \in \mathcal{Z}$  into an adversarial file  $z' \in \mathcal{Z}$ .

*Definition 10 (Optimal Evasion 1 or OE1; Adapted from [24]).*  $\mathcal{A}$  attempts to achieve the following for  $z \in \mathcal{Z}$  with  $+\leftarrow f(z)$ :

$$\min_{z'} \Gamma(z', z) \text{ s.t. } (z' \leftarrow \mathcal{A}(z, \delta_z)) \wedge (\delta_z \subseteq \mathcal{M}) \wedge (-\leftarrow f(z')).$$

As shown in Definition 11, the attacker attempts to maximize  $\mathcal{I}$ 's loss for waging high-confidence evasion attacks, while noting the small perturbations may be incorporated.

*Definition 11 (Optimal Evasion 2 or OE2; Adapted from [16]).*  $\mathcal{A}$  attempts to achieve the following for  $z \in \mathcal{Z}$  with  $+\leftarrow f(z)$ :

$$\max_{z'} L(F_{\theta}(\phi_c(S, z')), +) \text{ s.t. } (z' \leftarrow \mathcal{A}(z, \delta_z)) \wedge (\delta_z \subseteq \mathcal{M}) \wedge (-\leftarrow f(z')).$$

Let  $D'_{poison} \subset \mathcal{D}$  be a set of adversarial file-label pairs obtained by manipulating non-adversarial files in  $D_{poison}$ . Let  $D'_{train} \leftarrow D_{train} \cup D'_{poison}$  be the contaminated training data for learning a classifier  $f'$  with parameters  $\theta'$ . As shown in Definition 12, the BP attack is that the attacker aims at making  $f'$  mis-classify the files in a dataset  $D_{target}$ , while accommodating the attacks that  $\mathcal{A}$  manipulates labels of the files in  $D_{poison}$  [95].

*Definition 12 (Basic Poisoning or BP [9]).* Given a set  $D_{target}$  of files where  $+ \leftarrow f(z)$  for  $z \in D_{target}$  and a set  $D_{poison}$  of non-adversarial files,  $\mathcal{A}$  attempts to perturb files in  $D_{poison}$  to adversarial ones  $D'_{poison} = \{(\mathcal{A}(z, \delta_z), \mathcal{A}(y)) : ((z, y) \in D_{poison}) \wedge (\delta_z \subseteq \mathcal{M}) \wedge (\mathcal{A}(y) \in \{+, -\})\}$  such that classifier  $f'$  learned from  $D'_{train} \leftarrow D_{train} \cup D'_{poison}$  mis-classifies the files in  $D_{target}$ . Formally, the attacker intends to achieve the following for  $\forall z \in D_{target}$ :  $- \leftarrow f'(z)$  where  $f'$  is learned from  $D'_{train} \leftarrow D_{train} \cup D'_{poison}$ .

As shown in Definition 13, the OP attack is the same as BF, except that  $\mathcal{A}$  attempts to maximize the loss when using classifier  $f'$  with parameter  $\theta'$  to classify files in  $D_{target}$ . Definition 13 can have multiple variants by considering bounds on  $|D'_{poison}|$  [116] or bounds on the degree of perturbations  $|\delta_z|$  [118].

*Definition 13 (Optimal Poisoning or OP [87]).* Given  $D_{poison}$ ,  $\mathcal{A}$  perturbs  $D_{poison}$  into  $D'_{poison}$  for achieving:

$$\max_{D'_{poison}} \mathcal{L}(\theta', D_{target}) \text{ where } \theta' \leftarrow \arg \min_{\theta} \mathcal{L}(\theta, D_{train} \cup D'_{poison}).$$

(viii)  $A_8$ : it describes  $\mathcal{A}$ 's attack techniques, such as **Gradient-based Optimization (GO)**, **Sensitive Features (SF)**, **Mimicry (MI)**, **TRansferability (TR)**, **Heuristic Search (HS)**, **Generative Model (GM)**, and **Mixture Strategy (MS)**. We denote this by  $A_8 \in \{\text{GO, SF, MI, TR, HS, GM, MS}\}$ . Let  $\mathcal{A}$  have a classifier  $\hat{f}$ , which consists of a hand-crafted feature extraction  $\hat{\phi}_c$  and a parameterized model  $\hat{F}_{\hat{\theta}}$ . Let  $\mathcal{A}$  also have an objective function  $L_{\mathcal{A}} : [0, 1] \times \mathcal{Y} \rightarrow \mathcal{R}$ , which measures  $\hat{f}$ 's error or  $\mathcal{A}$ 's failure in evasion [16, 24]. Note that  $\hat{f}$  and  $L_{\mathcal{A}}$  can be the same as, or can mimic (by leveraging  $\mathcal{A}$ 's knowledge about  $I$ 's attributes  $A_1, \dots, A_5$ ),  $I$ 's classifier  $f$  and loss function  $L$ , respectively.

The attack technique specified by Definition 14 is that  $\mathcal{A}$  solves the feature-space optimization problems described in Definitions 10, 11, and 13 by using some GO method and then leverages the invertibility Assumption 5 to generate adversarial malware examples.

*Definition 14 (Gradient-based Optimization or GO, Adapted from [24, 87]).* Let  $\mathbf{x} \leftarrow \hat{\phi}_c(\hat{S}, z)$  and  $\mathbf{x}' \leftarrow \mathbf{x} + \delta_x$ . The feature-space optimization problem in Definition 10 can be written as

$$\min_{\delta_x} C(\mathbf{x}, \mathbf{x} + \delta_x) \text{ s.t. } (\delta_x \in [\underline{\mathbf{u}}, \bar{\mathbf{u}}]) \wedge (\hat{F}_{\hat{\theta}}(\mathbf{x}') < \tau), \quad (3)$$

where  $\underline{\mathbf{u}}$  and  $\bar{\mathbf{u}}$  are, respectively, the lower and upper bounds on  $\mathbf{M}$  (e.g.,  $\delta_x \in [-\mathbf{x}, 1 - \mathbf{x}]$  for binary representation  $\mathbf{x}$ ). The feature-space optimization problem in Definition 11 can be written as

$$\max_{\delta_x} L_{\mathcal{A}}(\hat{F}_{\hat{\theta}}(\mathbf{x} + \delta_x), +) \text{ s.t. } (\delta_x \in [\underline{\mathbf{u}}, \bar{\mathbf{u}}]). \quad (4)$$

The feature-space optimization problem specified in Definition 13 can be written as

$$\max_{\delta_x \in [\underline{\mathbf{u}}, \bar{\mathbf{u}}]} \mathbb{E}_{(z, y) \in D_{target}} L_{\mathcal{A}}(\hat{F}_{\hat{\theta}}(\hat{\phi}_c(\hat{S}, z), y)), \forall (z, y) \in D_{poison} \quad (5)$$

$$\text{where } \hat{\theta}' \leftarrow \arg \min_{\hat{\theta}} \mathbb{E}_{(z_t, y_t) \in \hat{D}_{train} \cup \{(\hat{\phi}_c^{-1}(\hat{\phi}_c(z) + \delta_x), y')\}} L_{\mathcal{A}}(\hat{F}_{\hat{\theta}}(\hat{\phi}_c(\hat{S}, z_t), y_t)).$$

In order to calculate the gradients of loss function  $L_{\mathcal{A}}$  with respect to  $\delta_x$  in Equations(3) and (4), inequality constraints can be handled by appending penalty items to the loss function in question and box-constraints can be coped with by using gradient projection [24, 78]. Since  $\mathbf{x} + \delta_x$  is continuous, the GO attack technique needs to map  $\delta_x$  to a discrete perturbation vector in  $\mathbf{M}$ , for instance by using the nearest neighbor search [78]. The gradients of loss function  $L_{\mathcal{A}}$  with respect to  $\delta_x$  in Equation (5) are delicate to deal with. One issue is the indirect relation between  $L_{\mathcal{A}}$  and

$\delta_x$ , which can be handled by the chain rule [73]. Another issue is the difficulty that is encountered when computing the partial derivatives  $\partial \hat{\theta}' / \partial \delta_x$  [87]. For dealing with this, researchers often relax the underlying constraints (e.g., by supposing that  $\hat{F}_{\hat{\theta}}$  is a linear model).

The attack technique specified by Definition 15 is that  $\mathcal{A}$  perturbs malware examples by injecting or removing a small number of features to decrease the classification error measured by the loss function  $L_{\mathcal{A}}$  as much as possible.

*Definition 15 (Sensitive Features or SF, Adapted from [74]).* For evasion attacks,  $\mathcal{A}$  aims at maximizing the following with respect to a given malware example-label pair  $(z, +)$ :

$$\max_{z'} L_{\mathcal{A}}(\hat{F}_{\hat{\theta}}(\hat{\phi}(\hat{S}, z')), +) \text{ s.t. } (z' \leftarrow \mathcal{A}(z, \delta_z)) \wedge (\delta_z \subseteq \mathcal{M}) \wedge (|\delta_z| \leq m),$$

where  $m$  is the maximum degree of manipulations.

For poisoning attacks,  $\mathcal{A}$  aims at maximizing the following with respect to the given  $D_{poison}$  and  $D_{target}$ ,

$$\max_{D'_{poison}} \mathbb{E}_{(\hat{z}, \hat{y}) \in D_{target}} L_{\mathcal{A}}(\hat{F}_{\hat{\theta}'}(\hat{\phi}_c(\hat{S}, \hat{z}), \hat{y})), \quad (6)$$

where  $\hat{\theta}'$  is learned from  $\hat{D}_{train} \cup D'_{poison}$  such that  $\forall z' \in D'_{poison}$  is obtained via the perturbation  $\delta_z$  with obeying  $(z' \leftarrow \mathcal{A}(z, \delta_z)) \wedge (\delta_z \subseteq \mathcal{M}) \wedge (z \in D_{poison}) \wedge (|\delta_z| \leq m)$ .

The attack technique specified by Definition 16 is that  $\mathcal{A}$  perturbs malware example  $z$  by mimicking a benign example, while noting that this attack technique can be algorithm-agnostic.

*Definition 16 (MImicry or MI, Adapted from [114]).* Given a set of benign examples  $D_{ben}$  and a malware example  $z$ ,  $\mathcal{A}$  aims at achieving the following minimization:

$$\min_{\delta_z \in \mathcal{M}} \Gamma(\mathcal{A}(z, \delta_z), z_{ben}) \text{ s.t. } (\exists z_{ben} \in D_{ben}). \quad (7)$$

The attack technique specified by Definition 16 can be extended to accommodate the similarity between representations in the feature space [16, 114]. The attack technique specified by Definition 17 is that  $\mathcal{A}$  generates adversarial examples against a surrogate model  $\hat{f}$ .

*Definition 17 (TRansferability or TR, Adapted from [91]).*  $\mathcal{A}$  learns a surrogate model  $\hat{f}$  of  $f$  from  $\hat{D}_{train}$ ,  $\hat{S}$ ,  $\hat{\phi}_c$  and  $\hat{F}$ . For evasion attacks,  $\mathcal{A}$  achieves  $- \leftarrow \hat{f}(z')$  by perturbing malware example  $z$  to  $z'$  and then attacks  $f$  with  $z'$ . For poisoning attacks,  $\mathcal{A}$  contaminates  $\hat{f}$  to  $\hat{f}'$  such that  $- \leftarrow \hat{f}'(\hat{z})$  for  $\forall (\hat{z}, \hat{y}) \in D_{target}$ , by poisoning the training set  $\hat{D}_{train}$  with  $D'_{poison}$  and the attacks  $f$  with  $D'_{poison}$ .

The attack technique specified by Definition 18 is that  $\mathcal{A}$  searches perturbations in  $\mathcal{M}$  via some heuristics, while leveraging oracle  $\mathcal{O}$ 's responses to  $\mathcal{A}$ 's queries and  $f$ 's responses to  $\mathcal{A}$ 's queries. Since  $\mathcal{M}$  is defined with respect to the problem space, this attack technique does not need the invertibility Assumption 5.

*Definition 18 (Heuristic Search or HS).* Let  $h$  be a function taking  $\mathcal{O}$ 's response and  $f$ 's response as input. Given a malware example  $z$ ,  $\mathcal{A}$  looks for an  $m$ -length manipulation path

$$\langle z_{(0)}, z_{(1)}, \dots, z_{(m)} \rangle \text{ s.t. } z_{(i+1)} = \mathcal{A}(z_{(i)}, \delta_{z_{(i)}}) \wedge (\delta_{z_{(i)}} \in \mathcal{M}) \wedge (h(\mathcal{O}, f, z, z_{(i)}) \leq h(\mathcal{O}, f, z, z_{(i+1)}))$$

where  $z_{(0)} = z$ .

The attack technique specified by Definition 19 is that  $\mathcal{A}$  uses a generative model  $G$  with parameters  $\theta_g$  to perturb malware representation vectors and then leverages the invertibility Assumption 5 to turn the perturbed vector into an adversarial malware example.

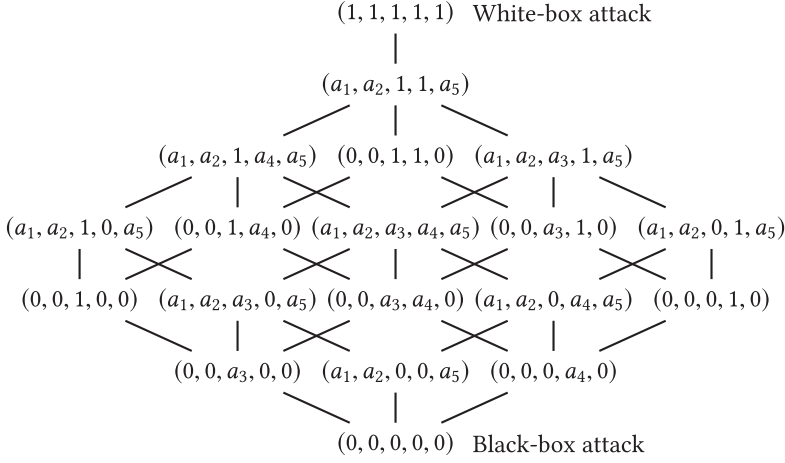


Fig. 3. A portion of the partial order defined over  $(a_1, \dots, a_5)$ .

**Definition 19 (Generative Model or GM).** Given a malware representation vector  $\mathbf{x} = \hat{\phi}_c(\hat{S}, z)$ ,  $\mathcal{A}$  achieves

$$\max_{\theta_g} L_{\mathcal{A}}(\hat{F}_{\hat{\theta}}(G_{\theta_g}(\mathbf{x})), +) \text{ s.t. } G_{\theta_g}(\mathbf{x}) \in [\underline{\mathbf{u}} - \mathbf{x}, \bar{\mathbf{u}} - \mathbf{x}]$$

and leverages the invertibility Assumption 5 to obtain an adversarial example  $z' = \hat{\phi}_c^{-1}(G_{\theta_g}(\mathbf{x}))$ .

The attack technique specified by Definition 20 is that  $\mathcal{A}$  combines multiple perturbation methods to perturb an example.

**Definition 20 (Mixture Strategy or MS [76]).** Let  $\mathcal{H}_A$  denote the space of generative methods and  $\mathcal{W}_a = \{\mathbf{w}_a : \mathbf{w}_a = (w_{a,1}, \dots, w_{a,K}), w_{a,i} \geq 0\}$  with  $i = 1, \dots, K$  denote the weights space. Given a malware example  $z$ ,  $\mathcal{A}$  aims at achieving

$$\max_{\mathbf{w}_a} L_{\mathcal{A}}(\hat{F}_{\hat{\theta}}(\hat{\phi}(z')), +) \text{ s.t. } \left( z' = \sum_{i=1}^K w_{a,i} g_i(z) \right) \wedge (O(z, z') = \text{true}) \wedge (g_i \in \mathcal{H}_A) \wedge (\mathbf{w}_a \in \mathcal{W}_a).$$

(ix)  $A_9$ : it corresponds to  $\mathcal{A}$ 's adversarial files. Given file manipulation set  $\mathcal{M}$ , the corresponding set of adversarial files is defined as  $\mathcal{Z}_{\mathcal{M}} = \{\mathcal{A}(z, \delta_z) : (z \in \mathcal{Z}) \wedge (\delta_z \subseteq \mathcal{M})\}$ . Given feature manipulation set  $\mathbf{M}$ , the set of adversarial feature vectors is:  $\mathcal{X}_{\mathbf{M}} = \{\mathbf{x}' : (\mathbf{x}' = \mathbf{x} + \delta_{\mathbf{x}}) \wedge (\delta_{\mathbf{x}} \in \mathbf{M})\}$ .

**On the Usefulness of the Preceding Specification.** The preceding specification can be applied to formulate a partial order in the attribute space, which allows to compare attacks unambiguously. Figure 3 depicts how vector  $(a_1, \dots, a_5)$  formulates a partial order between the widely-used informal notions of *black-box* attack, namely  $(a_1, a_2, a_3, a_4, a_5) = (0, 0, 0, 0, 0)$ , and *white-box* attack, namely  $(a_1, a_2, a_3, a_4, a_5) = (1, 1, 1, 1, 1)$ ; there are many kinds of gray-box attacks in between.

**2.2.3 Systematizing Defenses.** Similarly, we systematize defenses from two perspectives: *defender's objective* (i.e., what the defender aims at achieving) and *defender's input* (i.e., what leverages the defender can use). We also discuss how to apply the specification to formulate a partial-order structure for comparing defenses.

**Defender's Objectives.**  $\mathcal{I}$  aims at detecting ideally all of the malicious files, adversarial and non-adversarial alike, while suffering from small side-effects (e.g., increasing false-positives).

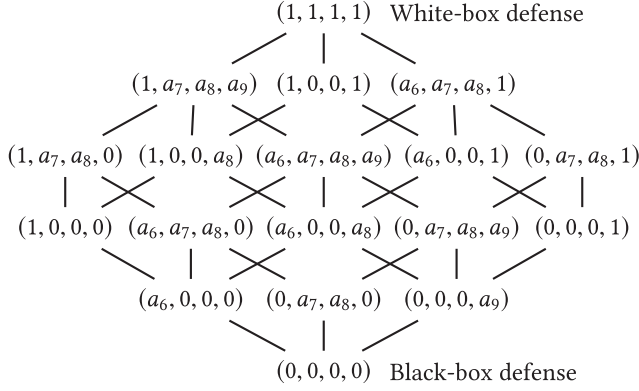


Fig. 4. A portion of the partial order defined over  $(a_6, \dots, a_9)$ .

**Defender's Input.** As highlighted in Table 3,  $\mathcal{I}$ 's input includes attributes  $A_1, \dots, A_5$ , which are under  $\mathcal{I}$ 's control, and the extent  $a_6, \dots, a_9$  at which  $\mathcal{I}$ , respectively, knows about attributes  $A_6, \dots, A_9$ , which are under  $\mathcal{A}$ 's control. Note that  $A_1, \dots, A_9$  have been defined above.

- We define  $a_6 \in [0, 1]$  to represent the extent at which  $\mathcal{I}$  knows  $\mathcal{A}$ 's manipulation set  $\mathcal{M}$ . Let  $\hat{\mathcal{M}} \subseteq \mathcal{M}$  denote the subset of  $\mathcal{A}$ 's manipulation set known to  $\mathcal{I}$ . Then, we set  $a_6 = |\hat{\mathcal{M}}|/|\mathcal{M}|$ .
- We define  $a_7 \in \{0, 1\}$  such that  $a_7 = 0$  means  $\mathcal{I}$  does not know  $\mathcal{A}$ 's attack tactic  $A_7 \in \{\text{BE}, \text{OE1}, \text{OE2}, \text{BP}, \text{OP}\}$  and  $a_7 = 1$  means  $\mathcal{I}$  knows  $\mathcal{A}$ 's tactic.
- We define  $a_8 \in \{0, 1\}$  such that  $a_8 = 1$  ( $a_8 = 0$ ) means the defender does (not) know  $\mathcal{I}$ 's attack technique  $A_8 \in \{\text{GO}, \text{SF}, \text{TR}, \text{MI}, \text{HS}, \text{GM}, \text{MS}\}$ .
- We use  $a_9 = |\hat{\mathcal{Z}}_{\mathcal{M}}|/|\mathcal{Z}_{\mathcal{M}}|$  to represent the extent at which  $\mathcal{I}$  knows about  $\mathcal{A}$ 's adversarial files, where  $a_9 \in [0, 1]$  and  $\mathcal{Z}_{\mathcal{M}}$  is  $\mathcal{A}$ 's adversarial files and  $\hat{\mathcal{Z}}_{\mathcal{M}} \subseteq \mathcal{Z}_{\mathcal{M}}$  is known to  $\mathcal{I}$ .

**On the Usefulness of the Preceding Specification.** Similarly, the defense specification can be used to formulate a partial order in the attribute space, paving the way for comparing defenses unambiguously. Figure 4 depicts how vector  $(a_6, \dots, a_9)$  formulates a partial order between the widely-used informal notions of black-box defense  $(a_6, a_7, a_8, a_9) = (0, 0, 0, 0)$  and white-box defense  $(a_6, a_7, a_8, a_9) = (1, 1, 1, 1)$ ; there are many kinds of gray-box defenses in between.

### 2.3 Systematizing Security Properties

Since  $f = \varphi(\phi(\cdot))$ , we decompose  $f$ 's security properties into  $\varphi$ 's and  $\phi$ 's. We consider: **Representation Robustness (RR)**, meaning that two similar files have similar feature representations; **Classification Robustness (CR)**, meaning that two similar feature representations lead to the same label; **Detection Robustness (DR)**, meaning that feature extraction function  $\phi$  returns similar representations for two files with the same functionality; **Training Robustness (TR)**, meaning that small changes to the training set does not cause any significant change to the learned classifier. With respect to small perturbations, Definitions 21 and 22 below collectively say that when two files  $z$  and  $z'$  are similar, they would be classified as the same label with a high probability. Since the classification function  $\varphi$  is linear, we can obtain a  $\epsilon$ -robust  $\varphi$  analytically, where  $\epsilon$  is a small scalar that bounds the perturbations applied to feature vectors [80]. This means that the main challenge is to achieve RF extraction.

*Definition 21 (RR or  $(\epsilon, \eta)$ -robust Feature Extraction; Adapted from [126]).* Given constants  $\epsilon, \eta \in [0, 1]$ , and files  $z, z' \in \mathcal{Z}$  such that  $(\Gamma(z, z') \approx 0) \wedge (\text{true} \leftarrow O(z, z'))$ , we say feature extraction



function  $\phi$  is  $(\epsilon, \eta)$ -robust if

$$\mathbb{P}(C(\mathbf{x}, \mathbf{x}') \leq \epsilon) = \mathbb{P}(C(\phi(z), \phi(z')) \leq \epsilon) > 1 - \eta.$$

*Definition 22 (CR or  $\epsilon$ -robust Classification [12]).* Given constant  $\epsilon \in [0, 1]$  as in Definition 21 and any feature vectors  $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$ , we say classification function  $\phi$  is  $\epsilon$ -robust if

$$(C(\mathbf{x}, \mathbf{x}') \leq \epsilon) \rightarrow ((\phi(\mathbf{x}) > \tau) \wedge (\phi(\mathbf{x}') > \tau)).$$

Definition 23 specifies DR, which says that feature extraction function  $\phi$  returns similar representations for two different files as long as they have the same functionality. Note that Definitions 22 and 23 collectively produce a malware detector with DR.

*Definition 23 (DR or  $(O, \eta)$ -robust Feature Extraction; Adapted from [2]).* Given constant  $\eta \in [0, 1]$  and two files  $z, z' \in \mathcal{Z}$  such that  $(\Gamma(z, z') > 0) \wedge (\text{true} \leftarrow O(z, z'))$ , we say feature extraction  $\phi$  is  $(O, \eta)$ -robust if  $\mathbb{P}(C(\phi(z), \phi(z')) \leq \epsilon) > 1 - \eta$ .

Suppose, we impose a restriction on the adversarial files set  $D'_{\text{poison}}$  such that  $|D'_{\text{poison}}| \leq \gamma |D_{\text{train}}|$  for some constant  $\gamma \in [0, 1]$ . Let classifier  $f'$  be learned from  $D_{\text{train}} \cup D'_{\text{poison}}$ . Definition 24 says that a classifier  $f'$  learned from poisoned training set can predict as accurately as  $f$  learned from  $D_{\text{train}}$  with a high probability.

*Definition 24 (TR or  $(\gamma, \zeta)$ -robust Training; Adapted from [116]).* Given classifiers  $f$  learned from  $D_{\text{train}}$  and  $f'$  learned from  $D_{\text{train}} \cup D'_{\text{poison}}$  where  $|D'_{\text{poison}}| \leq \gamma |D_{\text{train}}|$ , and small constants  $\zeta \in [0, 1]$ , we say  $f'$  is  $(\gamma, \zeta)$ -robust if  $\forall z \in \mathcal{Z}$

$$((f(z) > \tau) \wedge (|D'_{\text{poison}}| \leq \gamma |D_{\text{train}}|)) \rightarrow (\mathbb{P}(f'(z) > \tau) > 1 - \zeta).$$

### 3 SYSTEMATIZING AMD ARMS RACE

We systematize attacks according to  $\mathcal{A}$ 's objective, input, assumptions, the security properties that are broken, and the types of victim malware detectors (e.g., Windows vs. Android). Similarly, we systematize defenses according to  $\mathcal{I}$ 's objective, input, assumptions, the security properties that are achieved, and the types of enhanced malware detectors (e.g., Windows vs. Android). We group attacks (defenses) according to the attacker's (defender's) techniques and then summarize them in a table according to the publication date in chronological order. For convenience, we will use wildcard  $*$  to indicate any value in a domain (e.g.,  $[0, 1]$ ); we will use  $\vee$  to describe  $\mathcal{A}$ 's and  $\mathcal{I}$ 's "broader" input (if applicable). For example,  $(0, 1, 0, 1, 0 | A_6, \dots, A_9) \vee (1, 0, 1, 1, 1 | A_6, \dots, A_9)$  means that  $\mathcal{A}$  has either  $(a_1, a_2, a_3, a_4, a_5) = (0, 1, 0, 1, 0)$  or  $(a_1, a_2, a_3, a_4, a_5) = (1, 0, 1, 1, 1)$ . Finally, we will present the attack-defense escalation.

#### 3.1 Systematizing Attack Literature

*3.1.1 Attacks Using GO.* Biggio et al. [16] propose solving the problem of optimal evasion attacks by leveraging GO techniques. They focus on high-confidence evasion attacks with small perturbations (cf. Definition 11). Given a malware representation-label pair  $(\mathbf{x}, y = +)$ , the optimization problem specified in Equation(4) with respect to GO is instantiated as

$$\begin{aligned} \max_{\delta_{\mathbf{x}}} L_{\mathcal{A}}(\hat{F}_{\hat{\theta}}(\mathbf{x} + \delta_{\mathbf{x}}), y = +) &= \min_{\delta_{\mathbf{x}}} (L(F_{\theta}(\mathbf{x} + \delta_{\mathbf{x}}, y = -)) - \beta_a \mathcal{K}(\mathbf{x} + \delta_{\mathbf{x}})) \\ \text{s.t. } (\delta_{\mathbf{x}} \in [0, \bar{\mathbf{u}}]) &\wedge (C(\mathbf{x}, \mathbf{x} + \delta_{\mathbf{x}}) \leq m), \end{aligned}$$

where  $\beta_a \geq 0$  is a balance factor and  $\mathcal{K}$  is a density estimation function for lifting  $\mathbf{x} + \delta_{\mathbf{x}}$  to the populated region of benign examples. Since  $\delta_{\mathbf{x}} \geq \mathbf{0}$ , the manipulation only permits object injections to meet the requirement of preserving malicious functionalities. The attack is validated

Table 4. Summary of AMD attacks (✓ means applicable, ● means 0, ○ means 1, and ⊙ means a value in [0, 1])

Attack (in chronological order)	Attack Objective	Attack Input									Assumptions				Broken Properties				Malware detector		
		Indiscriminate Targeted Availability	$A_1$ : Training set $D_{train}$	$A_2$ : Defense technique	$A_3$ : Feature set	$A_4$ : Learning algorithm	$A_5$ : Response	$A_6$ : Manipulation set	$A_7$ : Attack tactic	$A_8$ : Attack technique					$A_9$ : Adversarial example set	RR: Representation Robustness	CR: Classification Robustness	DR: Detection Robustness	TR: Training Robustness	Windows Program	Android Package
Smutz and Stavrou [109]	✓		○	○	○	○	○	M	OE2	MI	$\mathcal{X}_M$		✓				✓			✓	
Biggio et al. [16]	✓		○	○	○	○	○	M	OE2	GO	$\mathcal{X}_M$	✓	✓	✓			✓			✓	
Maiorca et al. [82]	✓		●	●	●	●	●	M	BE	MI	$\mathcal{Z}_M$	✓					✓			✓	
Šrndić and Laskov [114]	✓		○	○	○	○	○	M	BE	TR	$\mathcal{X}_M$							✓			
			○	○	○	○	○	M	OE2	TR	$\mathcal{X}_M$	✓						✓		✓	
			○	○	○	○	○	M	OE2	TR	$\mathcal{Z}_M$										
Xu et al. [134]	✓		○	○	○	○	○	M	BE	HS	$\mathcal{Z}_M$							✓		✓	
Carmony et al. [25]	✓		○	○	○	○	○	M	BE	MI	$\mathcal{Z}_M$		✓					✓		✓	
Hu and Tan [58]	✓		●	●	○	○	○	M	BE	GM	$\mathcal{X}_M$	✓	✓		✓			✓	✓		
Hu and Tan [59]	✓		●	●	○	○	○	M	BE	GM	$\mathcal{X}_M$	✓	✓		✓			✓	✓		
Demontis et al. [39]	✓		○	○	○	○	○	M	OE2	SF	$\mathcal{X}_M$	✓	✓		✓			✓		✓	
Grosse et al. [53]	✓		●	○	○	○	○	M	OE2	SF	$\mathcal{X}_M$	✓	✓	✓			✓	✓		✓	
Chen et al. [29]	✓		○	○	○	○	○	M	OE2	SF	$\mathcal{X}_M$	✓	✓	✓			✓	✓			
Khasawneh et al. [65]	✓		●	●	●	○	○	M	BE	TR	$\mathcal{X}_M$	✓			✓			✓			
Dang et al. [36]	✓		●	●	●	●	●	M	BE	TR	$\mathcal{Z}_M$								✓		
			○	○	○	○	○	M	BE	HS	$\mathcal{Z}_M$								✓	✓	
Muñoz-González et al. [87]	✓		○	○	○	○	○	M	OP	GO	$\mathcal{X}_M$	✓			✓			✓	✓		
Yang et al. [136]	✓		●	●	●	●	○	M	BE	HS	$\mathcal{Z}_M$	✓	✓					✓		✓	
Rosenberg et al. [100]	✓		●	●	○	○	○	M	BE	TR	$\mathcal{X}_M$	✓			✓		✓	✓		✓	
Anderson et al. [5]	✓		●	●	●	○	○	M	BE	TR	$\mathcal{Z}_M$	✓			✓		✓	✓		✓	
Kreuk et al. [70]	✓		●	○	○	○	○	M	OE2	GM	$\mathcal{Z}_M$	✓	✓	✓			✓	✓		✓	
Chen et al. [30]	✓		○	○	○	○	○	M	OE2	GO	$\mathcal{X}_M$		✓		✓						
			○	○	○	○	○	M	BP	SF	$\mathcal{X}_M$	✓	✓		✓			✓		✓	
Al-Dujaili et al. [2]	✓		●	○	○	○	○	M	OE2	GO	$\mathcal{X}_M$	✓			✓			✓		✓	
Suciu et al. [118]	✓		○	○	○	○	○	M	BP	SF	$\mathcal{X}_M$	✓	✓		✓				✓		✓
			○	○	○	○	○	M	BP	SF	$\mathcal{Z}_M$	✓	✓		✓						
			○	○	○	○	○	M	BP	SF	$\mathcal{X}_M$	✓	✓		✓						
Kolosnjaji et al. [68]	✓		●	○	○	○	○	M	OE2	GO	$\mathcal{X}_M$	✓			✓		✓	✓		✓	
Suciu et al. [117]	✓		●	○	○	○	○	M	OE2	GO	$\mathcal{X}_M$	✓			✓		✓	✓		✓	
Chen et al. [31]	✓		●	●	○	○	○	M	OE1	GO	$\mathcal{X}_M$	✓	✓		✓			✓			✓
			○	○	○	○	○	M	OE2	SF	$\mathcal{X}_M$	✓			✓						
			○	○	○	○	○	M	OE2	MI	$\mathcal{Z}_M$	✓									
Pierazzi et al. [97]	✓		○	○	○	○	○	M	OE2	MI	$\mathcal{Z}_M$	✓						✓		✓	
Li and Li [76]	✓		○	○	○	○	○	M	OE2	MS	$\mathcal{X}_M$	✓						✓			✓
			○	○	○	○	○	M	OE2	MS	$\mathcal{Z}_M$	✓			✓			✓			✓

by using the PDF malware detector and the feature representation is the number of appearances of hand-selected keywords (e.g., JavaScript). Because the perturbation is continuous, the authors suggest searching a discrete point close to the continuous one and aligning the point with  $\nabla \mathcal{L}_{\mathcal{A}}(\mathbf{x} + \delta_{\mathbf{x}}, y = +)$ . This attack makes the invertibility Assumption 5 because it operates in the feature space. Experimental results show that when  $\mathcal{I}$  employs no countermeasures, knowing  $\mathcal{I}$ 's feature set  $S$  and learning algorithm  $F$  are sufficient for  $\mathcal{A}$  to evade  $\mathcal{I}$ 's detector. This attack and its variants have been shown to evade PDF malware detectors [17, 102, 114, 141], PE malware detectors [68], Android malware detectors [76], and Flash malware detectors [83]. The kernel density estimation item makes the perturbed representation  $\mathbf{x} + \delta_{\mathbf{x}}$  similar to the representations of benign examples,

explaining the successful evasion. In summary, the attack works under the Oracle, Measurability, and Invertibility assumptions.  $\mathcal{A}$ 's input is, or  $\mathcal{A}$  can be characterized as,  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 1, 1, 1, 1 | \mathbf{M}, \text{OE2}, \text{GO}, \mathcal{X}_{\mathbf{M}}) \vee (0, 0, 1, *, 0 | \mathbf{M}, \text{OE2}, \text{GO}, \mathcal{X}_{\mathbf{M}})$  and  $\mathcal{A}$  breaks the CR property.

Al-Dujaili et al. [2] propose evasion attacks against DNN-based malware detectors in the feature space. In this attack,  $\mathcal{A}$  generates adversarial examples with possibly large perturbations in the feature space. More precisely, given a representation-label pair  $(\mathbf{x}, y = +)$ , the optimization problem of Equation (4) with respect to GO is instantiated as:  $\max_{\delta_{\mathbf{x}}} L(F_{\theta}(\mathbf{x} + \delta_{\mathbf{x}}), y = +)$  s.t.  $\delta_{\mathbf{x}} \in [0, 1 - \mathbf{x}]$ . The attack has four variants, with each perturbing the representation in a different direction (e.g., normalized gradient of the loss function using the  $\ell_{\infty}$  norm). A “random” rounding operation is used to map continuous perturbations into a discrete domain. When compared with the basic rounding (which returns 0 if the input is smaller than 0.5, and returns 1 otherwise), the “random” rounding means that the threshold of rounding is sampled from the interval  $[0, 1]$  uniformly. For binary feature representation, the manipulation set  $\mathbf{M}_{\mathbf{x}} = [0, 1 - \mathbf{x}]$  assures the flipping of 0–1. The effectiveness of the attack is validated using Windows malware detector in the feature space. In summary, the attack works under the Oracle and Invertibility assumptions with  $\mathcal{A}$  input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 1, 1, 1, 1 | \mathbf{M}, \text{OE2}, \text{GO}, \mathcal{X}_{\mathbf{M}})$  and breaks the DR property.

Kreuk et al. [70] propose an evasion attack in the feature space against MalConv, which is an end-to-end Windows PE malware detector (as reviewed in Section 2.1) [99]. Given a malware embedding code  $\mathbf{x}$ , the optimization problem of Equation (4) with respect to GO is instantiated as:  $\min_{\delta_{\mathbf{x}}} L(F_{\theta}([\mathbf{x} | \delta_{\mathbf{x}}]), y = -)$  s.t.  $\|\delta_{\mathbf{x}}\|_p \leq \epsilon$ , where  $|$  means concatenation and  $\|\cdot\|_p$  is the  $p$  norm where  $p \geq 1$ . Because MalConv is learned from sequential data, perturbation means appending some content to the end of a PE file. Perturbations are generated in a single step by following the direction of the  $\ell_{\infty}$  or  $\ell_2$  normalized gradients of the loss function [51, 71]. For instance, the attack based on the  $\ell_{\infty}$  norm is  $\tilde{\mathbf{x}}' = \mathbf{x} - \epsilon \cdot \text{sign}(\nabla_{\mathbf{x}}(L(F_{\theta}(\mathbf{x}), -)))$ , where  $\text{sign}(x) = +1$  ( $-1$ ) if  $x \geq 0$  ( $x < 0$ ). Since the embedding operation uses a look-up table to map discrete values (0, 1, ..., 255) to the learned real-value vectors, the attack uses a nearest neighbor search to look for the learned embedding code close to  $\tilde{\mathbf{x}}'$ . In summary, the attack works under the Oracle and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 1, 1, 1, 1 | \mathbf{M}, \text{OE2}, \text{GO}, \mathcal{X}_{\mathbf{M}})$  and breaks the RR and CR properties.

Kolosnjaji et al. [68] and Suciú et al. [117] independently propose gradient-based attacks in the feature space to evade MalConv [99]. Both studies also use the loss function exploited by Kreuk et al. [70]. Kolosnjaji et al. [68] use the manipulation set  $\mathcal{M}$  corresponding to appending instructions at the end of a file. This attack proceeds iteratively and starts with randomly initialized perturbations. In each iteration, continuous perturbations are updated in the direction of the  $\ell_2$  normalized gradient of the loss function with respect to the input, and then a nearest neighbor search is applied to obtain discrete perturbations. Suciú et al. [117] perturb embedding codes in the direction of the  $\ell_{\infty}$  normalized gradient of the loss function, while adding instructions in the mid of a PE file (e.g., between PE sections) while noting that appended content could be truncated by MalConv. Both attacks work under the Oracle and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 1, 1, 1, 1 | \mathbf{M}, \text{OE2}, \text{GO}, \mathcal{X}_{\mathbf{M}})$  and break the RR and CR properties.

Muñoz-González et al. [87] propose the OP attack in the feature space (Definition 13), which is NP-hard. In this case, the optimization problem of Equation (5) is relaxed by supposing that the classifier is linear to render the optimization problem tractable [20, 87, 132]. The attack is waged against Windows PE malware detectors. Feature set includes API calls, actions, and modifications in the file system; each file is represented by a binary vector. The attack has two variants: one uses white-box input, where  $\mathcal{A}$  derives  $D'_{\text{poison}}$  from  $\mathcal{I}$ 's detector  $f$ ; the other uses gray-box input, where  $\mathcal{A}$  knows  $\mathcal{I}$ 's training set as well as feature set and trains a surrogate detector. The

attack works under the Oracle and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 1, 1, 1, 1 | \mathbf{M}, \text{OP}, \text{GO}, \mathcal{X}_{\mathbf{M}}) \vee (1, 0, 1, 0, 0 | \mathbf{M}, \text{OP}, \text{GO}, \mathcal{X}_{\mathbf{M}})$  and breaks TR.

**3.1.2 Attacks Using SF.** Demontis et al. [39] propose the OE2 in the feature space to perturb important features in terms of their weights in the linear function  $\varphi(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$ , where  $\mathbf{w} = (w_1, w_2, \dots, w_d)$  is a weight vector,  $b$  is the bias, and  $d$  is the dimension of feature space. The attack is waged against Drebin malware detector (which is reviewed in Section 2.1).  $\mathcal{A}$  manipulates the  $x_i$ 's with largest  $|w_i|$ 's as follows: flip  $x_i = 1$  to  $x_i = 0$  if  $w_i > 0$ , flip  $x_i = 0$  to  $x_i = 1$  if  $w_i < 0$ , and do nothing otherwise, while obeying the manipulation set  $\mathbf{M}$  corresponding to the injection or removal of features. The attack works under the Oracle, Measurability, and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 1, 1, 1, 1 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (0, 0, 1, *, 0 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}})$  and breaks the CR property.

Grosse et al. [53] propose a variant of the **Jacobian-based Saliency Map Attack (JSMA)** [92] in the feature space against the Drebin malware detector (which is reviewed in Section 2.1). Instead of using SVM, **Deep Neural Network (DNN)** is used to build a detector. Important features are identified by leveraging the gradients of the softmax output of a malware example with respect to the input. A large gradient value indicates a high important feature.  $\mathcal{A}$  only injects manifest features to manipulate Android Packages and generates adversarial files from  $\mathcal{I}$ 's detector  $f$ . The attack works under the Oracle, Measurability, and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 1, 1, 1, 1 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}})$  and breaks the RR and CR properties.

Chen et al. [29] propose an evasion attack in the feature space by perturbing the important features derived from a wrapper-based feature selection algorithm [27, 29, 96, 141]. The attacker's loss function  $L_{\mathcal{A}}$  has two parts: (i) the classification error in the mean squared loss and (ii) the manipulation cost  $C(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^d c_i |x_i - x'_i|$ , where  $\mathbf{x} = (x_1, \dots, x_d)$ ,  $\mathbf{x}' = (x'_1, \dots, x'_d)$ , and  $c_i$  is the hardness of perturbing the  $i$ th feature while preserving malware's functionality. The attack is waged against Windows PE malware detector that uses hand-crafted Windows API calls as features and the binary feature representation. However, there are no details about the composition of manipulation set. This attack works under the Oracle, Measurability, and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_7, \dots, A_9) = (1, 1, 1, 1, 1 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}})$  and breaks CR.

Chen et al. [31] propose evasion attacks in the feature space against two Android malware detectors, MaMaDroid [84], and Drebin [8]. The manipulation set  $\mathbf{M}$  corresponds to the injection of manifest features (e.g., *activities*) and API calls.  $\mathcal{A}$  evades MaMaDroid by using the OE1 (Definition 10) and OE2 (Definition 11), and evades Drebin by using OE2. The optimization problem of OE1 Equation (3) is solved using an advanced gradient-based method known as C&W [24]. OE2 is solved using JSMA [92]. Because JSMA perturbs SF, we categorize this attack into the SF group. The OE2 attack works under the Oracle, Measurability, and Invertibility assumptions, with four kinds of input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 1, 0, 0 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (0, 0, 1, 0, 1 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (1, 0, 1, 0, 0 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (1, 0, 1, 0, 1 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}})$ , and breaks the CR property. The OE1 attack works under the same assumptions with the same input except using attack technique GO, and breaks the CR property.

Chen et al. [30] propose a BP attack in the feature space against Android malware detectors. The feature set contains syntax features (e.g., permission, hardware, and API) and semantic features (e.g., sequence of pre-determined program behaviors such as `getDeviceID` → `URL` → `openConnection`). The ML algorithm used is SVM, random forest, or  $K$ -Nearest Neighbor (KNN) [22, 107]. The malware representations are perturbed using a JSMA variant [92] against the SVM-based classifier (while noting JSMA is applicable neither to random forests nor to KNN because they are gradient-free). Feature manipulation set  $\mathbf{M}$  corresponds to the injection of syntax features.  $\mathcal{A}$  poisons  $\mathcal{I}$ 's training set by injecting perturbed perturbations

with label  $-$ . The attack works under the Oracle, Measurability, and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 1, 1, 1, 1 | \mathbf{M}, \text{BP}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (0, 0, 0, 1, 1 | \mathbf{M}, \text{BP}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (1, 0, *, 1, 1 | \mathbf{M}, \text{BP}, \text{SF}, \mathcal{X}_{\mathbf{M}})$  and breaks TR.

Suciu et al. [118] propose a BP attack in both feature and problem spaces. The authors obtain  $D'_{\text{poison}}$  by applying small manipulations to non-adversarial benign files and then obtain their labels as given by VirusTotal service [108].  $\mathcal{A}$ 's objective is to make  $\mathcal{I}$ 's classifier  $f$  mis-classify a targeted malware file  $z_{\text{mal}}$  as benign.  $\mathcal{A}$  proceeds as follow: (i) obtain an initial benign file  $z_{\text{ben}}$ , where  $z_{\text{ben}} \approx z_{\text{mal}}$  in the feature space with respect to the  $\ell_1$  norm; (ii) use the JSMA method [92] to manipulate  $z_{\text{ben}}$  to  $z'_{\text{ben}}$  by making a small perturbation so that they have similar feature representations; (iii) add  $z'_{\text{ben}}$  and its label obtained from VirusTotal to  $D'_{\text{poison}}$  and use  $D_{\text{train}} \cup D'_{\text{poison}}$  to train classifier  $f'$  (Definition 15); (iv) undo the addition if  $z'_{\text{ben}}$  lowers the classification accuracy significantly, and accept it otherwise. The attack is waged against the Drebin malware detector and the manipulation set corresponds to the feature injection of permission, API, and strings. This attack works under the Oracle, Measurability, and Inversibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (*, 0, 1, *, 0 | \mathbf{M}, \text{BP}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (1, 1, 1, 1, 1 | \mathbf{M}, \text{BP}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (1, 0, *, *, 0 | \mathbf{M}, \text{BP}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (1, 0, 1, 0, 0 | \mathbf{M}, \text{BP}, \text{SF}, \mathcal{X}_{\mathbf{M}})$  and breaks the TR property. The study generates adversarial malware examples, but does not test their malicious functionalities.

**3.1.3 Attacks Using MI.** Smutz and Stavrou [109] propose a mimicry attack in the feature space to modify features of a malicious file to mimic benign ones, where  $\mathcal{A}$  knows  $\mathcal{I}$ 's classifier  $f$ . Discriminative features are identified by observing their impact on classification accuracy. The attack perturbs features of malware examples by replacing their value with the mean of the benign examples. The attack is leveraged to estimate the robustness of PDF malware detectors without considering the preservation of malware functionality. The attack works under the Measurability assumption with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 1, 1, 1, 1 | \mathbf{M}, \text{OE2}, \text{MI}, \mathcal{X})$  and breaks the CR property.

Maiorca et al. [82] propose a reverse mimicry attack against PDF malware detectors in the problem space. Instead of modifying malicious files to mimic benign ones,  $\mathcal{A}$  embeds malicious payload (e.g., JavaScript code) into a benign file. The attack can be enhanced by using parser confusion strategies, which make the injected objects being neglected by feature extractors when rendered by PDF readers [25]. The attack works under the Oracle assumption with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 0, 0, 0 | \mathcal{M}, \text{BE}, \text{MI}, \mathcal{Z}_{\mathcal{M}})$  and breaks the DR property.

Pierazzi et al. [97] propose a white-box evasion attack against the Drebin malware detector and then an enhanced version of the detector in the problem space [8, 39]. They intend to bridge the gap between the attacks in the problem space and the attacks in the feature space. In addition, four realistic constraints are imposed on the manipulation set  $\mathcal{M}$ , including available transformation, preserved semantics, robustness to preprocessing, and plausibility. In order to cope with the side-effect features when incorporating gradient information of  $\mathcal{I}$ 's classifier, the attacker first harvests a set of manipulations from benign files; Manipulations in the problem space are used to query  $\mathcal{I}$ 's feature extraction for obtaining perturbations in the feature space; an adversarial malware example is obtained by using the manipulations corresponding to the perturbations that have a high impact on the classification accuracy. This attack works under the Oracle assumption with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 1, 1, 1, 1 | \mathcal{M}, \text{OE2}, \text{MI}, \mathcal{Z}_{\mathcal{M}})$  and breaks the DR property.

**3.1.4 Attacks Using TR.** Šrndić and Laskov [114] investigate the mimicry attack and the aforementioned gradient descent and kernel density estimation attack against the PDFrate service, where  $\mathcal{A}$  knows some features used by  $\mathcal{I}$ .  $\mathcal{A}$  makes the representation of an adversarial malware example similar to a benign one. Manipulation set  $\mathcal{M}$  corresponds to adding objects into PDF files.



Both attacks perturb feature vectors against a surrogate model, and then map the perturbed feature representations to the problem space by injecting manipulations between the body and the trailer of a PDF file. For the mimicry attack,  $\mathcal{A}$  uses  $N_{ben} > 0$  benign examples to guide manipulations, resulting in  $N_{ben}$  perturbed examples. The example incurring the highest classification error is used as an adversarial example. The attack works under the Oracle and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, *, 0, 0 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{X}_{\mathcal{M}}) \vee (0, 0, *, *, 0 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{X}_{\mathcal{M}}) \vee (1, 0, *, 0, 0 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{X}_{\mathcal{M}}) \vee (1, 0, *, *, 0 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{X}_{\mathcal{M}}) \vee (0, 0, *, 0, 0 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{Z}_{\mathcal{M}}) \vee (0, 0, *, *, 0 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{Z}_{\mathcal{M}}) \vee (1, 0, *, 0, 0 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{Z}_{\mathcal{M}}) \vee (1, 0, *, *, 0 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{Z}_{\mathcal{M}})$  and breaks DR. The gradient-based attack neglects the constraint of small perturbations and works under the same assumptions with the same input except using the attack technique OE2.

Khasawneh et al. [65] propose an evasion attack in both the feature and problem spaces against malware detectors learned from dynamic hardware features (e.g., instruction frequency), where  $\mathcal{A}$  knows some features used by  $\mathcal{I}$ . The attack proceeds as follows.  $\mathcal{A}$  first queries  $\mathcal{I}$ 's classifier to obtain a surrogate model and then generates adversarial files against the surrogate model. Manipulation set  $\mathcal{M}$  corresponds to the injection of some features because the others (e.g., memory access) are uncontrollable. Perturbations are conducted to the important features that are identified by large weights in the model. The attack works under the Oracle and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, *, 0, 1 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{X}_{\mathcal{M}}) \vee (0, 0, *, 0, 1 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{Z}_{\mathcal{M}})$  and breaks the CR property.

Rosenberg et al. [100] propose an evasion attack in both the feature and problem spaces against a **Recurrent Neural Network (RNN)** based surrogate model, which is learned from API call sequences. In this attack,  $\mathcal{A}$ 's training data is different from  $\mathcal{I}$ 's, but the labels are obtained by querying  $\mathcal{I}$ 's detector. In order to reduce the number of queries to  $\mathcal{I}$ 's detector,  $\mathcal{A}$  augments its training data using the Jacobian-based augmentation technique [91] and modifies the API sequence of an example in the direction of the  $\ell_{\infty}$  normalized gradient of the loss function. Manipulation set  $\mathcal{M}$  corresponds to inserting no-op API calls. Experimental results show that adversarial examples generated from a surrogate RNN model can evade SVM, DNN, and RNN detectors. The attack works under the Oracle and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 1, 0, 1 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{X}_{\mathcal{M}}) \vee (0, 0, 1, 0, 1 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{Z}_{\mathcal{M}})$  and breaks the RR and CR properties.

**3.1.5 Attacks Using HS.** Xu et al. [134] propose black-box evasion attacks in the problem space against two PDF malware detectors known as PDFrate [109] and Hidost [115], respectively. Given a malicious file  $z$ ,  $\mathcal{A}$  uses a genetic algorithm to iteratively generate  $z'$  from  $z$  as follows: (i)  $\mathcal{A}$  manipulates a set of candidates (or  $z$  in the initial iteration) via object deletion, insertion, or replacement. (ii)  $\mathcal{A}$  queries these variants to  $\mathcal{O}$  and  $f$ . (iii)  $\mathcal{A}$  succeeds when obtaining a successful adversarial example  $z'$ , namely  $(\text{True} \leftarrow \mathcal{O}(z, z')) \wedge (- \leftarrow f(z'))$ ; otherwise,  $\mathcal{A}$  uses a score function to select candidates for the next iteration or aborts after reaching a threshold number of iterations. The score function  $h$  varies with classifiers; for PDFrate,  $h(\mathcal{O}, f, z, z') = 0.5 - f(z')$  if  $\mathcal{O}(z, z') = \text{true}$ , and returns -0.5 if  $\mathcal{O}(z, z') = \text{false}$ . This attack models an Oracle and works with the input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 0, 0, 1 | \mathcal{M}, \text{BE}, \text{HS}, \mathcal{Z}_{\mathcal{M}})$  and breaks the DR property.

Yang et al. [136] propose evasion attacks against Android malware detectors in the problem space. In this attack,  $\mathcal{A}$  also uses a genetic algorithm to perturb a malware example  $z$  iteratively. In each iteration,  $\mathcal{A}$  extracts some features and calculates similarity scores between the malicious APKs in the feature space; the features that have high impact on the similarity scores are selected; the manipulations are to perturb the selected features. The attack works under the Oracle and Measurability assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 0, 0, 1 | \mathcal{M}, \mathcal{Z}, \text{BE}, \text{HS}, \mathcal{Z}_{\mathcal{M}})$  and breaks the DR property.



Dang et al. [36] propose a black-box evasion attack against malware detectors (e.g., PDFrate) in the problem space. Given a malicious file  $z$ ,  $\mathcal{A}$  uses the hill-climbing algorithm to iteratively generate adversarial file  $z'$  from  $z$ . In each iteration,  $\mathcal{A}$  generates a path of variants sequentially, each of which is perturbed from its predecessor using manipulations corresponding to object deletion, insertion, or replacement. A score function  $h$  is leveraged to select candidates, such as  $h(O, f, z, z') = \text{mal}_{z'} - \text{clf}_{z'}$  or  $h(O, f, z, z') = \text{mal}_{z'}/\text{clf}_{z'}$ , where  $\text{mal}_{z'}$  denotes the length of the first example turned from malicious to benign (obtaining by using an oracle) on the manipulation path (cf. Definition 18) and  $\text{clf}_{z'}$  denotes the length of the first malware example that has successfully misled the classifier  $f$ . Both examples of interest are obtained by a binary search, effectively reducing the number of queries to oracle  $O$  and  $f$ . The attack models an Oracle and works with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 0, 0, 0 | \mathcal{M}, \text{BE}, \text{HS}, \mathcal{Z}_{\mathcal{M}})$  and breaks the DR property.

**3.1.6 Attacks Using GM.** Hu and Tan [58] propose an evasion attack against Windows malware detectors in the feature space, by using **Generative Adversarial Networks (GAN)** [50]. In this attack,  $\mathcal{A}$  modifies the binary representation of Windows API calls made by malicious files, namely flipping some feature values from 0 to 1.  $\mathcal{A}$  learns a generator  $G_{\theta_g}$  and a discriminator from  $\mathcal{A}$ 's training dataset. The discriminator is a surrogate detector learned from feature vectors corresponding to  $\mathcal{A}$ 's benign files and those produced by  $G_{\theta_g}$ , along with labels obtained by querying  $\mathcal{I}$ 's detector  $f$ . An adversarial example feature vector is generated by using  $\mathbf{x}' = \max(\mathbf{x}, \text{round}(G_{\theta_g}(\mathbf{x}, \mathbf{a})))$ , where  $\mathbf{a}$  is a vector of noises,  $\text{round}$  is the round function, and  $\max$  means element-wise maximum. Hu and Tan [59] also propose another evasion attack using the Seq2Seq model [33]. Both attacks work under the IID, Oracle, and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 1, 0, 1 | \mathcal{M}, \text{BE}, \text{GM}, \mathcal{X}_{\mathcal{M}})$  and break the DR property.

Anderson et al. [5] propose a **Reinforcement Learning (RL)**-based evasion attack against Windows PE malware detectors in the problem space. Manipulation set  $\mathcal{M}$  is the RL action space, which includes some bytecode injections (e.g., API insertion) and some bytecode deletion. Attacker  $\mathcal{A}$  learns an RL agent on  $\mathcal{A}$ 's data, with labels obtained by querying defender  $\mathcal{I}$ 's detector  $f$ . The learned agent predicts manipulations sequentially for a given malware example. Moreover,  $\mathcal{A}$  is restricted by only applying a small number of manipulations to a malicious PE file. Experimental results show that the attack is not as effective as others (e.g., gradient-based methods). The attack works under the Oracle and Measurability assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 0, 0, 1 | \mathcal{M}, \text{OE2}, \text{GM}, \mathcal{Z}_{\mathcal{M}})$  and breaks the RR and CR properties.

**3.1.7 Attacks Using MS.** Li and Li [76] propose evasion attacks against DNN-based Android malware detectors in both feature and problem spaces. Given four gradient-based attack methods, the attack looks for the best one to perturb malware representations.  $\mathcal{A}$  can iteratively perform this strategy to modify the example obtained in the previous iteration. Experimental results show that the mixture of attacks can evade malware detectors effectively. The attack works under the IID, Oracle, and Invertibility assumptions with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 1, 1, 1, 1 | \mathcal{M}, \text{BE}, \text{MS}, \mathcal{X}_{\mathcal{M}}) \vee (1, 1, 1, 1, 1 | \mathcal{M}, \text{BE}, \text{MS}, \mathcal{Z}_{\mathcal{M}})$  and breaks the DR property.

**3.1.8 Drawing Observations and Insights.** We summarize the preceding reviews with the following observations. (i) Indiscriminate attacks have been much more extensively investigated than targeted attacks and availability attacks. (ii) Evasion attacks have been much more extensively studied than poisoning attacks. (iii) The Oracle assumption has been widely made. In addition, we draw the following insights.

**INSIGHT 1.** (i) *Knowing the defender's feature set is critical to the success of transfer attacks, highlighting the importance of keeping the defender's feature set secret (e.g., randomizing the defender's feature set).* (ii) *The effectiveness of evasion attacks largely depends on the attacker's degree of*

Table 5. Summary of AMD Defenses (✓ Means Applicable, ● Means 0, ○ Means 1, and ⊙ Means a Value in [0, 1])

Defense (in chronological order)	Defense Objective	Defense Input									Assumptions				Achieved Properties				Malware Detector				
		malware detection	$A_1$ : Training set $D_{train}$	$A_2$ : Defense technique	$A_3$ : Feature set	$A_4$ : Learning algorithm	$A_5$ : Response	$A_6$ : Manipulation set	$A_7$ : Attack tactic	$A_8$ : Attack technique	$A_9$ : Adversarial example set	IID assumption	Oracle assumption	Measurability assumption	Smoothness assumption	Invertibility assumption	RR: Representation Robustness	CR: Classification Robustness	DR: Detection Robustness	TR: Training Robustness	Windows Program	Android Package	PDF
Biggio et al. [15]	✓	$D_{train}$	EL	$S$	$F_\theta$	FQ	●	○	●	●	✓						✓						✓
Smutz and Stavrou [110]	✓	$D_{train}$	SE	$S$	$F_\theta$	FQ	●	○	●	●	✓							✓					✓
Zhang et al. [141]	✓	$D_{train}$	RF	$S$	$F_\theta$	FQ	○	○	●	●	✓	✓	✓				✓	✓					✓
Demontis et al. [39]	✓	$D_{train}$	WR	$S$	$F_\theta$	FQ	○	○	●	●	✓	✓					✓	✓			✓		
Wang et al. [127]	✓	$D_{train}$	IT	$S$	$F_\theta$	FQ	○	○	●	●	✓						✓				✓		
Grosse et al. [53]	✓	$D_{train}$	WR	$S$	$F_\theta$	FQ	●	○	●	●	✓						✓	✓					✓
Grosse et al. [53]	✓	$D_{train}$	AT	$S$	$F_\theta$	FQ	○	○	○	●	✓	✓					✓	✓					✓
Chen et al. [29]	✓	$D_{train}$	AT	$S$	$F_\theta$	FQ	○	○	○	●	✓	✓					✓				✓		
Khasawneh et al. [65]	✓	$D_{train}$	CD	$S$	$F_\theta$	FQ	●	○	○	●	✓						✓				✓		
Dang et al. [36]	✓	$D_{train}$	SE	$S$	$F_\theta$	LQ	●	○	●	●	✓								✓				✓
Yang et al. [136]	✓	$D_{train}$	AT	$S$	$F_\theta$	FQ	●	○	●	⊙	✓								✓				✓
Yang et al. [136]	✓	$D_{train}$	SE	$S$	$F_\theta$	FQ	○	○	○	●	✓								✓				✓
Chen et al. [27]	✓	$D_{train}$	RF	$S$	$F_\theta$	FQ	○	○	○	●	✓	✓	✓	✓			✓	✓					✓
Incer et al. [61]	✓	$D_{train}$	VL	$S$	$F_\theta$	FQ	○	○	○	●	✓						✓	✓	✓		✓		
Chen et al. [30]	✓	$D_{train}$	SE	$S$	$F_\theta$	FQ	●	○	●	●	✓	✓								✓			✓
Al-Dujaili et al. [2]	✓	$D_{train}$	AT	$S$	$F_\theta$	FQ	○	○	○	●	✓								✓		✓		
Chen et al. [28]	✓	$D_{train}$	IT	$S$	$F_\theta$	FQ	●	○	○	●	✓						✓						✓
Jordan et al. [62]	✓	$D_{train}$	RF	$S$	$F_\theta$	FQ	○	○	○	●	✓						✓	✓	✓				✓
Li et al. [77]	✓	$D_{train}$	AT	$S$	$F_\theta$	FQ	●	○	○	●	✓	✓	✓	✓			✓	✓			✓		
Tong et al. [122]	✓	$D_{train}$	RF	$S$	$F_\theta$	FQ	○	○	○	●	✓						✓	✓	✓				✓
Li and Li [76]	✓	$D_{train}$	AT	$S$	$F_\theta$	FQ	○	○	○	●	✓								✓				✓
Chen et al. [32]	✓	$D_{train}$	VL	$S$	$F_\theta$	FQ	○	○	○	●	✓	✓	✓	✓			✓	✓					✓
Li et al. [78]	✓	$D_{train}$	EL+AT+RF	$S$	$F_\theta$	FQ	○	○	○	●	✓	✓		✓	✓				✓				✓

$D_{train}^*$  contains  $D_{train}$  and a portion of  $\mathcal{A}$ 's adversarial examples.

freedom in conducting manipulations in the problem space (i.e., a smaller degree of freedom means it is harder for the attack to succeed).

### 3.2 Systematizing Defense Literature

**3.2.1 Defenses Using EL.** Biggio et al. [15] propose a one-and-a-half-class SVM classifier against evasion attacks, by leveraging an interesting observation (i.e., decision boundaries of one-class SVM classifiers are tighter than that of two-class SVM classifiers) to facilitate outlier detection. Specifically, the authors propose an ensemble of a two-class classifier and two one-class classifiers, and then combine them using another one-class classifier. The defense can enhance PDF malware detectors against gradient-based attacks [16], which can be characterized as  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 1, 1, 1, 1 | \text{M}, \text{OP2}, \text{GO}, \mathcal{X}_M)$ . However, the defense cannot thwart attacks incurring large perturbations. Independent of this study, other researchers propose using the random subspace and bagging techniques to enhance SVM-based malware detectors, dubbed **Multiple Classifier System SVM (MCS-SVM)**, which leads to evenly distributed weights [18, 39]. These defenses work under the IID assumption with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{train}, \text{EL}, S, F_\theta, \text{FQ} | 0, 1, 0, 0)$  and achieves the CR property.

**3.2.2 Defenses Using WR.** Demontis et al. [39] propose enhancing the Drebin malware detector  $\varphi(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$  by using box-constraint weights. The inspiration is that the classifier's sensitivity to

perturbations based on the  $\ell_1$  norm is bounded by the  $\ell_\infty$  norm of the weights. This defense hardens the Drebin detector against a mimicry attack with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 1, 0, 0 | \mathcal{M}, \text{BE}, \text{MI}, \mathcal{X}_\mathcal{M})$ , obfuscation attack [41] with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 0, 0, 0 | \mathcal{M}, \text{BE}, -, \mathcal{Z}_\mathcal{M})$ , and the attack that modifies important features [39] with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 1, 1, 1, 1 | \mathcal{M}, \text{OE2}, \text{SF}, \mathcal{X}_\mathcal{M})$ , here “-” means inapplicable. Experimental results show this defense outperforms MSC-SVM [18]. The defense works under the IID, Oracle, and Measurability assumptions with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{\text{train}}, \text{WR}, S, F_\theta, \text{FQ} | 1, 1, 0, 0)$  and achieves CR.

Grosse et al. [53] investigate how to apply two defense techniques known as distillation [93] and retraining [120] to enhance the DNN-based Drebin malware detector. The distillation technique can decrease a model’s generalization error by leveraging a teacher to relabel the training data represented by real-value vectors (rather than one-hot encoding). It uses retraining to tune a learned model with respect to an augmented training set with adversarial examples. Both defenses are estimated against a variant of JSMA and can be characterized by their input as  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (0, 1, 1, 1, 1 | \mathcal{M}, \text{OE2}, \text{SF}, \mathcal{X}_\mathcal{M})$ . Experimental results show the two defenses achieve limited success. The defense based on the distillation technique works under the IID assumption with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{\text{train}}, \text{WR}, S, F_\theta, \text{FQ} | 0, 1, 0, 0)$  and achieves the RR and CR properties. The defense based on the retraining technique works under the IID and Measurability assumptions with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{\text{train}}, \text{AT}, S, F_\theta, \text{FQ} | 1, 1, 1, 0)$  and achieves the RR and CR properties.

**3.2.3 Defenses Using AT.** Chen et al. [29] adapt a generic retraining framework proposed in the AML context [75] to enhance linear malware detectors. The defense uses a label smoothness regularization technique to mitigate the side-effect of AT [135]. The defense is evaluated using Windows malware detectors against “feature selection”-based evasion attacks, which can be characterized as  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (1, 1, 1, 1, 1 | \mathcal{M}, \text{OE2}, \text{SF}, \mathcal{X}_\mathcal{M})$ . The defense works under the IID and Measurability assumptions and can be characterized as  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{\text{train}}, \text{AT}, S, F_\theta, \text{FQ} | 1, 1, 1, 0)$ , while assuring the CR property.

Yang et al. [136] propose a defense against genetic algorithm-based evasion attacks that can be characterized as  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (0, 0, 0, 0, 1 | \mathcal{M}, \text{BE}, \text{HS}, \mathcal{Z}_\mathcal{M})$ . The defense uses three techniques: AT, SE, and WR [39]. The AT uses one half of  $\mathcal{A}$ ’s adversarial examples. The defense works under the IID assumption and can be characterized as  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D'_{\text{train}}, \text{AT}, S, F_\theta, \text{FQ} | 0, 1, 0, *)$ , where  $D'_{\text{train}}$  is the union of  $D_{\text{train}}$  and a portion (e.g., one half) of  $\mathcal{A}$ ’s adversarial examples. The defense of SE is learned from manipulations used by the attacker and works under the IID assumption with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{\text{train}}, \text{SE}, S, F_\theta, \text{FQ} | 1, 1, 1, 0)$ . Both defenses achieve the DR property. The defense of wight regularization is reviewed in Section 3.2.2.

Al-Dujaili et al. [2] adapt the idea of minmax AT (proposed in the AML context) to enhance DNN-based malware detectors. In this defense, the inner-layer optimization generates adversarial files by maximizing the classifier’s loss function; the outer-layer optimization searches for the parameters  $\theta$  (of DNN  $F_\theta$ ) that minimize the classifier’s loss with respect to the adversarial files. The defense enhances Windows malware detectors against attacks with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (0, 1, 1, 1, 1 | \mathcal{M}, \text{OE2}, \text{GO}, \mathcal{X}_\mathcal{M})$ . Experimental results show that malware detectors that are hardened to resist one attack may not be able to defend against other attacks. By observing this phenomenon, researchers propose using a mixture of attacks to harden DNN-based malware detectors [76]. The defense works under the IID assumption and can be characterized as  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{\text{train}}, \text{AT}, S, F_\theta, \text{FQ} | 1, 1, 0, 0)$ . The defense assures the DR property.

Li et al. [77] propose a DNN-based attack-agnostic framework to enhance adversarial malware detectors. The key idea is dubbed adversarial regularization, which enhances malware detectors via the (approximately) optimally small perturbation. The framework wins the AICS'2019 adversarial malware classification challenge organized by MIT Lincoln Lab researcher [131], without knowing anything about the attack. The defense works under the IID, Measurability, and Smoothness assumptions with input  $(A_1, \dots, A_5|a_6, \dots, a_9) = (D_{train}, AT, S, F_\theta, FQ|0, 1, 0, 0)$  and assures the RR and CR properties. In the extended study [78], the authors further enhance the framework with six defense principles, including EL, AT, and RR learning. The enhanced defense is validated with 20 attacks (including 11 gray-box attacks and 9 white-box attacks) against Android malware detectors. The enhanced defense works under the IID and Measurability assumptions with input  $(A_1, \dots, A_5|a_6, \dots, a_9) = (D_{train}, AT + EL + RF, S, F_\theta, FQ|1, 1, 0, 0)$  and assures the DR property.

**3.2.4 Defenses Using Verifiable Learning (VL).** Incer et al. [61] propose using monotonic malware classifiers to defend against evasion attacks, where *monotonic* means  $\varphi(\mathbf{x}) \leq \varphi(\mathbf{x}')$  when  $\mathbf{x} \leq \mathbf{x}'$  [54]. Technically, this can be achieved by using (i) RFs that can only be removed or added but not both and (ii) monotonic classification function (e.g., linear models with non-negative weights). The resulting classifier can thwart any attack that perturbs feature values monotonically. The defense works under the IID assumption with input  $(A_1, \dots, A_5|a_6, \dots, a_9) = (D_{train}, VL, S, F_\theta, FQ|1, 1, 0, 0)$  and assures the RR, CR, and DR properties.

Chen et al. [32] propose a defense to enhance PDF malware detectors against evasion attacks, by leveraging the observation that manipulations on PDF files are subtree additions and/or removals. They also propose new metrics for quantifying such structural perturbations. This allows to adapt the *symbolic interval analysis* technique proposed in the AML context [128] to enhance the PDF malware detectors. The defense can cope with attacks leveraging small perturbations in the training phase. This defense works under the IID, Measurability, and Smoothness assumptions with input  $(A_1, \dots, A_5|a_6, \dots, a_9) = (D_{train}, VL, S, F_\theta, FQ|1, 1, 0, 0)$  and achieves the RR and CR properties.

**3.2.5 Defenses Using RF.** Zhang et al. [141] propose leveraging optimal adversarial attacks for feature selection. The defense enhances PDF malware detectors against gradient-based attacks, which can be characterized as  $(A_1, \dots, A_5|a_6, \dots, a_9) = (1, 1, 1, 1, 1|M, OE2, GO, \mathcal{X}_M)$ . The defense works under the IID, Measurability, and Smoothness assumptions and can be characterized as  $(A_1, \dots, A_5|a_6, \dots, a_9) = (D_{train}, RF, S, F_\theta, FQ|1, 1, 0, 0)$ . The defense assures the RR and CR properties.

Tong et al. [122] propose refining features into invariant ones to defend against genetic algorithm-based evasion attacks with input  $(A_1, \dots, A_5|a_6, \dots, a_9) = (0, 0, 0, 0, 1|M, BE, HS, \mathcal{Z}_M)$ . Experimental results show that AT can be further leveraged to enhance the robustness of the defense. The defense works under IID assumption with input  $(A_1, \dots, A_5|a_6, \dots, a_9) = (D_{train}, RF, S, F_\theta, FQ|1, 1, 0, 0)$ , and achieves RR, CR, and DR.

Chen et al. [27] propose mitigating evasive attacks by filtering features according to their importance  $|w_i|/c_i$  with respect to the linear function  $\varphi(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$ , where  $x_i$ ,  $w_i$ , and  $c_i$  denote, respectively, the  $i$ th component of  $\mathbf{x}$ ,  $\mathbf{w}$ , and the constraint on manipulation cost  $c$ . The defense enhances Android malware detectors against three attacks: a random attack with input  $(A_1, \dots, A_5|a_6, \dots, a_9) = (0, 0, 1, 0, 0|M, BE, -, \mathcal{X}_M)$ , a variant of the mimicry attack with input  $(0, 0, 1, 0, 0|M, BE, MI, \mathcal{X}_M)$ , and the attack that modifies important features with input  $(A_1, \dots, A_5|a_6, \dots, a_9) = (1, 1, 1, 1, 1|M, BE, SF, \mathcal{X}_M)$ , where “-” means inapplicable. The defense works under the IID, Measurability, and Smoothness assumptions with input  $(A_1, \dots, A_5|a_6, \dots, a_9) = (D_{train}, RF, S, F_\theta, FQ|1, 1, 0, 0)$  and achieves RR and CR.

Jordan et al. [62] propose a robust PDF malware detector against evasion attacks by interpreting JavaScript behaviors using static analysis. A PDF file is classified as malicious when it calls a vulnerable API method or when it exhibits potentially malicious or unknown behaviors. The defense is validated against the *reverse mimicry* attack [82] with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (0, 0, 0, 0, 0 | \mathcal{M}, \text{BE}, \text{MI}, \mathcal{Z}_{\mathcal{M}})$ . The defense has input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{train}, \text{RF}, S, F_{\theta}, \text{FQ} | 1, 1, 0, 0)$  and achieves RR, CR, and DR.

**3.2.6 Defenses Using IT.** Wang et al. [127] propose the *random feature nullification* to enhance DNN-based malware detectors against the attack of **Fast Gradient Sign Method (FGSM)** [51] by nullifying (or dropping) features randomly in both training and testing phases. This offers a probabilistic assurance in preventing a white-box attacker from deriving adversarial files by using gradients of the loss function with respect to the input. The defense enhances Windows malware detectors against the FGSM attack with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (0, 1, 1, 1, 1 | \mathcal{M}, \text{OE2}, \text{GO}, \mathcal{X}_{\mathcal{M}})$ . The defense works under IID assumption with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{train}, \text{IT}, S, F_{\theta}, \text{FQ} | 0, 1, 0, 0)$  and achieves CR.

DroidEye [28] defends Android malware detectors against evasion attacks by quantizing binary representations, namely transforming binary representations into real values and then using compression to reduce the effect of adversarial manipulations. The defense enhances linear malware detectors against a “feature selection”-based attack with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (1, 1, 1, 1, 1 | \mathcal{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathcal{M}})$  [29] and the FGSM attack with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (0, 1, 1, 1, 1 | \mathcal{M}, \text{OE2}, \text{GO}, \mathcal{X}_{\mathcal{M}})$  [51]. The defense works under IID assumption with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{train}, \text{IT}, S, F_{\theta}, \text{FQ} | 0, 1, 0, 0)$  and achieves CR.

**3.2.7 Defenses Using CD.** Khasawneh et al. [65] propose randomizing classifiers (i.e., using one randomly chosen from a pool of classifiers that use heterogeneous features) to defend against transfer attacks. The defense is validated against an attack which perturbs important features with input  $(a_1, \dots, a_5 | a_6, \dots, a_9) = (0, 0, *, 0, 1 | \mathcal{M}, \text{BE}, \text{SF}, \mathcal{Z}_{\mathcal{M}})$ . The defense works under the IID assumption with input  $(a_1, \dots, a_5 | a_6, \dots, a_9) = (D_{train}, \text{CD}, S, F_{\theta}, \text{FQ} | 0, 1, 1, 0)$  and achieves the CR property.

**3.2.8 Defenses Using SE.** Smutz and Stavrou [110] propose an ensemble classifier to defend against gray-box evasion attacks by returning classification results as benign, uncertain and malicious according to the voting result (e.g., [0%, 25%] classifiers saying malicious can be treated as benign, [25%, 75%] saying malicious can be treated as uncertain, and [75%, 100%] saying malicious can be treated as malicious). The defense enhances a PDF malware detector against three types of evasion attacks: gradient-based attack [114] with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 0, *, *, 0 | \mathcal{M}, \text{OE2}, \text{TR}, \mathcal{Z}_{\mathcal{M}})$ , mimicry attack with input  $(1, 0, *, *, 0 | \mathcal{M}, \text{BE}, \text{TR}, \mathcal{Z}_{\mathcal{M}})$ , and reverse mimicry attack with input  $(0, 0, 0, 0, 0 | \mathcal{M}, \text{BE}, \text{MI}, \mathcal{Z}_{\mathcal{M}})$  [82]. The defense works under the IID assumption with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{train}, \text{SE}, S, F_{\theta}, \text{FQ} | 0, 1, 0, 0)$  and achieves DR.

Dang et al. [36] propose enhancing PDF malware detectors by lowering the classification threshold  $\tau$  and restricting the maximum query times, rendering genetic algorithm-based evasion attacks harder to succeed. This defense works under the IID assumption with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{train}, \text{SE}, S, F_{\theta}, \text{LQ} | 0, 1, 0, 0)$  and achieves DR.

Chen et al. [30] investigate defending Android malware detectors against poisoning attacks with input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (1, 1, 1, 1, 1 | \mathcal{M}, \text{BP}, \text{SF}, \mathcal{X}_{\mathcal{M}})$ . The idea is to filter adversarial files that are distant from non-adversarial ones, where distance is measured by the Jaccard index, Jaccard-weight similarity, and cosine similarity. The defense works under the Measurability assumption with input  $(A_1, \dots, A_5 | a_6, \dots, a_9) = (D_{train}, \text{SE}, S, F_{\theta}, \text{FQ} | 0, 1, 0, 0)$  and achieves TR.



**3.2.9 Drawing Observations and Insights.** Summarizing the preceding discussions, we draw the following observations. (i) Most studies focus on black-box defenses (i.e., the defender knows little about the attacker), which is against the principle of “knowing yourself and knowing your enemy”. (ii) Most studies focus on defenses against evasion attacks rather than poisoning attacks. (iii) There is no silver bullet defense against evasion attacks or poisoning attacks, at least for now. (iv) Sanitizing adversarial files as outliers is effective against black-box and gray-box attacks, but not white-box attacks. (v) The security properties achieved by defenses have been evaluated empirically rather than rigorously proven (despite that provable security is emerging on the small degree of perturbations; see for example [32, 48]). (vi) There is no theoretical evidence to support that the effectiveness of defense tactics on the training set (e.g., AT and verifiable learning) can generalize to other adversarial examples. In addition, we draw the following insights:

**INSIGHT 2.** (i) *Effective defenses often require the defender to know the attacker’s manipulation set. In the real world, it is hard to achieve this, explaining from one perspective why it is hard to design effective defenses.* (ii) *The effectiveness of adversarial training depends on the defender’s capability in identifying the most powerful attack.*

### 3.3 Systematizing AMD Arms Race

Figure 5 displays AMD attack-defense arms race surrounding three malware detectors: PDFrate, Drebin, and DNN-based detector. For a better visual effect, we group papers that proposed defense methods in terms of a common input  $(a_6, \dots, a_9)$ . For example, we group [136], [53], and [29] together because the defenders in both papers have input  $(a_6, \dots, a_9) = (1, 1, 1, 0)$ , while noting that their input on  $(A_1, \dots, A_5)$  may or may not be different. We also simplify attack and defense inputs while preserving the *critical information* when an attack (defense) works for multiple inputs. For example,  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 1, 0, 0 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}})$  is the *critical information* for attack input  $(a_1, \dots, a_5 | A_6, \dots, A_9) = (0, 0, 1, 0, 0 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (0, 0, 1, 0, 1 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (1, 0, 1, 0, 0 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}}) \vee (1, 0, 1, 0, 1 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}})$  because it is the weakest attack input in the partial order formulated by these  $(a_1, \dots, a_5)$ ’s. This suggests us to focus on attack input  $(0, 0, 1, 0, 0 | \mathbf{M}, \text{OE2}, \text{SF}, \mathcal{X}_{\mathbf{M}})$  because it is already able to break some defense and automatically implies that a stronger input can achieve the same (while noting some special cases, see discussion in Section 3.2.1). Multiple defense inputs are simplified in the same manner.

**Arms race in PDF malware detection:** We summarize two sequences of escalations caused by PDFrate [109]. In one sequence, PDFrate is defeated by transfer attacks, which are realized by gradient-based and mimicry methods against surrogate models [114]. These attacks trigger the defense escalation to an ensemble detector built on top of some diversified classifiers [110]. This defense [110] triggers attack escalation to *reverse mimicry attacks* [82], which trigger the defense escalation of using robust hand-crafted features [62]. This defense represents the state-of-the-art PDF malware detector, but still incurs a high false-positive rate. In the other sequence of arms race, PDFrate is defeated by genetic algorithm-based attacks [134]. These attacks trigger the defense escalation to [36] and [122]. The former defense [36] restricts the responses to attacker queries, but can be defeated by the escalated attack that leverages the hill-climbing algorithm (also shown in [36]). The latter defense [122] uses invariant features to thwart the attacks and represents another state-of-the-art PDF malware detectors.

**Arms race in android malware detection:** Drebin is defeated by the attack that modifies a limited number of important features [39], which also proposes the new defense to defeat the escalated attack. This defense [39] triggers the attack escalation to, and is defeated by, the genetic algorithm-based attack [136] and the mimicry-alike attack [97]. The former attack [136] triggers the escalated defense (also presented in [136]) that leverages attack mutations to detect adversarial examples



[136]. The latter attack [97] injects objects in APKs and (in principle) can be defeated by the monotonic classifier [61, 97]. These escalated defenses represent the state-of-the-art Android malware detectors, but still incur a high false-positive rate.

*Arms race in DNN-based malware detection:* The DNN-based detector [53] triggers four gradient-based evasion attacks presented in [2], which also hardens the DNN malware detector by using an *minmax adversarial training* instantiation to incorporate the  $\ell_\infty$  normalized gradient-based attack. This escalated defense [2] triggers the mixture of attacks presented in [76]. The defense of *minmax adversarial training* incorporating a mixture of attacks can defeat a broad range of attacks, but still suffers from the mimicry attack and other mixtures of attacks [76]. As a consequence, there are no effective defenses can thwart all kinds of attacks.

*Independent arms race:* There are studies that have yet to trigger cascading arms races, including: (i) Studies [29, 30, 118, 127] propose independent attacks and then show how to defeat these attacks. (ii) Studies [31, 58, 59, 68, 70, 87, 100, 117] propose attacks to defeat naive malware detectors. (iii) Studies propose defenses to counter some attacks [15, 27, 28, 32, 77].

#### 4 FUTURE RESEARCH DIRECTIONS (FDRS)

**FRD 1: Pinning down the root cause(s) of adversarial malware examples.** Speculations on root cause(s) include: (i) invalidity of the IID assumption because of distribution drifting, namely that testing files and training files are drawn from different distributions [16, 19, 52]; (ii) incompetent feature extraction [39, 134]; (iii) high dimensionality of malware representations [48]; (iv) insufficient scale of training data [104]; (v) low-probability “pockets” in data manifolds [120]; (vi) linearity of DNNs [51]; and (vii) large curvature of decision boundaries [46, 85]. Although these speculations may be true, more studies are needed in order to (in)validate them.

**FRD 2: Characterizing the relationship between transferability and vulnerability.** In the AMD context, an attacker may use a surrogate model to generate adversarial examples and a defender may use a surrogate model for AT. Transferability is related to the extent at which knowledge gained by a surrogate model may be the same as, or similar to, what is accommodated by a target model. The wide use of surrogate models in the AMD context suggests that there may be a fundamental connection between knowledge transferability and model vulnerability.

**FRD 3: Investigating adversarial malware examples in the wild.** In the AMD context, it is challenging to generate practical adversarial malware examples to correspond to perturbations conducted in the feature space, owing to realistic constraints. On the other hand, an attacker can directly search for manipulations in the problem space. This may cause large perturbations, putting the value of studies on small perturbations in question. This represents a fundamental open problem that distinguishes the field of AMD from its counterparts in other application settings. This issue is largely unaddressed by assuming that there is an oracle for telling whether manipulated or perturbed features indeed correspond to a malware sample or not.

**FRD 4: Quantifying the robustness and resilience of malware detectors.** Robustness and resilience of malware detectors against adversarial examples need to be quantified, ideally with a provable guarantee. For this purpose, one may adapt the reduction-based paradigm underlying the provable security of cryptographic primitives and protocols.

**FRD 5: Designing malware detectors with provable robustness and resilience guarantees.** Having understood the root cause(s) of adversarial examples, characterized the effect of transferability, investigated the effectiveness of practical attacks, and designed metrics for quantifying the robustness and resilience of malware detectors, it is imperative to investigate robust malware detectors with provable robustness, ideally as rigorous as what has been achieved in the field of cryptography. In this regard, RF extraction, AL, and VL are promising candidates for making breakthroughs.

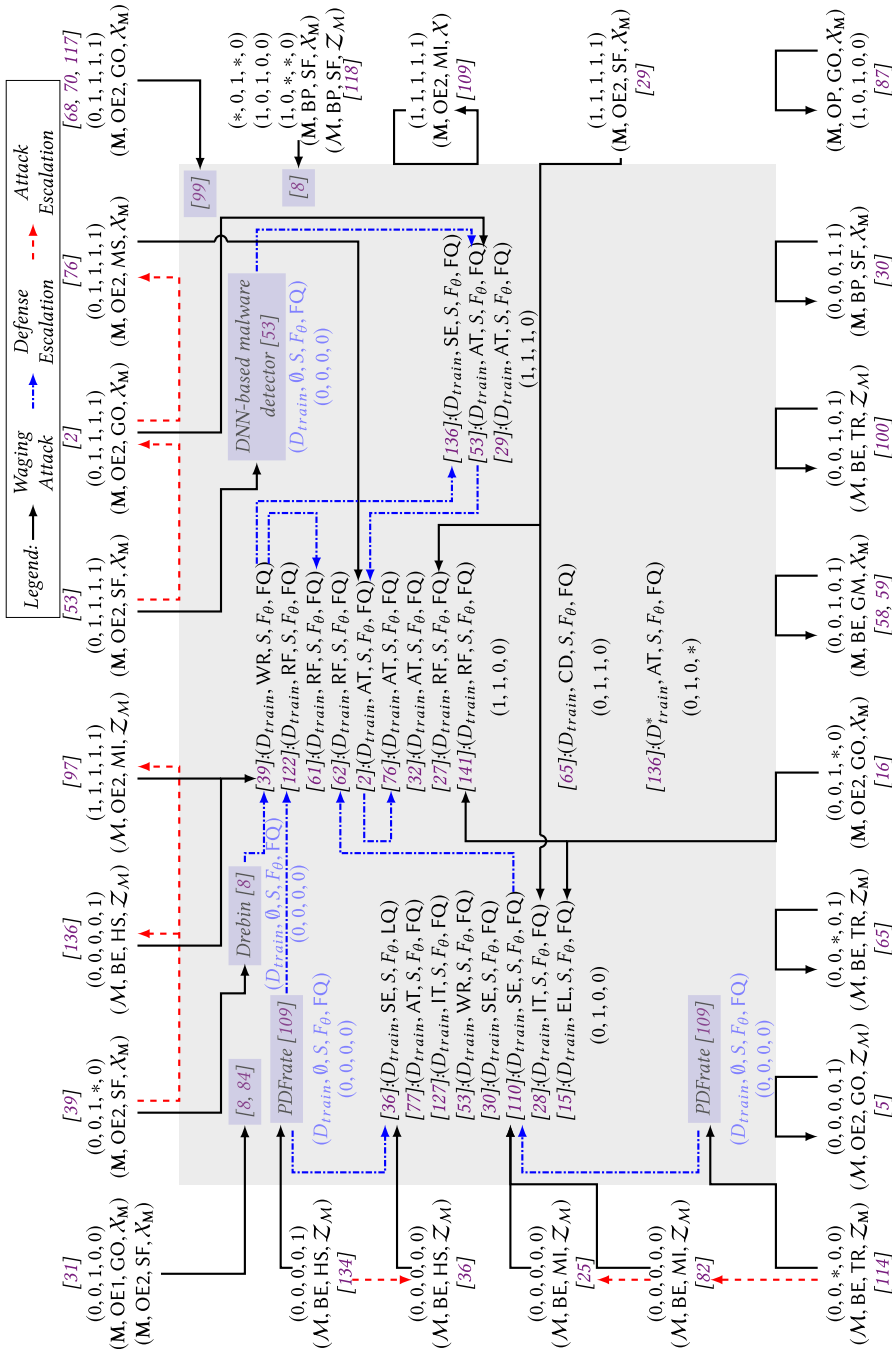


Fig. 5. Arms race in AMD attack and defense escalations.

**FRD 6:** *Forecasting the arms race in malware detection.* Arms race is a fundamental phenomenon inherent to the cybersecurity domain. In order to effectively defend against adversarial malware, one approach is to deploy proactive defense, which requires the capability to forecast the arms race between malware writers and defenders. For instance, it is important to predict how

attacks will evolve and what kinds of information would be necessary in order to defeat such attacks.

## 5 CONCLUSION

We have presented a framework for systematizing the field of AMD through the lens of assumptions, attacks, defenses, and security properties. This paves the way for precisely relating attacks and defenses. We have also shown how to apply the framework to systematize the AMD literature, including the arms race between AMD attacks and defenses. We have reported a number of insights.

The study leads to a set of future research directions. In addition to the ones described in Section 4, we mention the following two, which are discussed here, because there are rarely studies on these aspects. (i) To what extent explainability (or interpretability) of ML models can be leveraged to cope with adversarial malware examples? It is intuitive that explainability could be leveraged to recognize adversarial examples because they may not be explainable [37]. (ii) To what extent uncertainty quantification can be leveraged to cope with adversarial malware examples? If the uncertainty associated with detectors' predictions on adversarial malware examples are inherently and substantially higher than the uncertainty associated with non-adversarial malware examples, this fact can be leveraged to recognize adversarial malware examples. Finally, we reiterate that the research community should seek to establish a solid foundation for AMD. Although this foundation can leverage ideas and techniques from AML, the unique characteristics of AMD warrant the need of a unique foundation.

## ACKNOWLEDGMENTS

We thank the anonymous reviewers for their constructive comments that guided us in improving the article.

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Received June 2020; revised July 2021; accepted August 2021