Robust Learning against Logical Adversaries

Yizhen Wang  
Visa Research  
yizhewan@visa.com

Xiaozhu Meng  
Rice University  
Xiaozhu.Meng@rice.edu

Mihai Christodorescu  
Visa Research  
mihai.christodorescu@visa.com

Somesh Jha  
University of Wisconsin, Madison  
jha@cs.wisc.edu

Abstract

Test-time adversarial attacks have posed serious challenges to the robustness of machine learning models, and in many settings the adversarial manipulation needs not be bounded by small $\ell_p$-norms. Motivated by semantic-preserving attacks in security domain, we investigate logical adversaries, a broad class of attackers who create adversarial examples within a reflexive-transitive closure of a logical relation. We analyze the conditions for robustness and propose normalize-and-predict—a learning framework with provable robustness guarantee. We compare our approach with adversarial training and derive a unified framework that provides the benefits of both approaches. Driven by the theoretical findings, we apply our framework to malware detection. We use our framework to learn new detectors and propose two generic logical attacks to validate model robustness. Experiment results on real-world data set show that attacks using logical relations can evade existing detectors, and our unified framework can significantly enhance model robustness.

1 Introduction

The robustness of machine learning (ML) systems has been challenged by test-time attacks using adversarial examples [1, 2]. These adversarial examples are intentionally manipulated inputs that preserve the essential characteristics of the original inputs, and thus are expected to have the same test outcome as the originals by human standard; yet many ML models across different domains have reported significantly reduced performance on them [3, 4, 5, 6, 7, 8, 9]. As models in high-stake domains such as system security are also undermined by attacks [10, 11, 12, 13, 14], robust ML in adversarial test environment becomes an imperative task for the ML community.

While many defense mechanisms have been proposed [15, 16, 17, 18, 19, 20, 21], most existing work considers $\ell_p$-norm bounded adversarial manipulation. The $\ell_p$-norm constraint assumes that adversarial examples are syntactically similar to original inputs, e.g. two images close in pixel values. However, in many security-critical settings, the adversarial examples need only preserve the malicious semantics. For example, a spammer can add long wrapping texts to a phishing email: the bag-of-word features of the new email will have large $\ell_p$-distance from the original. Similarly, a malware author can choose different APIs to implement the same malicious function: the modified malware can have drastically different static program analysis features. Spam filters and malware detectors need to be robust to such semantic-preserving, adversarial manipulations that may have large $\ell_p$-norm.

Recent work also has started to examine defenses against adversarial transformations beyond $\ell_p$-norm constraints, including adversarial training [10, 11, 14, 22], verification-loss regularization [23]
and invariance-induced regularization [24]. Adversarial training in principle can achieve high robust accuracy when the adversarial example in the training loop maximizes the loss. However, finding such adversarial examples is in general NP-hard [25], and we show in Sec 3 that it is even PSPACE-hard for semantics-preserving attacks. [23, 24] add regularizers that indicate model robustness to the training objective. However, the regularizer’s value is not strictly enforced in training, and neither is model robustness. These limitations can still cause vulnerability to semantic-preserving attacks.

In this paper, we attempt to overcome these limitations using a learning framework that guarantees robustness by design. We investigate classification over binary inputs, and consider a logical adversary, whose admissible manipulation is specified by a logical relation. A logical relation is a set of input pairs, where each element specifies the source and target of an atomic input transformation and the source and target have the same semantic in the application domain. We consider a strong adversary that can apply arbitrary number of transformations because real-world attackers are often free to edit their malicious content. Our paper makes the following contribution towards the theoretical understanding of robust ML against logical adversaries:

1. We formally describe admissible adversarial manipulation using logical relations, and characterize the necessary and sufficient conditions for robustness to logical adversaries.

2. We propose normalize-and-predict, a learning framework that first converts each data input to a well-defined and unique normal form and then trains and classifies over the normalized inputs. We show that our framework has guaranteed robustness, and characterize conditions to different levels of robustness-accuracy trade-off.

3. We compare normalize-and-predict to the popular adversarial training framework, which directly optimizes for accuracy under attacks. We show that normalize-and-predict has the advantage in terms of explicit robustness guarantee and reduced training complexity, and in certain case has the same accuracy as adversarial training. Motivated by the comparison, we propose a unified framework, which selectively normalizes over more accuracy preserving relations and adversarially trains over the rest. Our unified approach gets the benefits from both frameworks.

We then apply our theoretical findings to malware detection. We formulate two types of common program transformation – 1) addition of redundant libraries and API calls, and 2) substitution of equivalent API calls – as logical relation. We instantiate our learning framework to these relations, and propose two generic logical adversarial attacks to determine robustness. Finally, we perform experiments over Sleipnir, a real-world WIN32 malware data set. Our results in Sec 5 show that:

1. Attacks using addition and substitution relation suffice to evade existing ML detectors.

2. Our unified approach using input normalization and adversarial training achieves highest robust accuracy among all baselines. The drop in accuracy on clean inputs is small and the computation cost is lower than pure adversarial training.

Finally, based on our theoretical and empirical results, we conclude that input normalization is vital to robust learning against logical adversaries. We believe that techniques that can improve the quality of normalization, such as transformation rule detection and semantic-aware feature extraction, are promising directions for future work.

**Related Work.** Test-time attacks in binary-input classification has recently caused severe security concerns, as ML models in security tasks are vulnerable to adversarial manipulation: [10, 11] evade API/library usage based malware detectors by adding redundant API calls and [12, 13, 14] attack running-time behavior based detectors via adding redundant execution traces. Instead of considering application-specific addition attacks, our paper extends the scope of adversarial attacks to general logical transformation: we unify the threat models into a powerful logical adversary, which can readily incorporate more complex input transformations. Our attacks surpass addition attacks on standard malware detection data set, suggesting the necessity of studying general logical adversary.

On the defense end, the work closest to ours in spirit is [24], which attempts to make model prediction invariant to input transformations. Their work however differs from ours in two major ways. First, they consider spatial transformation of images – the inputs form closed groups under transformation. Our logical adversary is more general as the transformations need not have an inverse. Second, their defense uses an invariance-induced regularizer, which may not enforce robustness on
finite sample. In contrast, our framework enforces robustness by design. [10, 11, 14] improve robustness via adversarial training; we show such approach is also hard to optimize. Last, [26, 27] enforce monotonicity over model outputs so that addition in feature values can only increase the maliciousness score. These approaches are specific for addition attacks and only protect one class.

Normalization is a technique to reduce the number of syntactically distinct instances that need to be considered by the detection system. First introduced to network security in the early 2000s in the context of network intrusion detection systems [28] and later applied to malware detection [29], it is used in various classical malware detectors [30, 31, 32, 33]. Our work addresses the open question whether normalization is useful for ML under logical adversary by investigating its impact on both robustness and accuracy.

2 Background

In this section, we introduce the learning setting and the threat model. We first describe the learning task, then formalize the potential adversarial manipulation as logical relations, and eventually derive the notion of robustness to logical adversaries.

**Learning Task.** We consider a data distribution \( D \) over a \( d \)-dimensional binary input space \( \mathcal{X} = \{0, 1\}^d \) and categorical label space \( \mathcal{Y} \). We use bold face letters, e.g. \( \mathbf{x} \), for input vectors and \( y \) for the label. Given a hypothesis class \( \mathcal{H} \), the learner wants to learn a classifier \( f : \mathcal{X} \to \mathcal{Y} \) in \( \mathcal{H} \) that minimizes the risk over the data distribution. In non-adversarial settings, the learner solves \( \min_{f \in \mathcal{H}} \mathbb{E}_{(x, y) \sim D} \ell(f, x, y) \), where \( \ell \) is a loss function. For classification, \( \ell(f, x, y) = 1(f(x) \neq y) \).

**Logical Relation.** A relation \( \mathcal{R} \) is a subset of \( \{0, 1\}^d \times \{0, 1\}^d \). We write \( \mathbf{x} \to_{\mathcal{R}} \mathbf{z} \iff (\mathbf{x}, \mathbf{z}) \in \mathcal{R} \). We write \( \mathbf{x} \to_{\mathcal{R}}^* \mathbf{z} \iff \mathbf{x} = \mathbf{z} \) or there exists \( \mathbf{z}_0, \mathbf{z}_1, \ldots, \mathbf{z}_k \) (\( k > 0 \)) such that \( \mathbf{x} = \mathbf{z}_0, \mathbf{z}_i \to_{\mathcal{R}} \mathbf{z}_{i+1} \) \((0 \leq i < k)\) and \( \mathbf{z}_k = \mathbf{z} \). In other words, \( \to_{\mathcal{R}}^* \) is the reflexive-transitive closure of \( \to_{\mathcal{R}} \). A relation is naturally ‘logical’ because its element can be described using logical statement, and the following illustrative examples show two common relations.

**Example 1** (Additive relation). In an additive relation \( \mathcal{R} \), \( \mathbf{x} \to_{\mathcal{R}} \mathbf{z} \iff x_i = 1 \implies z_i = 1 \) for all \( i \). Intuitively, it means \( \mathbf{x} \) can be transformed to \( \mathbf{z} \) by changing feature values from 0 to 1.

**Example 2** (Equivalence relation induced by equivalent coordinates). Let \( I = \{i_1, \cdots, d\} \) be the set of coordinate indices for inputs in \( \mathcal{X} \) and \( U = \{i_1, \cdots, i_m\} \subseteq I \). In an equivalence relation \( \mathcal{R} \) induced by \( U \), \( \mathbf{x} \to_{\mathcal{R}} \mathbf{z} \iff 1) x_i = z_i \text{ for all } i \in I \setminus U, \text{ and } 2) \bigvee_{i \in U} x_i = \bigvee_{i \in U} z_i \). Notice that \( \mathbf{x} \to_{\mathcal{R}} \mathbf{z} \iff \mathbf{z} \to_{\mathcal{R}} \mathbf{x} \). Intuitively, it means the presence of any combination of coordinates in \( U \) is equivalent to any other combination.

In this paper, we also consider unions of relations. Notice that a finite union \( \mathcal{R} \) of \( m \) relations \( \mathcal{R}_1, \cdots, \mathcal{R}_m \) is also a relation, and \( \mathbf{x} \to_{\mathcal{R}} \mathbf{z} \iff \mathbf{x} \to_{\mathcal{R}_i} \mathbf{z} \) for some \( i \in \{1, \cdots, m\} \).

**Threat Model.** A test-time adversary replaces a clean test input \( \mathbf{x} \) with an adversarially manipulated input \( A(\mathbf{x}) \), where \( A(\cdot) \) represents the attack algorithm. We consider an adversary who wants to maximize the classification error rate:

\[
\mathbb{E}_{(x, y) \sim D} 1(f(A(\mathbf{x})) \neq y).
\]

We assume white-box attacks\(^1\), i.e. the adversary knows all information about \( f \), including its structures, model parameters and any defense mechanism in place. To maintain the malicious semantics, the adversarial input \( A(\mathbf{x}) \) needs to be within a feasible set \( T(\mathbf{x}) \). In this paper, we focus on \( T(\mathbf{x}) \) described by logical relation. We consider a logical relation \( \mathcal{R} \) that is known to both the learner and the adversary, and we define a logical adversary as the following.

**Definition 1** (Logical adversary). An adversary is said to be \( \mathcal{R} \)-logical if \( T(\mathbf{x}) = \{\mathbf{z} \mid \mathbf{x} \to_{\mathcal{R}} \mathbf{z}\} \), i.e. each element in \( \mathcal{R} \) represents an admissible transformation, and the adversary can apply arbitrary number of transformation specified by \( \mathcal{R} \).

\(^1\)We consider a strong white-box attacker to avoid interference from security by obscurity, which is shown fragile in various other adversarial settings [16].
Definition 2 (Robustness and robust accuracy). Let \( Q(\mathcal{R}, f, x) \) be the following statement:
\[
\forall z (x \rightarrow_R^* z) \Rightarrow f(x) = f(z).
\]
Then, a classifier \( f \) is robust at \( x \) if \( Q(\mathcal{R}, f, x) \) is true, and the robustness of \( f \) to an \( \mathcal{R} \)-logical adversary is:
\[
\mathbb{E}_{x \sim D_X} \mathbb{I}_{Q(\mathcal{R}, f, x)},
\]
where \( \mathbb{I}(\cdot) \) indicates the truth value of a statement and \( D_X \) is the marginal distribution over inputs. The robust accuracy of \( f \) w.r.t. an \( \mathcal{R} \)-logical adversary is then:
\[
\mathbb{E}_{(x, y) \sim D} \mathbb{I}_{Q(\mathcal{R}, f, x) \land f(x) = y}.
\]

Notice that the robust accuracy of a classifier is no more than the robustness in value because of the extra requirement of \( f(x) = y \). Meanwhile, a classifier with the highest robustness accuracy may not always have the highest robustness and vice versa: an intuitive example is that a constant classifier is always robust but not necessarily robustly accurate. In Sec 3, we will discuss both objectives and characterize the trade-off between them.

3 Normalize-and-Predict – A Provably Robust Learning Framework

In this section, we introduce normalize-and-predict, a learning framework provably robust to an \( \mathcal{R} \)-logical adversary. We first analyze the conditions for robustness on a graph induced by logical relation. Inspired by the observation, we then propose a normalization procedure, which converts each input instance into a well-defined normal form. In the normalize-and-predict framework, the learner both trains and tests over the normal forms instead of the original inputs. Finally, we compare our approach with adversarial training and suggest a unified framework based on comparison.

3.1 Conditions for Robustness

We first define a directed graph \( G_{\mathcal{R}} = (V, E) \), which we call the relation graph of \( \mathcal{R} \), that is induced by a relation \( \mathcal{R} \). The vertex set \( V \) contains all elements in \( X \), i.e. all lattices in \( \{0, 1\}^d \). The edge set \( E \) contains an edge \((x, z) \in \mathcal{R} \). Then, a directed path exists from \( x \) to \( z \) if \( x \rightarrow_R^* z \). Let \( C_1, \cdots, C_k \) denote the weakly connected components in \( G \). We observe the following necessary and sufficient condition for robustness in a weakly connected component, which we prove in Appendix A.

Observation 1. A classifier \( f \) is robust for all \( x \in C_i \) iff \( f(x) \) returns the same label for all \( x \in C_i \).

The if direction holds because any \( x \in C_i \) can only be transformed into \( z \in C_i \) by the maximal property of weakly connected component. The contrapositive of the only if direction holds because if \( f(x) \neq f(z) \) for a pair \( x, z \in C_i \), then there must exist two adjacent nodes \( z_1, z_2 \) on the path between \( x \) and \( z \) such that one can be transformed to another yet \( f(z_1) \neq f(z_2) \).

3.2 The Normalize-and-Predict Framework

Observation 1 suggests that inputs in the same connected component must have the same prediction in order to obtain robustness. This motivates us to find a single input – a unique “normal” form – that represents all inputs in the connected component. If we can define a normal form and find a systematic way to convert all test inputs to their normal forms, then all adversarial examples of an input instance will share the same normal form, and thus have the same prediction.

Normal Form. Let \( C_i \) be any weakly connected component in \( G_{\mathcal{R}} \) induced by \( \mathcal{R} \). We first construct a new graph from \( C_i \) by condensing all nodes in the same cycle into a single node for all cycles in \( C_i \). Suppose \( S = \{x_1, \cdots, x_m\} \) is the set of nodes in a cycle. We only keep \( x_1 \) in the graph, and replace edge \((x_i, z)\) with \((x_1, z)\) and edge \((z, x_i)\) with \((z, x_1)\) for all \( x_i \in S \) and all \( z \) in the graph. We repeat this procedure until no cycle exists in the remaining graph, and we call the final graph \( C'_i \). Since \( C'_i \) is acyclic by construction, we can fix a topological order over its nodes.
Table 1: Comparison of training objective and test output for standard risk minimization learning scheme, normalize-and-predict and adversarial training. The upper row shows the training objectives; the lower row shows the test output, where \( f^* \) is the minimizer of the training objective.

|               | No Defense | Normalize-and-Predict | Adversarial Training |
|---------------|------------|-----------------------|---------------------|
| Train         | \( \min_{f \in \mathcal{H}} \sum_{(x, y) \in D} \ell(f, x, y) \) | \( \min_{f \in \mathcal{H}} \sum_{(x, y) \in D} \ell(f, N(x), y) \) | \( \min_{A \in \mathcal{A}} \max_{(x, y) \in D} \ell(f, A(x), y) \) |
| Test          | \( f^*(x) \) | \( f^*(N(x)) \) | \( f^*(x) \) |

**Definition 3** (Normal form). For any \( C_i \) and any node \( x \in C_i \), the normal form of \( x \), denoted by \( N(x) \), is the node in \( C'_i \) with the largest topological order.\(^2\)

**Normalize-and-Predict.** In the normalize-and-predict framework, the learner both trains the classifier and predicts the test label over the normal form of the original input. Let \( D \) denote the training set. In the empirical risk minimization learning scheme, the learner will now solve the following problem

\[
\min_{f \in \mathcal{H}} \sum_{(x, y) \in D} \ell(f, N(x), y),
\]

and use the minimizer \( f^* \) as the classifier. During test-time, the model will predict \( f^*(N(x)) \).

Table 1 compares the learning pipeline of normalize-and-predict to normal risk minimization and adversarial training. We characterize the robustness and robust accuracy of the classifier learned using the normalize-and-predict framework in the following theorem.

**Theorem 1.** Let \( f \) be a classifier obtained using the normalize-and-predict framework, and \( f(C_i) \) be the class label that \( f \) assigns to connected component \( C_i \). Let \( \mu(x) \) denote the probability mass of \( x \) and \( \eta(x, l) = \Pr(y = l | x) \) denote the probability that \( x \) has label \( l \). Then

1. \( f \) is always robust to \( \mathcal{R} \)-logical adversaries,
2. the accuracy of \( f \), denoted by \( \text{Acc}_f, \mathcal{R} \), will be: \( \sum_{C_i} \sum_{x \in C_i} \mu(x) \eta(x, f(C_i)) \).

In addition, the best robust accuracy using normalize-and-predict, denoted by \( \text{Acc}^*_{\mathcal{R}} \), has expression

\[
\text{Acc}^*_{\mathcal{R}} = \sum_{C_i} \max_{l \in Y} \sum_{x \in C_i} \mu(x) \eta(x, l),
\]

which happens when \( f(C_i) = \arg \max_{l \in Y} \sum_{x \in C_i} \mu(x) \eta(x, l) \).

The proof is in Appendix A.1. The robustness of \( f \) is guaranteed as a result of Observation 1. For accuracy, the term \( \max_{l \in Y} \sum_{x \in C_i} \mu(x) \eta(x, l) \) intuitively measures how concentrated the labels of random samples are within \( C_i \), and the accuracy will be high if \( x \in C_i \) shares the same label.

**Robustness-Accuracy Trade-off.** Theorem 1 suggests that robust accuracy depends on both the data distribution \( D \) and the relation \( \mathcal{R} \): the latter determines the graph structure. We observe that adding elements into \( \mathcal{R} \), which means allowing more admissible transformation, will always have negative impact on the robust accuracy except one special case as shown in Observation 2.

**Observation 2** (Robustness-accuracy trade-off). Let \( \mathcal{R}' \) and \( \mathcal{R} \) be two relations such that \( \mathcal{R}' = \mathcal{R} \cup \{(x, z)\} \), i.e. \( \mathcal{R}' \) allows an extra transformation from \( x \) to \( z \) than \( \mathcal{R} \). Let \( C_{x, \mathcal{R}} \) denote the weakly connected component in \( G_{\mathcal{R}} \) that contains \( x \), and \( l_C \) be the most likely label of inputs in a connected component \( C \). Then \( \text{Acc}^*_{\mathcal{R}'} - \text{Acc}^*_{\mathcal{R}} \leq 0 \) for all \( \mathcal{R}, \mathcal{R}' \) pairs, and the equality only holds when \( l_{C_{x, \mathcal{R}'}} = l_{C_{x, \mathcal{R}}} \).

The proof is in Appendix A.2; the intuition is that the extra edge on the relation graph may join two connected components, and the accuracy on one of the components will drop if the two components have different majority labels.

We further characterize three levels of trade-off with illustrative examples in Figure 1. First, if \( x, z \) have the same ground truth label, then the optimal classifier over the data distribution \( D \) after normalization should have the same natural accuracy as before normalization. Second, if both \( (x, z) \) and

\(^2\)In fact, the normal form can also be any element in \( C_i \) as long as it is consistent for all \( x \in C_i \). Topological order helps us to find such a consistent choice algorithmically.
(z, x) are in R, then as we show later in Theorem 2, the optimal classifier over D after normalization has the same robust accuracy as the optimal classifier under adversarial training, i.e. normalization preserves the best attainable robust accuracy. Last, if x can be transformed to different inputs with different ground truth labels, then having an absolutely robust classifier is at odds with robust accuracy. Suppose \( \mu(x) = 0.02, \mu(z_1) = \mu(z_2) = 0.49 \) in the rightmost example in Figure 1. The classifier after normalization will predict the same label and thus has accuracy at most 0.49, while the highest robust accuracy is 0.98 by predicting the ground truth label for \( z_1 \) and \( z_2 \).

3.3 Comparison and Synergy with Adversarial Training

Normalize-and-Predict differs from the popular adversarial training framework in their objectives: normalize-and-predict prioritizes robustness and then maximizes accuracy under the guarantee, while adversarial training maximizes robust accuracy at the cost of potential violation to robustness. In theory, adversarial training may have higher robust accuracy when ideally optimizing its objective. However, the following observations suggest that its training complexity may be prohibitively high.

Observation 3 (Hardness of training). The inner optimization problem of adversarial training is PSPACE-hard for logical adversary.

Observation 4 (Model capacity requirement). For some hypothesis class \( \mathcal{H} \) and relation \( R \), there exists \( f \in \mathcal{H} \) such that \( f(N_R(z)) \) is robustly accurate, but no \( f \in \mathcal{H} \) can be robustly accurate on the original inputs. In other words, robustly accurate classifier can only be obtained after normalization, suggesting that adversarial training may require larger model capacity. \(^3\)

The full statements and proofs of Observation 3 and 4 are in Appendix A.3 and A.4. In addition to the computational hardness of inner maximization and the potential higher model capacity requirements, previous work has also shown that robust learning may also have high sample complexity [34]. These factors together suggest that adversarial training may be suboptimal in practice.

Given the comparison of these two approaches, we propose a synergy of them that may enjoy the robustness guarantee and reduced training complexity of normalize-and-predict as well as the potential higher accuracy of adversarial training. For a relation \( R \), we strategically select a subset \( R' \subset R \), normalize inputs w.r.t. \( R' \), and adversarially train on the normalized inputs. Let \( N_{R'}(x) \) denote the normal form of \( x \) under \( R' \).

Formally, the learner solve the following problem

\[
\min_{f \in \mathcal{H}} \max_{A(\cdot)} \sum_{(x, y) \in D} \ell(f, A(N_{R'}(x)), y),
\]

during training to obtain a minimizer \( f^* \), and predicts \( f^*(N_{R'}(x)) \) at test-time. The classifier \( f^* \) will be robust to \( R' \)-logical adversary, and have potentially higher accuracy to transformations in \( R \setminus R' \) than using normalization alone. For choice of \( R' \), we characterize a condition for which normalize-and-predict and adversarial training have the same best attainable robust accuracy.

Theorem 2 (Preservation of robust accuracy). Consider \( \mathcal{H} \) to be the set of all labeling functions on \( \{0, 1\}^d \). Let \( f^* \) be the classifier that minimizes the objective of our unified framework over data distribution \( D \), i.e. the optimal solution to

\[
\min_{f \in \mathcal{H}} \max_{A(\cdot)} \mathbb{E}_{(x, y) \sim D} \ell(f, A(N_{R'}(x)), y), \]

where \( \ell \) is the 0-1 classification. Meanwhile, let \( f^*_{adv} \) be the classifier that minimizes the objective of adversarial training over \( D \), i.e. the optimal solution to

\[
\min_{f \in \mathcal{H}} \max_{A(\cdot)} \mathbb{E}_{(x, y) \sim D} \ell(f, A(x), y).
\]

\(^3\)We note that robust learning may already have high sample complexity [34]; reducing model capacity may help reduce the sample requirement too.
In addition, let \( G_{\mathcal{R}} \) denote the relation graph of \( \mathcal{R} \). Then, \( f^*(N_{\mathcal{R}}(\cdot)) \) and \( f_{adv}^* \) have the same robust accuracy if the connected components in \( G_{\mathcal{R}} \) are also strongly connected.

The proof is in Appendix A.5; the intuition is that we can find a classifier \( f \) in our unified framework such that \( f_{adv}^* \) is only robustly accurate when \( f(N_{\mathcal{R}}(\cdot)) \) is. Observation 2 and Theorem 2 provide a general guideline for selecting \( \mathcal{R}' \): we choose, with highest priority, the relation that leads to strongly connected components in its relation graph, and then consider relation that cause little drop in the best attainable robust accuracy.

4 Case Study: Robust Malware Detection

We now examine a security-critical domain – malware detection – in which robustness to logical adversary is crucial. Malware authors can edit the malware syntax while retain the malicious functionality in order to evade detection. We first show that common obfuscation techniques can be described by logical transformation on the feature vector, and then show two practical attacks, GREEDYBYGROUP and GREEDYBYGRAD, that use such logical transformation. Last, we describe our unified learning framework using both normalization and adversarial training, whose performance will be evaluated in the experiment section.

4.1 Adversarial Settings

One popular scheme of ML-based malware detection is to first extract a binary feature representation \( x \in \{0, 1\}^d \) of a program, which indicates its usage of libraries and API calls. The learner then builds classifiers over the extracted feature vectors, which ideally assign \( y = 1 \) to the malware and \( y = 0 \) otherwise. A common attack strategy studied in previous work is addition attack \([10, 11, 12, 13, 14]\): the attacker adds dummy API calls and import extra libraries to change the program syntax. Such transformation can be described using the additive relation in Example 1.

However, the attacker can perform a much richer set of transformation, which is not considered by previous work. We observe that the same program functionality typically can be implemented in different ways, using different sets of APIs. We consider a special case: API substitutions. APIs with similar functionality can be used interchangeably, without changing the program functionality. API substitution can be described by the equivalence relation in Example 2.

Formally, given a detector \( f : \{0, 1\}^d \rightarrow \{0, 1\} \), a malware instance \( x \) with label \( y = 1 \), and a relation \( \mathcal{R} \), the attacker wants to create a new malware with representation \( x^{adv} \) that solves: \( \max_{x : x \rightarrow x^{adv}} \ell(f, x, y) \).

**Algorithm 1 GREEDYBYGROUP (x, K)**

1. \( x^{adv} = x \), \( k = 0 \)
2. Partition \( \mathcal{R} \) into \( m \) groups \( \{\mathcal{R}_1, \ldots, \mathcal{R}_m\} \).
3. while \( k < K \) do
   - \( k = k + 1 \)
   - for \( \mathcal{R}_i \in \{\mathcal{R}_1, \ldots, \mathcal{R}_m\} \) do
     - \( x_i = \arg \max_{x : x^{adv} \rightarrow x} \ell(f, x, 1) \).
   - end
   - Combine \( x_i \)'s to obtain the new \( x^{adv} \)
4. end
5. return \( x^{adv} \)

**Algorithm 2 GREEDYBYGRAD(x, m, K)**

1. \( x^{adv} = x \), \( k = 0 \)
2. while \( k < K \) do
   - \( k = k + 1 \)
   - \( g = \nabla_x \ell(f, x, 1) \)
   - for \( (x^{adv}, z) \in \mathcal{R} \) do
     - \( c(x^{adv}, z) = \sum_{i=1}^d g_i (z_i - x_i^{adv}) \)
   - end
   - Apply the transformations with top \( m \) largest positive \( c(x^{adv}, z) \) to obtain the new \( x^{adv} \).
3. end
4. return \( x^{adv} \)

4.2 Attack Algorithms

We propose two logical attacks to validate the effectiveness of our unified approach. Both algorithms are greedy in nature and iteratively improve the adversarial objectives. We will explain the generic attack frameworks, followed by their instantiation for feature addition and substitution.
The **GREEDYBYGROUP** algorithm takes a test input vector \( x \) and a maximum number of iterations \( K \). In each iteration, it partitions \( R \) into subsets of relations \( R_1, \cdots, R_m \), and finds the instance within the transitive closure of each \( R_i \) that maximizes the loss. These instances from all \( R_i \)s are combined to create the new version of \( x^{adv} \).

We first break \( R \) into additive and equivalence relations. Each equivalence relation is characterized by an equivalent API group, which contains all APIs with the same functionality. Within each group, we search the combination of API usage that maximizes the test loss \( \ell \). For additive relation, we use attacks in [11] to find an additive adversarial example. In our experiments, we find that it is computationally intensive to search all equivalence and additive partitions in one iteration. An effective simplification is to search only additive partitions in the first half of iterations and then search only equivalence partitions in the second half of iterations.

The **GREEDYBYGRAD** algorithm takes a test input vector \( x \), a maximum number \( m \) of transformation to apply in each iteration, and a maximum number of iteration \( K \). In each iteration, it makes a first-order approximation of the change in \( \ell \) caused by each transformation, and then applies the transformations with top \( m \) approximated increases in \( \ell \) to create the new version of \( x^{adv} \).

In each iteration, we maintain a list of available transformation that includes 1) change any feature’s value from 0 to 1, and 2) change an API’s feature value from 1 to 0 and assign 1 to the feature of an equivalent API. We apply transformations with top \( m \) largest approximated increase in \( \ell \).

### 4.3 Robust Learning Strategy

We use normalization for equivalence relation and adversarial training for additive relation. The relation graph of equivalence relation satisfies the condition in Theorem 2, and therefore normalizing over the equivalence relation will not cause extra loss in robust accuracy compared to adversarial training. In contrast, transformations in additive relation may cause loss in robust accuracy, and thus is more suitable for adversarial training.

For each equivalent API group, we replace the API features with a single meta feature. The normalizer \( \mathcal{N}(\cdot) \) assigns 1 to the meta feature if any API in the equivalent group is present, and 0 otherwise. We then adversarially train the classifier over the normalized inputs.

### 5 Experiment

We evaluate the effectiveness of our unified framework to logical adversaries using **GREEDYBYGROUP** and **GREEDYBYGRAD**. Our evaluation aims to answer the following questions:

1. Do logical attacks pose real threats to existing ML-based malware detectors?
2. How effective is our unified framework in enhancing robustness, and do the results corroborate with the theory?

We investigate these aspects over **Sleipnir**, a real-world WIN32 malware data set that has also been a benchmark for addition attack [11]. Our result shows that our new logical attacks can effectively evade the detector adversarially trained with additive attacks. In contrast, the detector obtained from our unified approach has the highest robustness. In addition, our approach reduces the training time cost compared to pure adversarial training.

#### 5.1 Experiment Methodology

**Baselines Detectors and Attacks.** We compare four ML detectors. The **Unified** detector is trained with our synergy of normalization and adversarial training in Sec 4. The **Adv-Trained** detector is obtained via adversarial training, where the inner maximization returns the best adversarial example generated using our **GREEDYBYGRAD** and the addition attack in [11]. The **Al-Dujaili et al.** model is a benchmark from [11], which is adversarially trained against only addition attack. Finally, the

---

1 For small groups, we enumerate every possible combination. For large groups, we randomly sample a number of combinations and choose the one with the largest loss.

2 **GREEDYBYGROUP** is computationally expensive to be included in the training loop.
Table 2: Evaluation results. Each column represents a baseline detector, whereas each row represents one attack method, with Natural representing no attack. We present the False Negative Rate (FNR) and False Positive Rate (FPR) for each baseline in the format of mean±standard deviation.

|                   | Natural | Unified (Ours) | Adv-Trained | Al-Dujaili et al. [11] |
|-------------------|---------|----------------|-------------|------------------------|
|                   | FNR(%)  | FPR(%)         | FNR(%)      | FPR(%)                 |
| Natural           | 6.2±0.6 | 10.0±0.6       | 5.0±0.4     | 11.9±1.2               |
| META              | 100±0.0 | 10.0±0.6       | 5.5±0.5     | 11.9±1.2               |
| GREEDYBYGROUP     | 100±0.0 | 10.0±0.6       | 5.5±0.5     | 11.9±1.2               |

Natural model is trained with no defense. For attacks, we use GREEDYBYGRAD, GREEDYBYGROUP and the rfgsm_k addition attack in [11].

Data Sets. The data set contains Windows binary API usage features of 34,995 malware and 19,696 benign software, extracted from their Portable Executable (PE) files using LIEF. There are 22,761 unique API calls in the data set, so each PE file is represented by a binary indicator vector \( x \in \{0, 1\}^m \), where \( m = 22,761 \). We sample 19,000 benign PEs and 19,000 malicious PEs to construct the training (60%), validation (20%), and test (20%) sets.

Model Structure. We use a fully-connected neural net with three hidden layer, each with 300 ReLU nodes. This model structure is the same as in [11] to allow fair comparison to its baseline.

Equivalence Relation. We identify four types of patterns for extracting equivalent APIs:

- API with the same name but located in different Dynamically Linkable Libraries (DLLs). For example, memcpy, a standard C library function, is shipped in libraries with different names, including crtdll.dll, msvcr90.dll, and msvcr110.dll.
- API with and without the Ex suffix. The Ex suffix represents an extension to the same API without the suffix.
- API with and without the A or W suffixes. The A suffix represents the single character version. The W suffix represents the wide character version.
- API with/without _s suffix. The _s suffix represents the secure version of an API.

Using these four patterns, we extracted about 2,000 equivalent API groups. About 500 of the groups have more than 2 APIs and the maximal group has 23 APIs.

Experiment Procedure. For each baseline, we train to minimize the NLL loss for 20 epochs, and pick the model with the lowest loss on the validation set. We run five different train/test data set splits. The parameters for attacks in training and evading stages are set as follows.

1. rfgsm_k: we use the default attack parameters in [11] and set the number of attack iterations to 50.
2. META: we use both rfgsm_k and GREEDYBYGRAD attacks in the training loop to generate adversarial examples, and pick the adversarial example with the highest loss. For GREEDYBYGRAD, we run 5 iterations and in each iteration apply 10 transformations for both training and evading. We also consider two different GREEDYBYGRAD strategy, one considers both additive and equivalence relation and the other considers only additive relation.
3. GREEDYBYGROUP: We first run rfgsm_k for 50 iterations to create intermediate adversarial examples using additive relation. We then run 20 iterations for the equivalence relation, and in each iteration, sample \( 2^{10} \) different combinations of API usage within each equivalence relation.

In addition, we assign a higher weight (1.2x) to the loss on malware instances to encourage less FNR; users who desire more robustness to evasion attack are likely working in more security critical domains, and thus low FNR may better align with their interest.
5.2 Experiment Results

We present the results in Table 2. Each column represents a baseline detector, whereas each row represents one attack method. The first row reports the test error rate on clean inputs. The second row reports the error rate on adversarial examples created by the META attack used in the training loop of Adv-Trained. The third row reports the error rate against GreedyByGroup; this attack is omitted in adversarial training due to its high computational cost.

Effectiveness of Logical Attacks. As shown in Table 2, logical attacks are overwhelmingly effective to detectors that are oblivious to potential logical transformations. The adversarial examples can almost always (>99% FNR) evade the naturally trained model, and also can evade the detector in [11] most of the time (>89% FNR) as the detector does not consider API substitution.6

Robustness of Detectors. Our unified approach achieves the highest robustness, as the evasion rate (FNR) only increases by 0.5% on average. The Adv-Trained detector is the second robust but still has 22.1% increase in evasion rate. It is mostly evaded by GreedyByGroup, the attack that is too computationally expensive to be included in the training loop. This result corroborates with the expected advantage of normalization: its robustness guarantee does not depend on specific training algorithms. In contrast, the robustness of adversarial training depends on the strength of the attacks used in the inner maximization loop; when encountered with different attacks, its robustness may decrease. Last, in terms of accuracy on clean test inputs, all detectors using robust learning techniques have higher FPR compared to Natural, which is also expected because of the inevitable robustness-accuracy trade-off. However, the difference is much smaller compared to the cost due to evasion attacks, and thus the trade-off is worthwhile.

Training Time Cost. We run the experiment on a desktop computer with an Intel i7 CPU and a Nvidia 1080ti GPU. Our unified framework takes about 0.5 second to iterate 100 training inputs, which is comparable to [11]. In contrast, adversarial training using GreedyByGrad in the training loop takes more than 5 seconds for every 100 training inputs; the main bottleneck is finding the best adversarial transformation, which requires enumeration over all admissible transformations. In addition, we also note that GreedyByGroup takes hours to generate adversarial examples, and thus cannot be used in the training loop. Normalization shows its advantage in training complexity, as the normalizer for equivalence relation is simple and incurs only small overhead. In contrast, the computation cost of the inner maximization loop limits the use of strong but computationally intensive attacks.

6 Conclusion and Future Work

In this work, we set the first step towards robust learning against logical adversaries: we theoretically characterize the conditions for robustness and the sources of robustness-accuracy trade-off, and propose a provably robust learning framework. Our empirical evaluation shows that a combination of input normalization and adversarial training can significantly enhance model robustness. For future work, we see automatic detection of semantic-preserving transformation as a promising addition to our current expert knowledge approach, and want to explore semantically richer representation of program that enables better robustness-accuracy trade-off.

6For naturally trained models, there are a few test examples that can withstand evasion attack in some runs. However, the number is too small so the average and standard deviation in Table 2 are rounded to 100 and 0.0, respectively.
References

[1] Christian Szegedy, Wojciech Zaremba, Ilya Sutskever, Joan Bruna, Dumitru Erhan, Ian Goodfellow, and Rob Fergus. Intriguing properties of neural networks. arXiv preprint arXiv:1312.6199, 2013.

[2] Ian J Goodfellow, Jonathon Shlens, and Christian Szegedy. Explaining and harnessing adversarial examples. arXiv preprint arXiv:1412.6572, 2014.

[3] Seyed-Mohsen Moosavi-Dezfooli, Alhussein Fawzi, and Pascal Frossard. Deepfool: a simple and accurate method to fool deep neural networks. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 2574–2582, 2016.

[4] Pin-Yu Chen, Huan Zhang, Yash Sharma, Jinfeng Yi, and Cho-Jui Hsieh. Zoo: Zeroth order optimization based black-box attacks to deep neural networks without training substitute models. In Proceedings of the 10th ACM Workshop on Artificial Intelligence and Security, pages 15–26. ACM, 2017.

[5] Nicolas Papernot, Patrick McDaniel, Ian Goodfellow, Somesh Jha, Z Berkay Celik, and Ananthram Swami. Practical black-box attacks against machine learning. In Proceedings of the 2017 ACM on Asia conference on computer and communications security, pages 506–519, 2017.

[6] Kevin Eykholt, Ivan Evtimov, Earlene Fernandes, Bo Li, Amir Rahmati, Chaowei Xiao, Atul Prakash, Tadayoshi Kohno, and Dawn Song. Robust physical-world attacks on deep learning visual classification. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pages 1625–1634, 2018.

[7] Javid Ebrahimi, Anyi Rao, Daniel Lowd, and Dejing Dou. Hotflip: White-box adversarial examples for text classification. In Proceedings of the 56th Annual Meeting of the Association for Computational Linguistics (Volume 2: Short Papers), pages 31–36, 2018.

[8] Puyudi Yang, Jianbo Chen, Cho-Jui Hsieh, Jane-Ling Wang, and Michael I Jordan. Greedy attack and gumbel attack: Generating adversarial examples for discrete data. Journal of Machine Learning Research, 21(43):1–36, 2020.

[9] Yao Qin, Nicholas Carlini, Garrison Cottrell, Ian Goodfellow, and Colin Raffel. Imperceptible, robust, and targeted adversarial examples for automatic speech recognition. In International Conference on Machine Learning, pages 5231–5240, 2019.

[10] Kathrin Grosse, Nicolas Papernot, Praveen Manoharan, Michael Backes, and Patrick McDaniel. Adversarial examples for malware detection. In European Symposium on Research in Computer Security, pages 62–79. Springer, 2017.

[11] Abdullah Al-Dujaili, Alex Huang, Erik Hemberg, and Una-May O’Reilly. Adversarial deep learning for robust detection of binary encoded malware. In 2018 IEEE Security and Privacy Workshops (SPW), pages 76–82. IEEE, 2018.

[12] Ishai Rosenberg, Asaf Shabtai, Lior Rokach, and Yuval Elovici. Generic black-box end-to-end attack against state of the art api call based malware classifiers. In International Symposium on Research in Attacks, Intrusions, and Defenses, pages 490–510. Springer, 2018.

[13] Weiwei Hu and Ying Tan. Black-box attacks against rnn based malware detection algorithms. In Workshops at the Thirty-Second AAAI Conference on Artificial Intelligence, 2018.

[14] Ishai Rosenberg, Asaf Shabtai, Yuval Elovici, and Lior Rokach. Defense methods against adversarial examples for recurrent neural networks. arXiv preprint arXiv:1901.09963, 2019.

[15] Nicolas Papernot, Patrick McDaniel, Xi Wu, Somesh Jha, and Ananthram Swami. Distillation as a defense to adversarial perturbations against deep neural networks. In 2016 IEEE Symposium on Security and Privacy (SP), pages 582–597. IEEE, 2016.

[16] Nicholas Carlini and David Wagner. Towards evaluating the robustness of neural networks. In 2017 IEEE Symposium on Security and Privacy (SP), pages 39–57. IEEE, 2017.

[17] Matthias Hein and Maksym Andriushchenko. Formal guarantees on the robustness of a classifier against adversarial manipulation. In Advances in Neural Information Processing Systems, pages 2266–2276, 2017.
[18] Yizhen Wang, Somesh Jha, and Kamalika Chaudhuri. Analyzing the robustness of nearest neighbors to adversarial examples. In International Conference on Machine Learning, pages 5133–5142, 2018.

[19] Aleksander Madry, Aleksandar Makelov, Ludwig Schmidt, Dimitris Tsipras, and Adrian Vladu. Towards deep learning models resistant to adversarial attacks. In 6th International Conference on Learning Representations (ICLR), Vancouver, Canada, Apr. 2018.

[20] Hongyang Zhang, Yaodong Yu, Jianfao Jiao, Eric Xing, Laurent El Ghaoui, and Michael Jordan. Theoretically principled trade-off between robustness and accuracy. In International Conference on Machine Learning, pages 7472–7482, 2019.

[21] Yao-Yuan Yang, Cyrus Rashtchian, Yizhen Wang, and Kamalika Chaudhuri. Adversarial examples for non-parametric methods: Attacks, defenses and large sample limits. arXiv preprint arXiv:1906.03310, 2019.

[22] Qi Lei, Lingfei Wu, Pin-Yu Chen, Alexandros G Dimakis, Inderjit S Dhillon, and Michael Witbrock. Discrete adversarial attacks and submodular optimization with applications to text classification. Systems and Machine Learning (SysML), 2019.

[23] Po-Sen Huang, Robert Stanforth, Johannes Welbl, Chris Dyer, Dani Yogatama, Sven Gowal, Krishnamurthy Dvijotham, and Pushmeet Kohli. Achieving verified robustness to symbol substitutions via interval bound propagation. pages 4074–4084, 2019.

[24] Fanny Yang, Zuowen Wang, and Christina Heinze-Deml. Invariance-inducing regularization using worst-case transformations suffices to boost accuracy and spatial robustness. In Advances in Neural Information Processing Systems, pages 14757–14768, 2019.

[25] G. Katz, C. Barrett, D.L. Dill, K. Julian, and M.J. Kochenderfer. Reluplex: An efficient smt solver for verifying deep neural networks. In International Conference on Computer Aided Verification, 2017.

[26] Inigo Incer, Michael Theodorides, Sadia Afroz, and David Wagner. Adversarially robust malware detection using monotonic classification. In the Fourth ACM International Workshop on Security and Privacy Analytics (IWSPA), Tempe, AZ, USA, Mar. 2018.

[27] Alex Kouzemtchenko. Defending malware classification networks against adversarial perturbations with non-negative weight restrictions. arXiv preprint arXiv:1806.09035, 2018.

[28] Mark Handley, Vern Paxson, and Christian Kreibich. Network intrusion detection: Evasion, traffic normalization, and end-to-end protocol semantics. In Proceedings of the 10th Conference on USENIX Security Symposium - Volume 10, SSYM’01, Berkeley, CA, USA, 2001. USENIX Association.

[29] Mihai Christodorescu, Somesh Jha, Johannes Kinder, Stefan Katzenbeisser, and Helmut Veith. Software transformations to improve malware detection. Journal in Computer Virology, 3:253–265, 10 2007.

[30] Kevin Coogan, Gen Lu, and Saumya Debray. Deobfuscation of virtualization-obfuscated software: A semantics-based approach. In Proceedings of the 18th ACM Conference on Computer and Communications Security, CCS ’11, pages 275–284, New York, NY, USA, 2011. ACM.

[31] Benjamin Bichsel, Veselin Raychev, Petar Tsankov, and Martin Vechev. Statistical deobfuscation of android applications. In Proceedings of the 2016 ACM SIGSAC Conference on Computer and Communications Security, CCS ’16, pages 343–355, New York, NY, USA, 2016. ACM.

[32] Richard Baumann, Mykolai Protsenko, and Tilo Müller. Anti-proguard: Towards automated deobfuscation of android apps. In Proceedings of the 4th Workshop on Security in Highly Connected IT Systems, SHCIS ’17, pages 7–12, New York, NY, USA, 2017. ACM.

[33] Aleiiedin Salem and Sebastian Banescu. Metadata recovery from obfuscated programs using machine learning. In Proceedings of the 6th Workshop on Software Security, Protection, and Reverse Engineering, SSPREW ’16, pages 1:1–1:11, New York, NY, USA, 2016. ACM.

[34] Pascale Gourdeau, Varun Kanade, Marta Kwiatkowska, and James Worrell. On the hardness of robust classification. In Advances in Neural Information Processing Systems, pages 7444–7453, 2019.

[35] Dexter Kozen. Lower bounds for natural proof systems. In FOCS, 1977.
A Proofs for Theorems and Observations

In this section, we present the omitted proofs for theorems and observations due to page limit of the main body.

A.1 Proof to Theorem 1

Proof. The robustness result is a natural consequence of Observation 1: the normalization procedure ensures that inputs in the same weakly connected component (WCC) on the relation graph will have the same normal form, and thus have the same prediction. The robustness is then guaranteed by the if direction of Observation 1.

The accuracy result is obtained by expressing robust accuracy in terms of the marginal distribution \( \mu \) over inputs and the labeling function \( \eta \) as the following.

\[
Acc_{f,R} = \mathbb{E}_{(x,y) \sim D} \mathbb{I}(R,f(x),y) = \mathbb{E}_{(x,y) \sim D} \mathbb{I}(f(x) = y) = \sum_{x} \mu(x) \mathbb{I}(f(x) = y) \quad (f \text{ is always robust})
\]

\[
= \sum_{C_i \in C} \sum_{x \in C_i} \mu(x) \mathbb{I}(f(x) = y) \quad \text{(partition of input space by WCC)}
\]

\[
= \sum_{C_i \in C} \sum_{x \in C_i} \mu(x) \eta(x, f(x)) \quad \text{(definition of labeling function } \eta) \]

\[
= \sum_{C_i \in C} \sum_{x \in C_i} \mu(x) \eta(x, f(C_i)). \quad (f \text{ predicts the same in } C_i)
\]

The best robust accuracy is then achieved when the accuracy in each weakly connected component is maximized.

A.2 Proof to Observation 2

We first write the full version for Observation 2 in the following claim.

Claim 1. Let \( R' \) and \( R \) be two relations such that \( R' = R \cup \{(x,z)\} \), i.e. \( R' \) allows an extra transformation from \( x \) to \( z \) than \( R \). Let \( G_R, G_{R'} \) denote their relation graphs and \( C_{x,R} \) be the weakly connected component (WCC) in \( G_{R_R} \) that contains \( x \). In addition, let \( \mu, \eta \) be the same as defined in Theorem 1, and \( l_C = \arg \max_{x \in Y} \sum_{x \in C} \mu(x) \eta(x, l) \), i.e. the most likely label of inputs in \( C \). Then the change of best attainable robust accuracy from \( R \) to \( R' \), denoted by \( \Delta_{R,R'} \), is

\[
\Delta_{R,R'} = Acc_{R'} - Acc_R
\]

\[
= \sum_{x' \in C_{x,R'}} \mu(x') \eta(x', l_{C_{x,R'}}) - \left( \sum_{x' \in C_{x,R}} \mu(x') \eta(x', l_{C_{x,R}}) + \sum_{x' \in C_{x,R} \setminus C_{x,R}} \mu(x') \eta(x', l_{C_{x,R}}) \right).
\]

The change \( \Delta_{R,R'} \) is always non-negative for any \( R, R' \) pairs, and the equality only holds when \( l_{C_{x,R}} = l_{C_{x,R'}} \).

Proof. First, we observe that \( C_{x,R'} = C_{x,R} \cup C_{z,R} \). Notice that \( (x,z) \) will not change the graph structure outside \( C_{x,R} \cup C_{z,R} \): the maximal property of WCC guarantees that neither \( x \) nor \( z \) connect to nodes outside their own WCC. If \( C_{x,R} \) and \( C_{z,R} \) are two disjoint WCCs, then the path \( x \rightarrow_R z \) will join them to form \( C_{x,R'} \). Otherwise, \( x, z \) are already in the same WCC, and thus \( C_{x,R'} = C_{x,R} = C_{z,R} \).

Since the graph structure outside \( C_{x,R} \) does not change, it suffices to only look at change of best robust accuracy within \( C_{x,R'} \). The term \( \sum_{x' \in C_{x,R'}} \mu(x') \eta(x', l_{C_{x,R'}}) \) is the best robust accuracy in \( C_{x,R'} \). When \( C_{x,R} \neq C_{z,R} \), the term \( \sum_{x' \in C_{x,R}} \mu(x') \eta(x', l_{C_{x,R}}) \) and \( \sum_{x' \in C_{x,R} \setminus C_{x,R}} \mu(x') \eta(x', l_{C_{x,R}}) \)
are the best robust accuracy in $C_{x,R}$ and $C_{z,R}$, respectively. When $C_{x,R} = C_{z,R}$, the latter term becomes zero and the former is the best robust accuracy in $C_{x,R}$. In both cases, the equation in Claim 1 holds by definition.

Next, we show $\Delta_{R,R'} \leq 0$. First, consider $l_{C_{x,R}} \neq l_{C_{z,R}}$. No matter what $l_{C_{x,R}}$ is, it will be different from at least one of $l_{C_{x,R}}$, $l_{C_{z,R}}$. Suppose, $l_{C_{x,R}} \neq l_{C_{z,R}}$, then the robust accuracy for inputs in $C_{x,R}$ will drop. Similarly, the accuracy in $C_{z,R}$ will drop if $l_{C_{x,R}} \neq l_{C_{z,R}}$. Therefore, $\Delta_{R,R'} < 0$. Second, when $l_{C_{x,R}} = l_{C_{z,R}}$, then we will have $l_{C_{x,R}} = l_{C_{x,R}} = l_{C_{z,R}}$ by definition, and the expression for $\Delta_{R,R'}$ will evaluate to 0.

We also note that if the majority label $l_{C,R}$ is not unique for $C_{x,R}$ and/or $C_{z,R}$, then we consider $l_{C_{x,R}} = l_{C_{z,R}}$ if any majority label for $C_{x,R}$ matches any one for $C_{z,R}$.

A.3 Proof to Observation 3

We first write the full statement of Observation 3 in the following theorem.

**Theorem 3.** Let $R \subseteq \{0, 1\}^n \times \{0, 1\}^n$ be a relation. Given a function $f$, an input $x \in \{0, 1\}^d$ and a feasible set $T(x) = \{z : x \rightarrow_R z\}$, solving the following maximization problem:

$$\max_{z \in T(x)} l(f, z, y)$$

is PSPACE-hard when $l(f, x, y)$ is the 0-1 classification loss.

**Proof.** Let $\alpha : \{0, 1\}^d \rightarrow \{0, 1\}$ be a predicate. Define a loss function $l(f, z, y)$ as follows: $l(f, z, y) = \alpha(z)$ (the loss function is essentially the value of the predicate). Note that $\max_{z \in T(x)} l(f, z, y)$ is equal to 1 iff there exists a $z \in T(x)$ such that $\alpha(z) = 1$. This is a well known problem in model checking called reachability analysis, which is well known to be PSPACE-complete (the reduction is from the problem of checking emptiness for a set of DFAs, which is known to be PSPACE-complete [35]).

Recall that the maximization problem $\max_{z \in B_r(x,y)} l(f, z, y)$ used in adversarial training for the image modality was proven to be NP-hard [25]. Hence it seems that the robust optimization problem in our context is in a higher complexity class than in the image domain.

A.4 Proof to Observation 4

We first write the formal statement of the observation in the following claim.

**Claim 2.** Consider $X = \{0, 1\}^d$ and $Y = \{0, 1\}$. Suppose there exist a set of features $\{x_1, x_1', x_2, x_3, x_4\}$ such that $x_1$ and $x_1'$ satisfy the equivalence relation in Example 2, and $y = 1$ iff any of the following is true: 1) $(x_2 = 1) \land (x_3 = 1)$, 2) $(x_1 \lor x_1' = 1) \land (x_2 = 1)$, 3) $(x_1 \lor x_1' = 1) \land (x_3 = 1) \land (x_4 = 1)$. Then

1. no linear model can classify the inputs with perfect robust accuracy, but
2. a robust and accurate linear model exists under normalize-and-predict.

**Proof.** Let $H = \{f_{w,b} : \text{sgn}(\langle w, x \rangle + b)\}$. Let $w_1, w_1', w_2, w_3, w_4$ denote the coordinates in $w$ that corresponds to $x_1, x_1', x_2, x_3, x_4$. Let $c$ be the contribution to the prediction score from features other than $x_1, x_1', x_2, x_3, x_4$, i.e.

$$c = \langle w, x \rangle + b - \left( \sum_{i \in \{1,2,3,4\}} w_i x_i \right) - w_1' x_1'.$$

In order to classify all possible $x$ correctly, the classifier $f_{w,b}$ must satisfy

$$w_2 + w_4 + c < 0 \quad (5)$$

$$w_2 + w_1' + c > 0 \quad (6)$$

$$w_3 + w_1 + w_1' + c < 0 \quad (7)$$

$$w_3 + w_4 + w_1 + c > 0 \quad (8)$$
First, by Formula 5 and 6, we have \( w_1 > w_2 \) and \( w_1' > w_4 \). However, by Formula 7 and 8, we have \( w_1 + w_1' < w_4 + w_1 \), which implies \( w_1' < w_4 \). Contradiction. Therefore, no linear classifier can satisfy all the equations.

On the other hand, if we perform normalization by letting \( x_1 = x_1 \lor x_1' \) and removing \( x_1' \), then a classifier \( f_{x,b} \) with \( w_1 = 0.4, w_2 = 0.7, w_3 = 0.5, w_4 = 0.2, b = -1 \) and the rest \( w_i \) set to 0 can perfectly classify \( x \).

\[ \]

A.5 Proof to Theorem 2

**Proof.** We know by definition that \( f_{adv}^* \) has the highest possible robust accuracy. Therefore, it suffices to show that there exists a classifier \( f(\mathcal{N}_R(\cdot)) \) under our unified framework that has at least as good robust accuracy as \( f_{adv}^* \).

We consider an \( f \) under our unified framework as follows. Let \( C \) denote a connected component (which is also strongly connected) \( C \) in \( G_R' \) and \( Y_C \) be the set of all labels that \( f_{adv}^* \) assigns to inputs in \( C \), i.e., \( Y_C = \{ y \in Y | \exists x \in C \ s.t. \ f_{adv}^*(x) = y \} \). Let \( C_x \) denote the connected component which contains \( x \). We consider a classifier \( f \) such that

\[
 f(x) = \arg \max_{l \in Y_{C_x}(x,y) \sim D} \mathbb{I}(z \in C_x \land y = l),
\]

i.e., \( f \) predicts the same label for all inputs in a connected component, and chooses the label that maximizes the clean accuracy in the connected component. Notice that \( f(x) = f(\mathcal{N}_R(x)) \) by construction, so we will use \( f(x) \) instead of \( f(\mathcal{N}_R(x)) \) for simplicity.

Recall that we say a classifier \( f \) is robustly accurate over an input-label pair \((x,y)\) under \( \mathcal{R} \) if and only if \( f(z) = y \) for all \( z : x \rightarrow_{R^*} z \). Now to show that \( f \) with the prediction rule in Equation 9 has the same robust accuracy as \( f_{adv}^* \), we prove the following claim.

**Claim 3.** The classifier \( f \) is robustly accurate over \((x,y)\) under \( \mathcal{R} \) if \( f_{adv}^* \) is robustly accurate \((x,y)\) under \( \mathcal{R} \).

We prove the contrapositive of the claim. Suppose \( f \) is not robustly accurate over \((x,y)\). Let \( z \) denote the input such that \( \mathcal{N}_{R'}(x) \rightarrow_{R^*} z \) and \( f(z) \neq y \).

First, we notice that \( \mathcal{N}_{R'}(x) \rightarrow_{R'} z \) implies \( x \rightarrow_{R'} z \): we know \( x \rightarrow_{R'} \mathcal{N}_{R'}(x) \) because the connected components in \( G_{R'} \) are strongly connected, and therefore an attacker can first transform \( x \) to \( \mathcal{N}_{R'}(x) \) using rules in \( R' \), and then transform \( \mathcal{N}_{R'}(x) \) to \( z \) using rules in \( R' \).

Second, by the definition of \( f(z) \), we know that there must be a \( z' \in C_z \) such that \( f_{adv}^*(z') = f(z) \neq y \) because \( f \) only predicts the label that has been used by \( f_{adv}^* \) over some input in the same connected component. Since \( C_x \) is strongly connected by our initial assumption, we must have \( z \rightarrow_{R^*} z' \).

Now, because \( x \rightarrow_{R^*} z \) and \( z \rightarrow_{R^*} z' \), we have \( x \rightarrow_{R^*} z' \). Since \( x \rightarrow_{R^*} z' \) but \( f_{adv}^*(z') \neq y \), we can conclude that \( f_{adv}^* \) is not robustly accurate at \( x \), and thus prove the claim.

Claim 3 suggests that \( f \) is at least as robustly accurate as \( f_{adv}^* \). Since we know 1) \( f^* \) is at least as robustly accurate as \( f \), and 2) \( f_{adv}^* \) has the highest possible robust accuracy by definition, we can conclude that \( f^*, f \) and \( f_{adv}^* \) have the same robust accuracy and thus complete the proof.