

A THEORETICAL FRAMEWORK FOR ROBUSTNESS OF (DEEP) CLASSIFIERS AGAINST ADVERSARIAL SAMPLES

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ABSTRACT

Adversarial samples are maliciously created inputs that lead a learning-based classifier to produce incorrect output labels. An adversarial sample is often generated by adding adversarial perturbation (AP) to a normal test sample. Recent studies that tried to analyze classifiers under such AP are mostly empirical and provide little understanding of why. To fill the gap, we propose a theoretical framework for analyzing learning-based classifiers, especially deep neural networks (DNN) in the face of AP. By using concepts from topology, this framework brings forth the key reasons why an adversarial can fool a classifier (f_1) and suggests a new focus on its oracle (f_2 , like human annotators of that specific task). By investigating the topological relationship between two (pseudo)metric spaces corresponding to predictor f_1 and oracle f_2 , we develop several conditions that can determine if f_1 is always robust (strong robust) against adversarial samples according to its f_2 . The theoretical framework leads to a set of novel and complementary insights that have not been uncovered by the literature. Surprisingly our theorems find that just one extra irrelevant feature can make a classifier not strong robust, and the right feature representation learning is the key to getting a classifier that is both accurate and strong robust. Empirically we find that "Siamese architecture" can be used to help DNN models get close to the desired topological relationship for strong robustness, which in turn effectively improves its performance against AP.

1 INTRODUCTION

Deep Neural Networks (DNNs) can efficiently learn highly accurate models from large corpora of training samples. As a result, DNNs have been demonstrated to perform exceptionally well on multiple machine learning tasks (Krizhevsky et al., 2012; Hannun et al., 2014), including many security-sensitive applications such as (Microsoft Corporation, 2015; Dahl et al., 2013; Sharif et al., 2016; Moosavi-Dezfooli et al., 2016; Papernot et al., 2016b).

Unlike machine learning used in other fields, security sensitive tasks involve intelligent and adaptive adversaries responding to the learning systems. Recent studies show that attackers can force many machine learning models, including DNNs, to produce an abnormal output behavior, such as a misclassification. A so-called "adversarial sample" (Goodfellow et al., 2014; Szegedy et al., 2013) is crafted by adding a carefully chosen adversarial perturbation to a correctly classified sample drawn from the data distribution. The goal of this paper is to analyze the adversarial robustness of machine learning classifiers and uncover the underlying principles that enable learning-based classification systems to achieve robust performance when being attacked by adversarial samples.

Investigating the behavior of machine learning systems in adversarial environments is an emerging topic (Huang et al., 2011; Barreno et al., 2006; 2010; Globerson & Roweis, 2006; Biggio et al., 2013; Kantchelian et al., 2015; Zhang et al., 2015). Recent studies can be roughly categorized into three types: (1) Poisoning attacks in which specially crafted attack points are injected into the training data. Multiple recent papers (Alfeld et al., 2016; Mei & Zhu, 2015b; Biggio et al., 2014; 2012; Mei & Zhu, 2015a) have considered the problem of an adversary being able to pollute the training data with the goal of influencing learning systems including support vector machines (SVM), autoregressive

models and topic models. (2) Evasion attacks are attacks in which the adversary’s goal is to create inputs that are misclassified by a deployed target classifier. Related studies (Szegedy et al., 2013; Goodfellow et al., 2014; Xu et al., 2016; Kantchelian et al., 2015; Rndic & Laskov, 2014; Biggio et al., 2013) assume the adversary does not have an opportunity to influence the training data, but instead finds “adversarial samples” to evade a trained classifier like DNN, SVM or random forest. (3) Privacy-aware machine learning (Duchi et al., 2014) is another important category relevant to data security in machine learning systems. Recent studies have proposed various strategies (Xie et al., 2014; Bojarski et al., 2014; Stoddard et al., 2014; Li & Zhou, 2015; Rajkumar & Agarwal, 2012; Dwork, 2011; Nock et al., 2015) to preserve the privacy of data such as differential privacy. This paper focuses on evasion attacks that are mostly used to attacking classifiers that try to distinguish malicious behaviors from benign behaviors. Here we extend it to a broader meaning – adversarial manipulation of test samples. Evasion attacks may be encountered during system deployment of machine learning methods in adversarial settings.

Several recent studies consider how to find adversarial perturbation to fool DNN classification and how to design corresponding strategies against such adversarial perturbation. (Szegedy et al., 2013) observed that convolution NNs are vulnerable to small artificial perturbations. They use box-constrained Limited-memory BFGS (L-BFGS) to create adversarial samples reliably. Their study also finds that adversarial perturbations generated from one network can also force other networks to produce wrong output. Then, (Goodfellow et al., 2014) try to clarify that the primary cause of such vulnerabilities is the linear nature of DNNs. They propose an algorithm – “fast gradient sign method” for generating adversarial examples quickly. Subsequent papers (Fawzi et al., 2015; Papernot et al., 2015a; Sabour et al., 2015; Nguyen et al., 2015) have explored other adversarial manipulations on DNN outputs or deep representations.

Meanwhile, researchers try to develop hardening strategies for making DNN systems robust to various kinds of noise, which in the worst-case include “adversarial perturbation”. For instance, denoising NN architectures (Vincent et al., 2008; Gu & Rigazio, 2014; Jin et al., 2015) can discover more robust features by using a noise-corrupted version of inputs as training samples. A modified distillation strategy (Papernot et al., 2015b) is proposed to improve the robustness of DNNs against adversarial examples, though it has been shown to be unsuccessful recently (Carlini & Wagner, 2016a). More recent techniques incorporate a smoothness penalty (Miyato et al., 2016; Zheng et al., 2016) or a layer-wise penalty (Carlini & Wagner, 2016b) as a regularization term in the loss function to promote the smoothness of the DNN model distributions. In the broader secure machine learning field, researchers also make attempts for hardening learning systems. For instance: (1) (Barreno et al., 2010) and (Biggio et al., 2008) propose a method to introduce some randomness in the selection of classification boundaries; (2) A few recent studies (Xiao et al., 2015; Zhang et al., 2015) consider the impact of using reduced feature sets on classifiers under adversarial attacks. (Xiao et al., 2015) proposes an adversary-aware feature selection model that can improve a classifier’s robustness against adversarial attacks by incorporating specific assumptions about the adversary’s data manipulation strategy. (3) Multiple studies model adversarial scenarios with formal frameworks representing the interaction between the classifier and the adversary. Related efforts include perfect information assumptions (Dalvi et al., 2004), assuming a polynomial number of membership queries (Lowd & Meek, 2005), formalizing the attack process as a two-person sequential Stackelberg game (Brückner & Scheffer, 2011; Liu & Chawla, 2010), a min-max strategy (training a classifier with best performance under the worst perturbation) (Dekel et al., 2010; Globerson & Roweis, 2006), exploring online and non-stationary learning (Dahlhaus, 1997; Cesa-Bianchi & Lugosi, 2006), and formalizing as an adversarial reinforcement learning problem (Uther & Veloso, 1997).

Despite previous studies (Zheng et al., 2016; Carlini & Wagner, 2016a;b), there exists little theoretical understanding of the underlying principles that determine the robustness of a machine-learning classifier against AP. Several important questions have not been answered yet:

- What makes a classifier always robust to AP ?
- Which parts of a classifier influence its robustness against AP more compared to the rest ?
- What is the relationship between a classifier’s generalization accuracy and its robustness against adversarial samples ?
- Why (many) DNN classifiers are not robust against AP ? How to improve ?

This paper tries to answer above questions and makes the following contributions:

Table 1: A list of important notations used in the paper.

f_1	A learned machine learning classifier $f_1 = c_1 \circ g_1$.
f_2	The oracle for the same task (see Definition (2.1)) $f_2 = c_2 \circ g_2$.
g_i	Part of f_i including operations that progressively transform input representations into a new form of learned representations in X_i .
c_i	Part of f_i including relatively simple decision functions for classifying.
X	Input space (e.g., $\{0, 1, 2, \dots, 255\}^{32 \times 32 \times 3}$ for cifar10 (Krizhevsky & Hinton, 2009)).
Y	Output space (e.g., $\{1, 2, 3, \dots, 10\}$ for cifar10 (Krizhevsky & Hinton, 2009)).
X_1	Feature space defined by the feature extraction module g_1 of a predictor f_1 .
X_2	Feature space defined by the feature extraction module g_2 of an oracle f_2 .
$d_1(\cdot, \cdot)$	The metric function for measuring distances in feature space X_1 with respect to a learned predictor f_1 .
$d_2(\cdot, \cdot)$	The metric function for measuring distance in feature space X_2 with respect to an oracle f_2 .
$d'_1(\cdot, \cdot)$	The Pseudometric function with respect to the learned predictor f_1 , $d'_1(x, x') = d_1(g_1(x), g_1(x'))$.
$d'_2(\cdot, \cdot)$	The Pseudometric function with respect to the oracle f_2 , $d'_2(x, x') = d_2(g_2(x), g_2(x'))$.
<i>a.e.</i>	almost everywhere (Folland, 2013) (defined by Definition (6.1) in Section 6.5)
$\epsilon, \delta_1, \delta_2, \delta, \eta$	small positive constants

- Section 2 points out that previous definitions of adversarial examples for a classifier (f_1) have overlooked the importance of the oracle function (f_2) of the same task. Section 2.2 also points out the second key piece being missed by recent literature: the decomposition of $f_i = c_i \circ g_i$ ($i \in \{1, 2\}$). Both predictor f_1 and oracle f_2 can be split into g_i including feature learning operations and c_i including simple decision functions for the classification. We then revise the definition of "adversarial sample" by considering the sample similarity in the feature space defined by g_2 . This is because the main property of "adversarial sample" is that they can "fool" the predictor f_1 and is treated as "similar" as its seed sample according to f_2 .
- Section 3 formally defines when a classifier f_1 is always robust ("strong-robust") against AP. It proves two theorems about sufficient and necessary conditions that make f_1 strong-robust according to f_2 . Our theorems lead to a number of interesting insights, like (1) when f_1 is continuous a.e., g_1 controls the strong-robustness of f_1 according to f_2 ; (2) even one extra unrelated features will make the predictor f_1 vulnerable to AP. Our theorems also provide a few possible guidance to harden classifiers, such as by learning a better g_1 or by removing unrelated features.
- Section 4 uses the framework of "strong-robustness" to analyze DNNs. Empirically we find that "Siamese architecture" can be used to help a DNN classifier learn a better g_1 and achieve better robustness against AP.

2 ORACLES MATTER FOR DEFINING ADVERSARIAL SAMPLES

This section provides a general definition of *adversarial samples at test time*¹, by including the notion of an oracle. All previous definitions of "adversarial samples" are special cases of our general formulation. Besides, the proposed general definition decomposes the influence of feature learning and classification decision that have been overlooked by the previous studies. Table 1 provides a list of necessary notations we use in the paper.

2.1 PREVIOUS FORMULATIONS OF ADVERSARIAL SAMPLES

For a particular classification task, a learned classifier is represented as $f_1 : X \rightarrow Y$, where X represents the input sample space and Y is the output space representing a categorical set. To attack f_1 in the test phase, the basic idea proposed in the recent literature (Biggio et al., 2013; Lowd &

¹ We use "adversarial perturbation", "adversarial samples", "adversarial attacks at test time", and "adversarial examples" interchangeably in the rest of this paper.

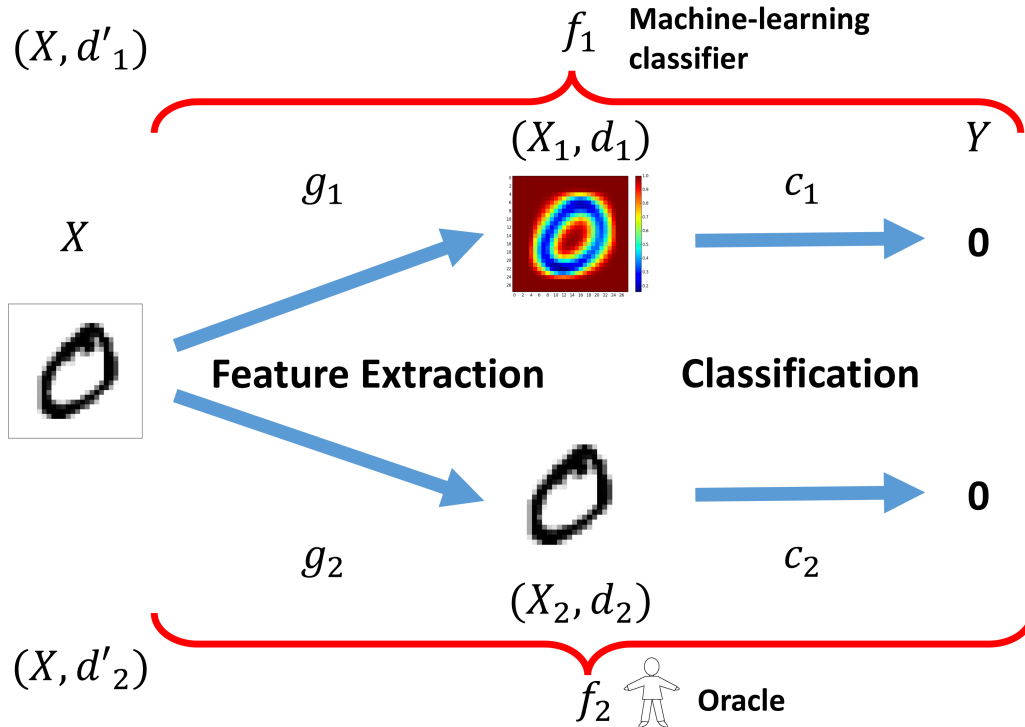


Figure 1: Example of a learned predictor and oracle for classifying images of hand-written “0”. Both include two steps: feature extraction and classification. The upper sub-figure is about the learned machine classifier f_1 and the lower sub-figure is about the oracle f_2 . The learned classifier f_1 transforms data samples from the original space X to an embedded metric space (X_1, d_1) using its feature extraction step. Here, d_1 is the similarity measure on the feature space X_1 . Classification models like DNN cover the feature extraction step in the model, though many other models like decision tree need hard-crafted or domain-specific feature extraction. Then f_1 can use a softmax function to decide the classification result $y \in Y$. Similarly, human oracle f_2 transforms data samples from the original space X into an embedded metric space (X_2, d_2) by its feature extraction. Here, d_2 is the corresponding similarity measure. Then the oracle get the classification result $y \in Y$ using the feature representation of samples (X_2, d_2) .

Meek, 2005) is to generate a misclassified sample x' by perturbing a correctly classified sample x , with an adversarial perturbation $\Delta(x, x')$. Formally, when given $x \in X$

$$\begin{aligned} &\text{Find } x' \\ &\text{s.t. } f_1(x) \neq f_1(x') \\ &\quad \Delta(x, x') < \epsilon \end{aligned} \tag{2.1}$$

Here $x, x' \in X$. $\Delta(x, x')$ represents the difference between x and x' . The meaning of $\Delta(x, x')$ depends on the specific data type that x and x' belong to².

For the purpose of “fooling” a classifier, naturally, the attacker wants to control the size of the perturbation $\Delta(x, x')$ to ensure the perturbed sample x' still stays close enough to the original sample x to satisfy the intended “fooling” purpose. For example, in the image classification case, Eq. (2.1) can use the gradient information to find a $\Delta(x, x')$ that makes *human annotators* still recognize x' as almost the same as x , though the classifier will predict x' into a different class. In another example with more obvious security implications about PDF malware (Xu et al., 2016), x' in Eq. (2.1) is found by genetic programming. A modified PDF file from a malicious PDF seed will still be recognized as malicious by *an oracle machine* (i.e., a virtual machine decides if a PDF file is malicious or not by

²For example, in the case of strings, $\Delta(x, x')$ represents the difference between two strings.

Table 2: Summary of the previous studies defining adversarial examples.

Previous studies	f_1	$\Delta(x, x')$	Formulation of $f_1(x) \neq f_1(x')$
(Goodfellow et al., 2014)	Convolutional neural networks	ℓ_∞	$\operatorname{argmax}_{x'} \operatorname{Loss}(f_1(x'), f_1(x))$
(Szegedy et al., 2013)	Convolutional neural networks	ℓ_2	$\operatorname{argmin}_{x'} \operatorname{Loss}(f_1(x'), l)$, subject to: $l \neq f_1(x')$
(Biggio et al., 2013)	Support vector machine (SVM)	ℓ_2	$\operatorname{argmin}_{x'} \operatorname{Loss}(f_1(x'), -1)$, subject to: $f_1(x) = 1$
(Kantchelian et al., 2015)	Decision tree and Random forest	$\ell_2, \ell_1, \ell_\infty$	$\operatorname{argmin}_{x'} \operatorname{Loss}(f_1(x'), -1)$, subject to: $f_1(x) = 1$
(Grosse et al., 2016)	Convolutional neural networks	ℓ_0	$\operatorname{argmax}_{x'} \operatorname{Loss}(f_1(x'), f_1(x))$
(Xu et al., 2016)	Random forest and SVM	ℓ_1, ℓ_∞	$\operatorname{argmin}_{x'} \operatorname{Loss}(f_1(x'), -1)$, subject to: $f_1(x) = 1$

actually running it), but are classified as benign by state-of-art machine learning classifiers (Xu et al., 2016). Various definitions for "adversarial samples" exist in the recent literature and are summarized in Appendix Section 6.

2.2 WHY ORACLE MATTERS FOR DEFINING ADVERSARIAL SAMPLES

The goal of machine learning is to train a learning-based predictor function $f_1 : X \rightarrow Y$ to approximate the oracle classifier $f_2 : X \rightarrow Y$ for the same classification task. For example, in image classification tasks, the oracle f_2 is often human annotators. In this paper, the notion of "oracle" is defined as follows:

Definition 2.1. An "**Oracle**" represents a decision process generating ground truth labels for the specific task of interest. Each oracle is task-specific, with finite knowledge and noise-free.³

Clearly in real applications when searching for adversarial samples, there exists a hidden assumption about the oracle f_2 for the same task. That is: $f_2(x) = f_2(x')$, the adversarial sample x' should be classified into the same category as the original sample x by the oracle f_2 . Therefore, a more precise definition of "adversarial samples" should be:

$$\begin{aligned}
 &\text{Find } x' \\
 &\text{s.t. } f_1(x) \neq f_1(x') \\
 &\quad \Delta(x, x') < \epsilon \\
 &\quad f_2(x) = f_2(x')
 \end{aligned} \tag{2.2}$$

Both Eq. (2.1) and Eq. (2.2) need to define a distance function to measure $\Delta(x, x')$. Previous studies have used functions including ℓ_2 -norm, ℓ_1 -norm, ℓ_0 -norm and ℓ_∞ -norm (Goodfellow et al., 2014; Szegedy et al., 2013; Grosse et al., 2016; Kantchelian et al., 2015). Table 2 summarizes different choices of f_1 and $\Delta(x, x')$ used in the recent literature. In addition, several algorithms have been implemented to generate "adversarial perturbations" by solving Eq. (2.1) as a constrained optimization. We summarize three of such attacking studies in Section 6.2.

2.3 MEASURING SAMPLE DIFFERENCE IN WHICH SPACE? MODELING & DECOMPOSING f_i

With the purpose of "fooling" a classifier, adversarial sample x' and its seed sample x should be regarded as "similar" by the oracle. This is reflected as the last two constraints in Eq. (2.2). Most previous studies have not explicitly specified in what space to calculate the distance (or similarity) among samples. Instead they just simply used norm functions on the original space X to get $\Delta(x, x')$. For instance, most studies listed in Table 2 assume (X_2, d_2) as $(X, \|\cdot\|)$ and $\|\cdot\|$ denotes a norm function.

³We leave all detailed analysis of when an oracle contains noise as future work.

Modeling Oracle f_2 : We want to argue that this simplification is not ideal. For most machine-learning tasks, an oracle does not make the classification decision and does not measure the difference among samples in space X . For instance, human annotators are oracle for a specific image-classification task. As illustrated by the seminal cognitive neuroscience paper "untangling invariant object recognition" (DiCarlo & Cox, 2007) and its follow-up study (DiCarlo et al., 2012), the information processing of visual object recognition by human brains takes place along the ventral visual stream, and this stream is considered to be a progressive series of visual re-representations, from V1 to V2 to V4 to IT cortex (DiCarlo & Cox, 2007). Experimental results support that human visual system makes classification decision at IT cortex. Appendix Section 6.3 provides more details of modeling oracle and points out that for many security-sensitive applications about machines, oracles f_2 do exist and use various (dynamic) traces for measuring and deciding classification⁴.

Therefore, in the context of AP we think the sample similarity should be defined according to the distance function and the feature space defined by the oracle f_2 of the same task. We denote this feature space and the distance function as (X_2, d_2) in the rest of this paper. Though it is hard to measure and define (X_2, d_2) , we want to argue that in the context of "adversarial samples", modeling f_2 is significant and necessary. Such analysis can bring forth the key causes of AP and leads to a set of novel insights we uncover in Section 3.4 that have not been uncovered by the literature.

Decomposing f_2 and f_1 : We can decompose an oracle function $f_2 : X \rightarrow Y$ as $f_2 = c_2 \circ g_2$ where $g_2 : X \rightarrow X_2$ represents the operations for feature extraction and $c_2 : X_2 \rightarrow Y$ performs the simple operation of classification. Essentially g_2 includes the operations that (progressively) transform input representations into an informative form of representations X_2 . c_2 applies relatively simple functions (like linear) in X_2 for the purpose of classification. d_2 is the metric function (details in Section 3) an oracle uses to measure the similarity among samples (by relying on representations learned in the space X_2). We illustrate the modeling and decomposition in Figure 1.

We then decompose f_1 in a similar way, to answer the question: "which parts of a learned classifier influence its robustness against AN more compared to the rest?". As shown in Figure 1, we assume a common machine learning classifier $f_1 = c_1 \circ g_1$, where $g_1 : X \rightarrow X_1$ represents the feature extraction⁵ and function $c_1 : X_1 \rightarrow Y$ performs the operation of classification. Appendix Section 6.4 provides a list of examples for decomposing state-of-the-art f_1 .

2.4 ASSUMPTION : ALMOST EVERYWHERE (A.E.) CONTINUITY OF f_i

Most previous studies (Table 2) have made an important and implicit assumption about f_1 and f_2 : f_i is almost everywhere (a.e.) continuous. $i \in \{1, 2\}$.

Definition 2.2. Suppose f_i is the classification function. f_i is continuous a.e., $i \in \{1, 2\}$, if $\forall x \in X$ a.e., $\exists \delta_i > 0$, such that $\forall x' \in X, d_i(g_i(x), g_i(x')) < \delta_i, f_i(x) = f_i(x')$.

Illustrated in Figure 1, d_i is the metric function (details in Section 3) f_i uses to measure the similarity among samples in the space X_i . For notation simplicity, we use the term "continuous a.e." for "continuous almost everywhere"⁶ in the rest of the paper. The above definition is a special case of almost everywhere continuity defined in (Folland, 2013) (see Definition (6.1) in Section 6.5), since we decompose f_i in a certain way (see Figure 1). The a.e. continuity has a few indications, like:

$$\forall x, x' \in X, \mathbb{P}(f_i(x) \neq f_i(x') | d_i(g_i(x), g_i(x')) < \delta_i) = 0 \quad (2.3)$$

See Section 6.5 for details of indications by a.e. continuity.

f_2 is assumed continuous a.e. previously: Most previous studies find "adversarial samples" by solving Eq. (2.1), instead of Eq. (2.2). This made an implicit assumption that if the adversarial sample x' is similar to the seed sample x , they belong to the same class according to f_2 . This assumption essentially is: f_2 is almost everywhere (a.e.) continuous.

f_1 is continuous a.e.: Almost all popular machine learning classifiers satisfy the a.e. continuity assumption. For instance, a deep neural network is certainly continuous a.e.. Similarly to the results shown by (Szegedy et al., 2013), DNNs satisfy that $|f_1(x) - f_1(x')| \leq W \|x - x'\|_2$ where $W \leq \prod W_i$ and $W_i \geq \|(w_i, b_i)\|_\infty$. Here $i = \{1, 2, \dots, L\}$ representing i -th linear layer in NN.

⁴Oracles f_2 do exist in many security-sensitive applications about machines. But machine-learning classifiers f_1 are used popularly due to speed or efficiency

⁵Notice that g_1 may also include implicit feature selection steps like ℓ_1 regularization.

⁶The measure (e.g., Lebesgue measure) of discontinuous set is 0.

Therefore, $\forall \epsilon > 0$, let $\delta = \epsilon/W$. Then $|f_1(x) - f_1(x')| < \epsilon$ when $d_1(x, x') = \|x - x'\|_2 < \delta$. This shows that a deep neural network is almost everywhere continuous when $d_1(\cdot) = \|\cdot\|_2$.

In appendix Section 6.5, we show that if f_1 is not continuous a.e., it is not robust to any types of noise. Considering the generalization assumption of machine learning, machine learning classifiers should satisfy the continuity a.e. assumption. Appendix Section 6.7 provides two examples of how popular machine learning classifiers satisfy this assumption.

For the rare cases when f_1 is not continuous a.e., see next Section 2.6 discussing "boundary points" that matter for analyzing adversarial perturbations.

2.5 A REVISED FORMULATION OF "ADVERSARIAL SAMPLES" USING f_2 AND d_2

By replacing $\Delta(x, x')$ in Eq. (2.2), we have a revised formulation of "adversarial samples":

Definition 2.3. Adversarial sample for a classification task: Suppose we have two functions f_1 and f_2 . $f_1 : X \rightarrow Y$ is the classification function learned from a training set and $f_2 : X \rightarrow Y$ is the classification function of the oracle that generates ground-truth labels for the same task. The adversarial examples at test time can be defined as: given a sample $x \in X$, find a similar "adversarial sample" $x' \in X$, such that (x, x') satisfies Eq. (2.4). If f_2 is continuous a.e., (x, x') just needs to satisfy Eq. (2.5)⁷.

$$\begin{array}{ccc} \text{Find } x' & & \text{Find } x' \\ \text{s.t. } f_1(x) \neq f_1(x') & \xrightarrow[\text{when } f_2 \text{ continuous a.e.}]{(2.4)} & \text{s.t. } f_1(x) \neq f_1(x') \\ d_2(g_2(x), g_2(x')) < \delta_2 & & d_2(g_2(x), g_2(x')) < \delta_2 \\ f_2(x) = f_2(x') & & \end{array} \quad (2.5)$$

Using $d_2(g_2(x), g_2(x'))$ to describe the difference between x and x' reflects the true properties of "fooling" by adversarial samples. Based on this definition, we uncover multiple early insights theoretically (see Section 3) about why a classifier might be not robust against such samples.

2.6 BOUNDARY POINTS OF f_1 MATTER WHEN f_1 IS NOT CONTINUOUS A.E. IN X

When f_1 is not continuous a.e., the analysis of adversarial samples needs to consider "boundary points" of f_1 with certain properties. This section tries to clarify the definition and related scope.

Definition 2.4. We define the set of boundary points of f_i as the following set of sample pairs: $\{(x, x') | f_i(x) \neq f_i(x'), d_i(g_i(x), g_i(x')) < \delta_i, x \in X, x' \in X\}$ (2.6)

Our definition of the boundary points describes such points as pairs of samples that are across the classification boundary. This format of definition makes the following analysis (notation-wise) easy and concise.

Lemma 2.5. f_i is not continuous a.e., if and only if $x \in X, x' \in X, \mathbb{P}(f_i(x) \neq f_i(x') | d_i(g_i(x), g_i(x')) < \delta_i) > 0$ (2.7)

This lemma shows that a case with probability of boundary points larger than 0 is exactly the situation when f_i being not continuous a.e..

In addition, we want to point out that all boundary pairs of f_2 (satisfying $f_2(x) \neq f_2(x')$ and $d_2(g_2(x), g_2(x')) < \delta_2$) are not considered in our analysis of adversarial samples. Figure 6 illustrates three types of boundary points, using the first two columns showing boundary points of f_2 .

The third column of Figure 6 describes "Boundary based adversarial attacks" that can only attack seed samples whose distance to the boundary of f_1 is smaller than δ_2 . Essentially this attack is about those boundary points of f_1 that are treated as similar and belong to the same class by f_2 . That is

$$\mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d_2(g_2(x), g_2(x')) < \delta_2, d_1(g_1(x), g_1(x')) < \delta_1) \quad (2.8)$$

- When f_1 is continuous a.e., Eq. (2.8) equals to 0. (derived from Eq. (2.3) in Section 2.4)
- When f_1 is not continuous a.e., Eq. (2.8) might be larger than 0. (derived from Eq. (2.7))

The value of this probability is critical for our analysis in Theorem (3.3) and in Theorem (3.5). Again, we want to emphasize that most machine learning methods assume f_1 is continuous a.e. and therefore "boundary based adversarial attacks" are not crucial.

⁷When f_2 is continuous a.e., $\mathbb{P}(f_2(x) = f_2(x') | d_2(g_2(x), g_2(x')) < \epsilon) = 1$

3 DEFINE AND UNDERSTAND STRONG-ROBUSTNESS

With a more accurate definition of "adversarial samples", now we try to answer the first central question: "What makes a classifier always robust against adversarial samples?". Section 3.1 defines a concept "strong-robust" describing a classifier always robust against adversarial samples. Section 3.2 and Section 3.3 present the sufficient and necessary conditions for "strong-robustness". Section 3.4 then provides a few surprising insights we derive from the analysis of "strong-robustness".

3.1 DEFINE " f_1 IS $\{\delta_2, \eta\}$ -STRONG-ROBUST AGAINST ADVERSARIAL SAMPLES"

We apply reverse-thinking on Definition (2.3) and derive the following definition of **strong-robustness** for a machine learning classifier against adversarial perturbation:

Definition 3.1. $\{\delta_2, \eta\}$ -**Strong-robustness of a machine-learning classifier:** A learned predictor $f_1(\cdot)$ is $\{\delta_2, \eta\}$ -strong-robust against adversarial samples if: $\forall x, x' \in X$ a.e., (x, x') satisfies Eq. (3.1).

$$\begin{aligned} \forall x, x' \in X \\ \mathbb{P}(f_1(x) = f_1(x') | f_2(x) = f_2(x'), d_2(g_2(x), g_2(x')) < \delta_2) > 1 - \eta \end{aligned} \quad (3.1)$$

When f_2 is continuous a.e., Eq. (3.1) becomes the following Eq. (3.2):

$$\forall x, x' \in X, \mathbb{P}(f_1(x) = f_1(x') | d_2(g_2(x), g_2(x')) < \delta_2) > 1 - \eta \quad (3.2)$$

Here η and δ_2 are two small positive constants. Eq. (3.1) defines the " $\{\delta_2, \eta\}$ -strong-robustness" as a claim with a high probability. To simplify notations, in the rest of this paper, we use the simplified term "strong-robust" representing " $\{\delta_2, \eta\}$ -strong-robust". Also in the rest of this paper, we propose and prove theorems and corollaries by using it more general form by Eq. (3.1). For all cases, if f_2 is continuous a.e., all proofs and equations can be simplified by using only the term $d_2(g_2(x), g_2(x')) < \delta_2$ (i.e. by removing the term $f_2(x) = f_2(x')$) according to Eq. (3.2). Our "strong-robustness" definition leads to four important theorems in next two subsections.

We want to emphasize that " f_1 is strong-robust" does not mean it is a good classifier. For example, a trivial example for strong-robust models is $f_1(x) \equiv 1, \forall x \in X$. However, it is a useless model since it doesn't have any prediction power. A learned classifier should be both strong-robust and accurate in an adversarial setting.

3.2 TOPOLOGICAL EQUIVALENCE OF TWO METRIC SPACES (X_1, d_1) AND (X_2, d_2) IS SUFFICIENT IN DETERMINING THE STRONG-ROBUSTNESS

In the appendix, Section 7.1 briefly introduces the concept of metric space and the definition of topological equivalence among two metric spaces. As shown in Figure 1, here f_1 defines a metric space (X_1, d_1) on X_1 with the metric function d_1 . Similarly f_2 defines a metric space (X_2, d_2) on X_2 with the metric function d_2 .

If the topological equivalence (Eq. (7.1)) exists between (X_1, d_1) and (X_2, d_2) , it means that for all pair of samples from X , we have the following relationship:

$$\forall x, x' \in X, d_1(g_1(x), g_1(x')) < \delta_1 \Leftrightarrow d_2(g_2(x), g_2(x')) < \delta_2 \quad (3.3)$$

When f_1 is continuous a.e., this can get us the following important theorem, indicating that the topological equivalence between (X_1, d_1) and (X_2, d_2) is a sufficient condition in determining whether or not f_1 is strong-robust against adversarial samples:

Theorem 3.2. *When f_1 is continuous a.e., if (X_1, d_1) and (X_2, d_2) are topologically equivalent, then the learned classifier $f_1(\cdot)$ is strong-robust to adversarial samples at test time.*

Proof. See its proofs in Appendix:Section 7.3.4 □

This theorem can actually guarantee that:

$$\forall x, x' \in X, \mathbb{P}(f_1(x) = f_1(x') | f_2(x) = f_2(x'), d_2(g_2(x), g_2(x')) < \delta_2) = 1 \quad (3.4)$$

Clearly Eq. (3.4) is a special (stronger) case of the "strong-robustness" defined by Eq. (3.1).

For more general cases including f_1 might not be continuous a.e., we also need to consider the probability of the boundary point attacks (Eq. (2.8)). Therefore, we revise and get a more general theorem as follows:

Theorem 3.3. *If (X_1, d_1) and (X_2, d_2) are topologically equivalent and $\mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d_1(g_1(x), g_1(x')) < \delta_1, d_2(g_2(x), g_2(x')) < \delta_2) < \eta$, then the learned classifier $f_1(\cdot)$ is strong-robust to adversarial samples at test time.*

Proof. See its proofs in Appendix:Section 7.3.3. □

3.3 FINER TOPOLOGY OF (X, d'_1) THAN (X, d'_2) IS SUFFICIENT AND NECESSARY IN DETERMINING THE STRONG-ROBUSTNESS OF f_1

Now we extend the discussion from two metric spaces into two pseudometric spaces. This extension finds the sufficient and necessary condition that determines the strong-robustness of f_1 . The related two pseudometrics are d'_1 (for f_1) and d'_2 (for f_2), both directly being defined on X . Appendix Section 7.2 includes detailed descriptions of pseudometric, pseudometric spaces, topology and a finer topology relationship between two pseudometric spaces.

Essentially, τ_1 (the topology in pseudometric space (X, d'_1)) is a finer topology than τ_2 (the topology in pseudometric space (X, d'_2)) means:

$$\forall x, x' \in X, d'_2(x, x') < \delta_2 \Rightarrow d'_1(x, x') < \delta_1 \quad (3.5)$$

Here δ_1 and δ_2 are two small scalars larger than 0. Also because $d'_1(x, x') = d_1(g_1(x), g_1(x'))$ and $d'_2(x, x') = d_2(g_2(x), g_2(x'))$, the above equation equals to:

$$\forall x, x' \in X, d_2(g_2(x), g_2(x')) < \delta_2 \Rightarrow d_1(g_1(x), g_1(x')) < \delta_1 \quad (3.6)$$

Using Eq. (3.6) and the continuity a.e. assumption, we can derive the following Theorem about the sufficient and necessary condition for f_1 's strong-robustness:

Theorem 3.4. *When f_1 is continuous a.e., f_1 is strong-robust against adversarial test samples if and only if τ_1 (the topology in (X, d'_1)) is a finer topology than τ_2 (the topology in (X, d'_2)).*

Proof. See its proof in appendix Section 7.3.1. □

This theorem provides a sufficient and necessary condition in determining whether or not f_1 is strong-robust.

Actually the above theorem can guarantee that when f_1 is continuous a.e.:

$$\forall x, x' \in X, \mathbb{P}(f_1(x) = f_1(x') | d_2(g_2(x), g_2(x')) < \delta_2) = 1 \quad (3.7)$$

Eq. (3.7) clearly is a special (stronger) case of strong-robustness defined by Eq. (3.1).

For more general cases where f_1 might not be continuous a.e., the probability of the boundary points attack (Eq. (2.8)) needs to be considered. We revise and get a more general sufficient condition for strong-robustness as follows:

Theorem 3.5. *When f_1 is not continuous a.e., If τ_1 (the topology in (X, d'_1)) is a finer topology than τ_2 (the topology in (X, d'_2)) and $\mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d_1(g_1(x), g_1(x')) < \delta_1, d_2(g_2(x), g_2(x')) < \delta_2) < \eta$, then f_1 is strong-robust against adversarial test samples.*

This theorem provides a sufficient condition in determining whether or not f_1 is strong-robust. ⁸

3.4 WHY THEOREMS ARE IMPORTANT

The four theorems proposed above lead to a set of key insights in this section about why and how an adversarial can fool a machine-learning classifier using adversarial samples. One of the most valuable insights is: feature learning step decides whether a predictor is strong-robust or not in an adversarial test setting. All the discussion in the subsection assumes f_1 is continuous a.e..

3.4.1 g_1 MATTERS FOR THE STRONG-ROBUSTNESS AND c_1 DOES NOT

Theorem (3.2) and Theorem (3.4) indicate that when f_1 is continuous a.e., the two feature spaces (X_1, d_1) and (X_2, d_2) or the functions g_1 and g_2 determine the strong-robustness of f_1 . This raises an important question that how c_1 and c_2 influence the strong-robustness of f_1 .

⁸When f_1 is not continuous a.e., it is difficult to find the necessary and sufficient condition for strong-robustness of f_1 . We leave this to future research.

In Figure 7 and Figure 8, we show two different cases in which f_1 is strong-robust according to f_2 . In both figures, f_1 is not accurate according to f_2 . Figure 7 shows the case of $X_1 = X_2 = \mathbb{R}^2$. Figure 8 shows the case of $X_1 = \mathbb{R}, X_2 = \mathbb{R}^2$ and $X_1 \subset X_2$. For such cases, strong-robustness means $\mathbb{P}(f_1(x) = f_1(x') | d_2(x, x') < \delta_2) = 1$. All pairs of test samples (x, x') can be categorized into the three cases shown in both figures.

- Test-case (a) is when x and x' are predicted as the same class and f_1 gets correct predictions according to f_2 . There exist no adversarial samples.
- Test-case (b) is when x and x' are predicted as the same class, but f_1 gets incorrect predictions according to f_2 . There exist no adversarial samples.
- Test-case (c) shows when $f_1(x) \neq f_1(x')$, $d_2(x, x') < \delta_2$ and $f_2(x) = f_2(x')$. This case is explained in Section 2.6. Essentially, this is about “Boundary based adversarial attacks” and can only attack points whose distance to the boundary of f_1 is smaller than δ_2 ($f_1(x) \neq f_1(x')$, $d_2(x, x') < \delta_2$ and $f_2(x) = f_2(x')$). When f_1 is continuous a.e., the probability of this set is 0.

Clearly from the two figures, c_1 does not determine the strong-robustness of f_1 .

3.4.2 EXTRA UNRELATED FEATURES RUIN THE STRONG-ROBUSTNESS

Based on Theorem (3.4), we can have another corollary as follows:

Corollary 3.6. *When f_1 is continuous a.e., if $X_1 = \mathbb{R}^{n_1}, X_2 = \mathbb{R}^{n_2}, n_1 > n_2, X_2 \subsetneq X_1, d_1, d_2$ are norm functions, then $f_1(\cdot)$ is not strong-robust against adversarial samples.*

This corollary shows that the feature learning is crucial in determining whether a predictor is strong-robust or not in adversarial test setting. By Corollary (3.6), if unrelated features are selected in the feature selection step, then no matter how accurate the model is trained, it is not strong-robust to adversarial samples.

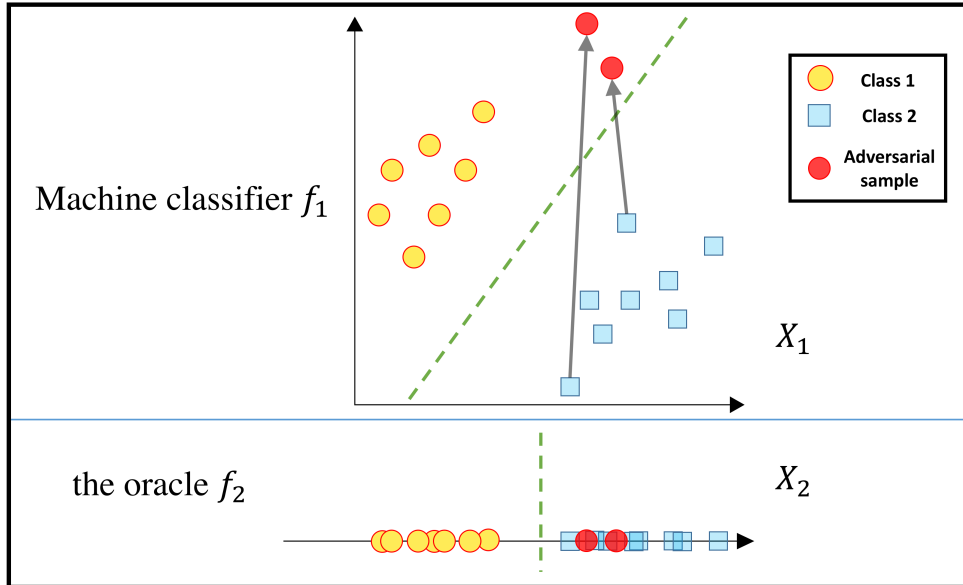


Figure 2: An example showing f_1 with one unrelated feature is prone to adversarial samples. The red circle denotes an adversarial sample, which is very close to its seed sample in the oracle feature space (according to d_2), but it is far from its seed sample in the feature space (according to d_1) of the trained classifier. Essentially "adversarial samples" can be easily found for all seed samples in this Figure. We only draw for two seeds. Besides, for each seed sample, we can generate a series of "adversarial samples" (by varying attacking power) after the attacking line crosses the decision boundary of f_1 . We only show one case of such an "adversarial sample" for each seed sample.

Here's an example. Figure 2 shows a situation that the oracle only uses one feature to classify samples correctly. A machine classifier uses an extra unrelated feature and successfully classifies all the items.

Table 3: Summary of theoretical conclusions that we can derive from our theorems. Here $X_1 = \mathbb{R}^{n_1}$ and $X_2 = \mathbb{R}^{n_2}$. The strong-robustness is determined by feature extraction function g_1 . The accuracy is determined by both the classification function c_1 and the feature extraction function g_1 .

	Cases:	d_1 & d_2 are norms	Can be accurate?	Based on	Illustration
(I)	$X_1 \setminus (X_1 \cap X_2) \neq \emptyset,$ $X_2 \not\subset X_1$	Not Strong-robust	may not be accurate	Theorem (3.4)	Figure 2
(II)	$n_1 > n_2, X_2 \subsetneq X_1$	Not strong-robust	may be accurate	Corollary (3.6)	Figure 2
(III)	$n_1 = n_2, X_1 = X_2$	Strong-robust	may be accurate	Corollary (3.7)	Figure 7
(IV)	$n_1 < n_2, X_1 \subset X_2$	Strong-robust	may not be accurate	Theorem (3.4)	Figure 8

However, it’s very easy to find adversary samples by only adding a perturbation using the additional feature. In Figure 2, red circles are such adversarial samples. The adversarial samples are very close to seed samples in the oracle space. But they are predicted into a different class by f_1 .

In real-world applications, such attacks can be, for example, adding words with a very tiny font size in a spam E-mail, that is invisible to a human annotator. When a learning-based classifier tries to utilize such extra words, it can lead to many easily generated adversarial emails.

For many security sensitive applications, previous studies using state-of-art learning-based classifiers normally believe that adding more features is always helpful. Apparently, our corollary indicates that this thinking is wrong and can lead to their classifiers vulnerable to adversarial samples (Xu et al., 2016).

3.4.3 FEATURE SPACE IS MORE IMPORTANT THAN A SPECIFIC FORM OF NORM FUNCTIONS

Corollary 3.7. *When f_1 is continuous a.e., if d_1 and d_2 are norms and $X_1 = X_2 = \mathbb{R}^n$, then $f_1(\cdot)$ is strong-robust to adversarial samples at test time.*

This corollary shows that if a learned classifier and its oracle share the same derived feature space ($X_1 = X_2$), the learned classifier is strong-robust when two metrics are both norm functions (even if not the same norm). We can call this corollary as “norm doesn’t matter”.

Many interesting phenomena can be answered by Corollary (3.7). For instance, for a norm regularized classifier, this corollary answers an important question that whether a different norm function will influence its robustness against adversarial samples. The corollary indicates that changing to a different norm function may not improve the robustness of the model under adversarial perturbation.

Summarizing Theorem (3.2), Theorem (3.4), Corollary (3.7) and Corollary (3.6), the robustness of a learned classifier is decided by two factors: (1) the difference between two derived feature spaces; and (2) the difference between the metric functions. Two corollaries show that the difference between the feature spaces is more important than the difference between the two metric functions.

3.4.4 ROBUSTNESS AND ACCURACY

In Table 3, we provide four situations in which the proposed theorems can be used to determine whether a classifier f_1 is strong-robust against adversarial samples or not.

- Case (I): If f_1 uses some extra and unrelated features, it will not be strong-robust to adversarial attacks. It may not be an accurate predictor if f_1 misses some related features used by f_2 .
- Case (II): If f_1 uses some extra and unrelated features, it will not be strong-robust to adversarial attacks. It may be an accurate predictor if f_1 uses all the features used by f_2 .
- Case (III): If f_1 and f_2 use the same set of features and nothing else, f_1 is strong-robust and may be accurate.
- Case (IV): If f_1 misses some related features and does not extract unrelated features, f_1 is strong-robust (even though its accuracy may be unsatisfactory).

Our theoretical analysis in Table 3 provides a much better understanding of the relationship between robustness and accuracy. For instance, two interesting cases from Table 3 are worth to emphasize again: (1) If f_1 misses related features used by f_2 and does not include unrelated features, f_1 is strong-robust (even though it may not be accurate). (2) If f_1 uses some extra and unrelated features,

it will not be strong-robust (though it may be a very accurate predictor). Clearly, in an adversarial setting, we should aim to get a classifier that is both strong-robust and precise. A better feature learning function g_1 is exactly the solution that may achieve both goals.

3.4.5 WHEN f_1 IS CONTINUOUS A.E., EITHER STRONG-ROBUST OR NOT ROBUST AT ALL A.E.

Table 3 indicates that training a strong-robust and accurate classifier in practice is extremely difficult. For instance, Figure 2 shows only one extra irrelevant feature, which does not hurt accuracy, makes the classifier not robust to adversarial perturbation at all (i.e., for samples a.e. in X , easy to find its adversarial samples.).

When f_1 is continuous a.e., $\mathbb{P}(f_1(x) = f_1(x') | f_2(x) = f_2(x'), d_2(g_2(x), g_2(x')) < \delta_2)$ equals to either 1 or 0. This means f_1 is either strong-robust or not robust under AN at all a.e.. One case with this probability as 0 is illustrated by Figure 2. Case (III) and Case (IV) from Table 3 have this probability equaling to 1.

When f_1 is not continuous a.e., for instance when X is a finite space, the probability of "adversarial samples" can be calculated as:

$$\begin{aligned} & \mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d_2(g_2(x), g_2(x')) < \delta_2) \\ &= \frac{\#\{(x, x') | f_2(x) = f_2(x') \& d_2(g_2(x), g_2(x')) < \delta_2 \& f_1(x) \neq f_1(x')\}}{\#\{(x, x') | f_2(x) = f_2(x') \& d_2(g_2(x), g_2(x')) < \delta_2\}} \end{aligned} \quad (3.8)$$

This is exactly the proportion of those pairs of points for which f_1 classifies them into different classes and f_2 treats them as similar and "same-class" samples. For this case, both g_1 and c_1 matter for the strong-robustness of f_1 . See Appendix Section 7.4.2 for an example showing how c_1 makes f_1 not strong robust.

3.5 WHY USEFUL FOR "ADVERSARIAL SAMPLE" STUDIES NOT MODELING f_2 ?

Our theoretical analyses bring forth the causes of the "adversarial samples" and leads to a set of novel early insights that have not been uncovered by the literature. For applications in which modeling f_2 is hard, this theoretical framework can still be useful. Most previous studies (reviewed in Section 2.2) assume (X_2, d_2) equals to $(X, \|\cdot\|)$, where $\|\cdot\|$ is a norm function. Replacing (X_2, d_2) into $(X, \|\cdot\|)$ in all theoretically conclusions presented above, our theorems can explain many studies in the literature.

- For instance, one previous study (Xu et al., 2016) shows that a genetic-programming based "adversarial sample" strategy can always evade two state-of-art learning-based PDF-malware classifiers (with "100%" evasion rates). The reason behind such good evasion rates is the Condition (3.6). Both state-of-art PDF-malware classifiers have used many superficial features (e.g., a feature representing "is there a long comment section") that are not relevant to "the malicious property" of a PDF sample at all !
- As another example, multiple DNN studies about adversarial samples claim that adversarial samples are transferable among different DNN models. This can be explained by Figure 2 (when X_1 is a much higher-dimensional space). Since different DNN models learn over-complete feature spaces (X_1), there is a high chance that these different X_1 involve a similar set of unrelated features. Therefore the adversarial samples are generated along similar gradient directions. That is why many such samples can evade multiple DNN models.

Besides, our theorems suggest a list of possible solutions that may improve the adversarial robustness of learning-based classifiers. Options include such as:

- **By learning a better g_1 :** Methods like DNNs directly learn the feature extraction function g_1 . To reach the strong-robustness, for example, we can force to learn a g_1 that helps (X, d'_1) to be a finer topology than (X_2, d'_2) . Next Section 4.2 explores this option and shows that Siamese architecture can be used to implement this solution and improves the adversarial robustness of a state-of-the-art DNN model.
- **By removing unrelated features:** As shown by Table 3, unrelated features ruin the strong-robustness of learning-based classifiers. Clearly if feature selection methods can be easily explored for an application, a simple way is to design techniques filtering out irrelevant features. One previous study (Zhang et al., 2015) explores this strategy against evasion attacks.

- **By obtaining more samples:** For cases when f_1 is not continuous a.e., obtaining more samples is clearly a good way to learn a better decision boundary that might improve the adversarial robustness of the classifier at the same time.

4 DNN CLASSIFIERS' ROBUSTNESS AGAINST ADVERSARIAL SAMPLES

In this section, we apply the above theorems for analyzing deep neural networks (DNN) classifiers.

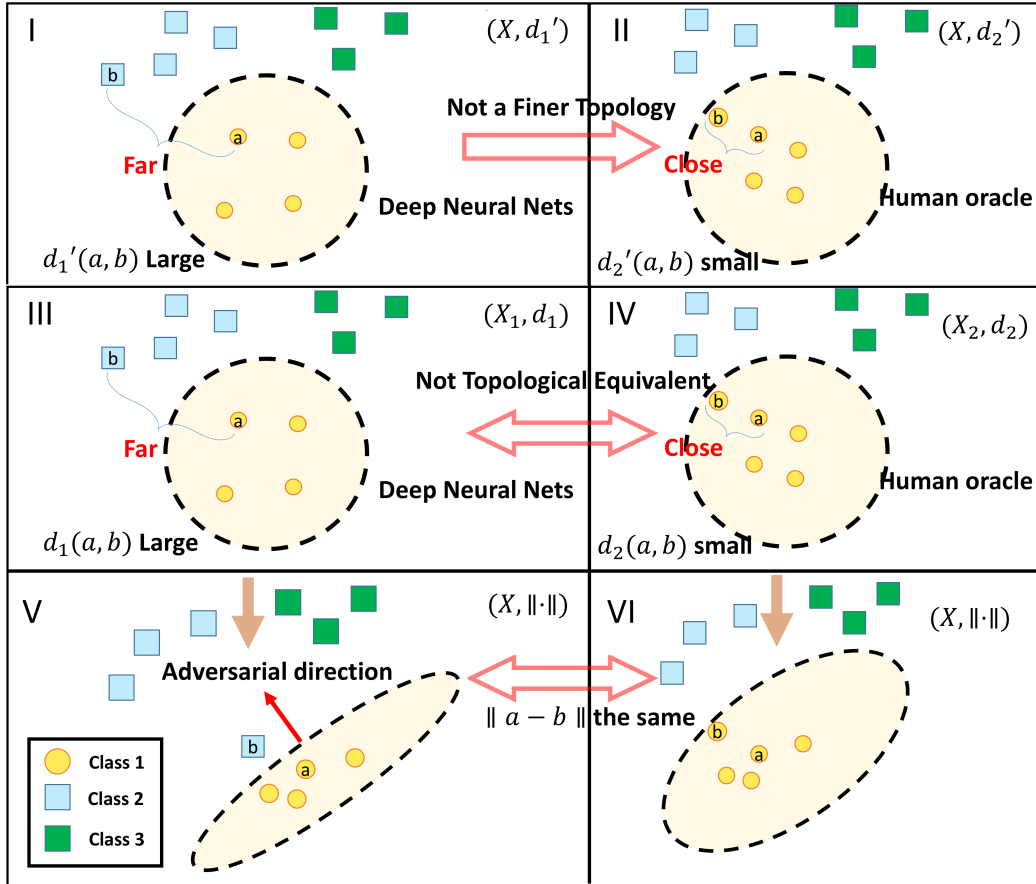


Figure 3: This figure shows one situation that (X, d_1') is not a finer topology than (X, d_2') (therefore, (X_1, d_1) and (X_2, d_2) are not topologically equivalent). According to Theorem (3.4), in this case, the DNN is vulnerable to adversarial samples. The two sample points a and b are close with regards to (w.r.t.) a norm $\|\cdot\|$ in X . They are also close w.r.t. d_2 in (X_2, d_2) space and close w.r.t. d_2' in (X, d_2') space. But they are far from each other in the space of (X, d_1') and in the space of (X_1, d_1) . In other words, while $d_2(a, b)$, $d_2'(a, b)$ and $\|a - b\|$ are small, $d_1(a, b)$ and $d_1'(a, b)$ are large. Clearly, DNN can be easily evaded by adding a small perturbation $\|a - b\|$ on sample a or sample b . NOTE: it is normally difficult to get the analytic form of (X_2, d_2) for most applications. Most previous studies (reviewed in Section 2.2) assume (X_2, d_2) equals to $(X, \|\cdot\|)$, where $\|\cdot\|$ is a norm function.

Researchers have proposed different strategies to generate adversarial samples attacking deep neural networks (e.g., (Szegedy et al., 2013; Nguyen et al., 2015; He et al., 2015; Papernot et al., 2016a; Moosavi-Dezfooli et al., 2015; Papernot et al., 2015b)). Here we focus on an image classification application with symbols defined as follows:

- $f_1(\cdot)$: $f_1(\cdot)$ is a DNN classifier with multiple layers, including linear perceptron layers, activation layers, convolutional layers and softmax decision layer.

Table 4: Accuracy of the deep residual network(He et al., 2015) obtained from two noise-perturbed testing cases. The second column shows the result on randomly perturbed samples, and the third column shows the result on adversarially perturbed samples.

Attack power (defined in Eq. (8.2))	Test accuracy on randomly perturbed samples	Test accuracy on adversarially perturbed samples
0	0.9411	0.9411
1	0.9409	0.5833
5	0.9369	0.3943
10	0.9288	0.3853

- (X_1, d_1) : X_1 denotes the feature space discovered by the layer right before the last fully connected layer. This feature space is automatically extracted from the original image space (e.g., RGB representation) by the DNN. (X, d'_1) is defined by d_1 using Eq. (7.2).
- (X_2, d_2) : X_2 denotes the feature space that oracle (e.g., human annotators) used to decide ground-truth labels of training images. For example, a human annotator needs to recognize a hand-written digit “0”. X_2 includes what patterns he/she needs for such a decision. (X, d'_2) is defined by d_2 using Eq. (7.3)

4.1 ARE STATE-OF-THE-ART DEEP NEURAL NETS STRONG-ROBUST ?

For DNN, it is difficult to derive a precise analytic form of d_1 (or d'_1). But we can observe some properties of d_1 through experimental results. For instance, Table 4 shows properties of d_1 (and d'_1) resulting from performing testing experiments on a state-of-art residual network. The model we use is a 200-layer residual network (He et al., 2015) trained on Imagenet dataset (Deng et al., 2009) by Facebook⁹.

In Table 4, we generate two types of test samples from 50000 images in the validation set of Imagenet: (1) 50000 randomly perturbed images. The random perturbations on each image are generated by first fixing the perturbation value on every dimension to be the same, and then randomly assigning the sign on every dimension as + or - (with probability 1/2). In this way, the size of the perturbation can be described by $\|x - x'\|_\infty$ that we name as the level of **attacking power** (later defined in Eq. (8.2)). (2) 50000 adversarially perturbed images. We use the fast-gradient sign method (introduced in Section 6.2) to generate such adversarial perturbations on each seed image. The “attacking power” of such adversarial perturbations uses the same formula as Eq. (8.2). The first column of Table 4 shows different attack powers (Eq. (8.2)) we use in the experiment. The second column shows the accuracy of running the DNN model on the first group of image samples and the third column shows the accuracy of running the DNN model on the second group of image samples. From Table 4, we can see that the accuracy of the DNN model in the adversarial setting is very bad. Clearly, the performance on randomly perturbed data is much better than performance on maliciously perturbed data. Comparing the second column and the third column in Table 4, we can conclude that d_1 (and d'_1) in a random direction is larger than d_1 (and d'_1) in the adversarial direction. This indicates that a round sphere in (X_1, d_1) (and (X, d'_1)) corresponds to a very thin high-dimensional ellipsoid in $(X, \|\cdot\|)$ (illustrated by the left half of Figure 3).

The phenomenon we observed can be explained by Figure 3. Figure 3 (I) shows a sphere in (X, d'_1) and Figure 3 (III) shows a sphere in (X_1, d_1) . They correspond to the very thin high-dimensional ellipsoid in $(X, \|\cdot\|)$ in Figure 3 (V). The norm function $\|\cdot\|$ is defined in space X and is application-dependent. In the case of Table 4, $\|\cdot\| = \|\cdot\|_\infty$.

Differently, for human oracles, a sphere in (X, d'_2) (shown in Figure 3 (II)) or in (X_2, d_2) (shown in Figure 3 (IV)) corresponds to an ellipsoid in $(X, \|\cdot\|)$, however, not including very-thin directions (shown in Figure 3 (VI)). When the attackers try to minimize the perturbation size using the approximated distance function $d_2 = \|\cdot\|$, the thin direction of ellipsoid in Figure 3 (V) is exactly the adversarial direction.

⁹<https://github.com/facebook/fb.resnet.torch>

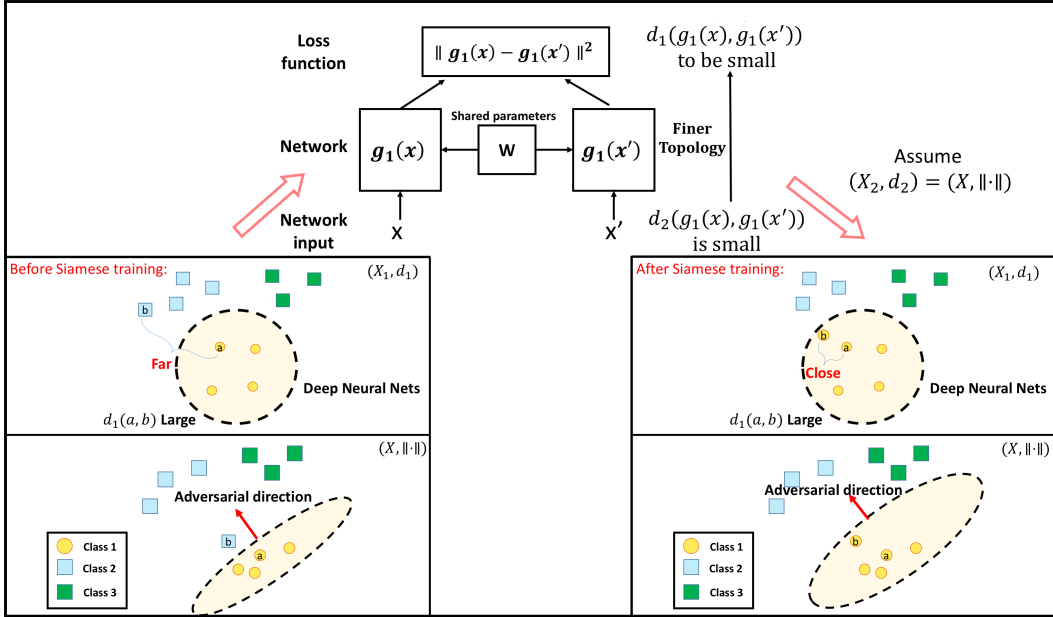


Figure 4: Sketch of Siamese training. Inputs are pairs of seed sample and their randomly perturbed version, while we suppose the d_2 distance between the pair is small. By forwarding a pair into the Siamese network and penalizing the outputs of the pair, this training intuitively limit the d_1 distance between two similar samples to be small. Backpropagation is used to update the weights of the network.

4.2 USING “SIAMESE ARCHITECTURE” TO IMPROVE DNNs’ ADVERSARIAL ROBUSTNESS

One intuitive formulation that we can use to improve a DNN’s adversarial robustness is by solving the following:

$$\forall x, x' \in X, \text{if } d_2(g_2(x), g_2(x')) < \epsilon, \operatorname{argmin}_w d_1(g_1(x; w), g_1(x'; w)) \quad (4.1)$$

This essentially forces the DNN to have the finer topology between (X_1, d_1) and (X_2, d_2) by learning a better g_1 . We name the strategy minimizing the loss defined in Eq. (4.1) as “Siamese Training” because this formulation uses the Siamese architecture (Bromley et al., 1993), a classical deep-learning approach proposed for learning embedding. We feed a slightly perturbed input x' together with its original seed x to the Siamese network which contains two copies (sharing the same weights) of a DNN model we want to improve. By penalizing the difference between middle-layer ($g_1(\cdot)$) outputs of (x, x') , “Siamese Training” can push two spaces (X, d_1) versus (X_2, d_2) to approach finer topology relationship, and thus increase the robustness of the model. This can be concluded from Figure 4. By assuming $d_2(g_2(x), g_2(x'))$ equals (approximately) to $\|\Delta(x, x')\|$, previous studies (summarized in Table 2) normally assume d_2 is a norm function $\|\cdot\|$. Because for a pair of inputs (x, x') that are close to each other (i.e., $\|x - x'\|$ is small) in $(X, \|\cdot\|)$, Siamese training pushes them to be close also in (X_1, d_1) . As a result, this means that a sphere in (X_1, d_1) maps to a not-too-thin high-dimensional ellipsoid in $(X, \|\cdot\|)$. Therefore the adversarial robustness of DNN model after Siamese training may improve.

The Siamese architecture (Bromley et al., 1993) has long been used in many real applications, like face recognition (Krizhevsky et al., 2012) and dimension reduction (Hadsell et al., 2006). A Siamese network contains two copies of a DNN model sharing the same weights. The loss function of the Siamese network can be any distance measure as long as it is differentiable. The process of Siamese Training is summarized by the Algorithm 1 in Section 8.1. In experiments, we choose Euclidean distance $\|\cdot\|_2$ for $d_1(\cdot)$ (however, many other choices are possible).

The primary purpose of covering Siamese training in this paper is to provide an empirical study showing how our theorems can be useful for analyzing a particular hardening strategy. Siamese

training is closely related to a recent study "stability training" from (Zheng et al., 2016). The authors tried to increase the model robustness by pushing the KL divergence between the outputs small. Another recent work (Lee et al., 2015) proposes a hardening process very similar to Siamese training. Differently, we use the randomly perturbed sample as x' , while this paper uses the adversarially perturbed sample as x' , though both try to match the middle layer outputs. More details have been included in Section 8.2 to connect "Siamese training" with similar state-of-the-art methods.

Details of our experimental set-up and datasets are included in Section 8.1. The results of running "Siamese training" on VGG model about CIFAR-10 dataset are summarized in Table 5. Six different training strategies are compared through testing on adversarial samples (details in Section 8.1): (1) original model; (2) stability training (Zheng et al., 2016)¹⁰; (3) Siamese training used as regularization (G); (4) Siamese training (G) alone; (5) Siamese training used as regularization (F); (6) Siamese training (F) alone. The first column of Table 5 shows different levels of attack power (defined in Eq. (8.2)). Test accuracy reported in Figure 5(a) and Table 5 shows that Siamese training greatly decreases the effectiveness of the adversarial attacks, especially by Siamese training (G).

In Appendix Section 8.3 we propose a new evaluation measure "Adversarial Robustness of Classifiers (ARC)" to quantify how far a classifier is away from the strong-robustness. This quantitative measure considers both the predictor f_1 and the oracle f_2 . By design, a classifier (f_1)'s ARC achieves the maximum (1 since ARC is rescaled to $[0, 1]$) if and only if f_1 is strong-robust (see Theorem (8.3)). In our experiments, interestingly, VGG models after four different Siamese training all obtain much higher ARC and ARCA¹¹ than "stability training". Figure 5(b) shows that the improvement ranges from 52% (by Siamese training as regularization (G)) to 100% (by Siamese training (G)).

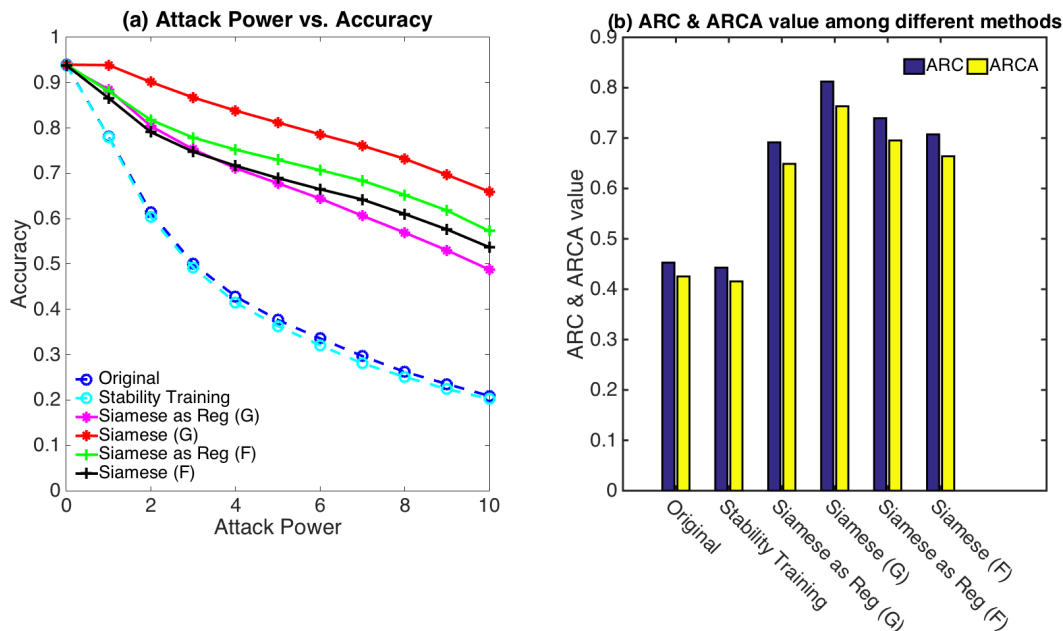


Figure 5: (a) Test accuracy under "adversarial sample" attacks: six different colors for six different training strategies. (Details in Section 8.1) (b). ARC and ARCA for six different training strategies under "adversarial sample" attacks.

¹⁰ATT: Stability training was shown to improve the model robustness against Gaussian noise in (Zheng et al., 2016). Differently, our experiments focus on testing a learning model's robustness against "adversarial perturbation". The sole purpose of including this baseline is to show where state-of-art hardening strategies are in our experimental setting.

¹¹Appendix Section 8.3 also combines accuracy and ARC into a unified measure ARCA: "Adversarial Robustness of Classifiers with Accuracy".

5 CONCLUSION

Most machine learning classifiers were not designed to withstand manipulations made by intelligent and adaptive adversaries. Recent literature has tried to analyze and harden learning-based classifiers under such adversarial perturbations (AP). However, previous studies are mostly empirical and provide little understanding of why many learning-based classifiers, including deep neural networks (DNNs), are vulnerable to AP. To fill this gap, we propose a theoretical framework using the notions of topological spaces to uncover such reasons. The central idea of our work is that the robustness of a classifier f_1 against AP is decided by both f_1 and its oracle f_2 (such as human annotators of that specific task). This motivates us to design a formal definition describing when a classifier f_1 is always robust ("strong-robustness") against AP according to its f_2 . The second key piece of our framework is the decomposition of $f_i = c_i \circ g_i$. g_i includes feature learning operations and c_i includes relatively simple decision functions for the classification. We theoretically prove that f_1 is strong-robust against AP if and only if a special topological relationship exists between the two feature spaces defined by g_1 and g_2 . Theorems of our framework provide two important insights: (1) The strong-robustness of f_1 is fully determined by its g_1 , not c_1 . (2) Extra irrelevant features ruin the strong-robustness of f_1 . Empirically we find that the Siamese architecture can be used to enhance the adversarial robustness of DNN models.

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6 APPENDIX OF PROBLEM FORMULATION

Various definitions for "adversarial samples" exist in the recent literature. For instance, Eq. (6.1) tries to find the x' by minimizing $\Delta(x, x')$ under some constraints. Eq. (2.1) is a more general formulation than Eq. (6.1) and can summarize most relevant studies. For example, (Xu et al., 2016) used genetic programming to generate multiple possible malicious variants from seed (one malicious PDF file). Here "adversarial samples" are those generated PDFs that can fool PDFRate (a learning-based classifier for detecting malicious PDFs) to classify them as benign. The distances of these variants to the seed are not necessarily minimal. For such cases, Eq. (2.1) still fits, while Eq. (6.1) does not.

6.1 MORE ABOUT PREVIOUS DEFINITIONS OF ADVERSARIAL SAMPLES AT TESTING TIME

Various definition of adversarial samples exist in the literature. Eq. (2.1) provides a more general formulation. The following Eq. (6.1) has been popular as well. Eq. (6.1) is a special case of Eq. (2.1).

$$\begin{aligned} & \underset{x' \in X}{\operatorname{argmin}} \Delta(x, x') \\ & \text{Subject to: } f_1(x) \neq f_1(x') \end{aligned} \tag{6.1}$$

Besides, in the field of security, machine learning has been popular in classifying the malicious ($y = 1$) behavior versus benign ($y = -1$) in computer security tasks. For such a context, two different definitions of adversarial samples exist:

For instance, (Biggio et al., 2013) uses a formula as follows:

$$\begin{aligned} & \underset{x'}{\operatorname{argmin}}(f_1(x')) \\ & \text{s.t. } \Delta(x, x') < d_{\max} \\ & \quad f_1(x) > 0 \end{aligned} \tag{6.2}$$

Differently, (Lowd & Meek, 2005) uses the following formula:

$$\begin{aligned} & \underset{x'}{\operatorname{argmin}}(\Delta(x, x')) \\ & \text{s.t. } f_1(x') < 0 \\ & \quad f_1(x) > 0 \end{aligned} \tag{6.3}$$

Here d_{\max} is a constant. Clearly, these two formulas are not equivalent.

6.2 BACKGROUND: PREVIOUS ALGORITHMS GENERATING "ADVERSARIAL SAMPLES"

To fool classifiers at test time, several approaches have been implemented to generate "adversarial perturbations" by solving Eq. (2.2). According to Eq. (2.2), an adversarial sample should be able to change the classification result $f_1(x)$, which is a discrete value. To solve Eq. (2.2), we need to transform the constraint $f_1(x) \neq f_1(x')$ into an optimizable formulation. Then we can easily use the Lagrangian multiplier to solve Eq. (2.2). All the previous studies define a loss function $Loss(\cdot, \cdot)$ to quantify the constraint $f_1(x) \neq f_1(x')$. This loss function can be the same with the training loss, or it can be chosen differently, such as hinge loss or cross entropy loss.

We summarize three typical attacking studies here:

Gradient ascent method (Biggio et al., 2013) Machine learning has been popular in classifying malicious ($y = 1$) versus benign ($y = -1$) in computer security tasks. For such contexts, a simple way to solve Eq. (2.2) is through gradient ascent. To minimize the size of the perturbation and maximize the adversarial effect, the perturbation should follow the gradient direction (i.e., the direction providing the largest increase of function value, here from $y = -1$ to 1). Therefore, the perturbation r in each iteration is calculated as:

$$r = \epsilon \nabla_x Loss(f_1(x + r), -1) \text{ Subject to: } f_1(x) = 1 \tag{6.4}$$

By varying ϵ , this method can find a sample x' with regard to $d_2(x, x')$ such that $f_1(x) \neq f_1(x')$.

Box L-BFGS adversary (Szegedy et al., 2013) This study views the adversarial problem as a constrained optimization problem, i.e., find a minimum perturbation in the restricted sample space.

The perturbation is obtained by using Box-constrained L-BFGS to solve the following equation:

$$\underset{r}{\operatorname{argmin}}(c \times d_2(x, x+r) + \operatorname{Loss}(f_1(x+r), l)), x+r \in [0, 1]^p \quad (6.5)$$

Here p is the total number of features, c is a term added for the Lagrange multiplier. (for an image classification task, it is 3 times the total number of pixels of an RGB image) l is a target label, which is different from the original label. The constraint $x+r \in [0, 1]^p$ means that the adversarial sample is still in the range of sample space.

Fast gradient sign method (Goodfellow et al., 2014) The fast gradient sign method proposed by (Goodfellow et al., 2014) views d_2 as the ℓ_∞ -norm. In this case, a natural choice is to make the attack strength at every feature dimension the same. The perturbation is obtained by solving the following equation:

$$\underset{r}{\operatorname{argmin}}(c \times d_2(x, x+r) - \operatorname{Loss}(f_1(x+r), f_1(x))), x+r \in [0, 1]^p \quad (6.6)$$

Therefore the perturbation can be calculated directly by:

$$r = \epsilon \operatorname{sign}(\nabla_z \operatorname{Loss}(f_1(z), f_1(x))) \quad (6.7)$$

Here the loss function is the function used to train the neural network. A recent paper (Kurakin et al., 2016) shows that adversarial examples generated by fast gradient sign method are misclassified even after these images have been recaptured by cameras.

6.3 MORE ABOUT MODELING ORACLE f_2

Though difficult, we want to argue that it is possible to theoretically model "oracles" for some state-of-the-art applications. For instance, as illustrated by the seminal cognitive neuroscience paper "untangling invariant object recognition" (DiCarlo & Cox, 2007) and its follow-up study (DiCarlo et al., 2012), the authors show that one can view the information processing of visual object recognition by human brains as the process of finding operations that progressively transform retinal representations into a new form of representation (X_2 in this paper), followed by the application of relatively simple decision functions (e.g., linear classifiers (Duda et al., 2012)). More specifically, in human and other primates, such visual recognition takes place along the ventral visual stream, and this stream is considered to be a progressive series of visual re-representations, from V1 to V2 to V4 to IT cortex (DiCarlo & Cox, 2007). Multiple relevant studies (e.g., (DiCarlo & Cox, 2007; Johnson, 1980; Hung et al., 2005)) have argued that this viewpoint of representation learning plus simple decision function is more productive than hypothesizing that brains directly learn very complex decision functions (highly non-linear) that operate on the retinal image representation. This is because the experimental evidence suggests that this view takes the problem apart in a way that is consistent with the architecture and response properties of the ventral visual stream. Besides, simple decision functions can be easily implemented in a single step of biologically plausible neuronal processing (i.e., a thresholded sum over weighted synapses).

As another example, the authors of (Xu et al., 2016) used genetic programming to find "adversarial samples" (by solving Eq. (2.2)) for a learning-based malicious-PDF classifier. This search needs an oracle to determine if a variant x' preserves the malicious behavior of a seed PDF x (i.e., $f_2(x) = f_2(x')$). The authors of (Xu et al., 2016) therefore used the Cuckoo sandbox (a malware analysis system through actual execution) to run a variant PDF sample in a virtual machine installed with a PDF reader and reported the behavior of the sample including network APIs calls. By comparing the behavioral signature of the original PDF malware and the manipulated variant, this oracle successfully determines if the malicious behavior is preserved from x to x' . One may argue that "since Cuckoo sandbox works well for PDF-malware identification, why a machine-learning based detection system is even necessary?". This is because Cuckoo sandbox is computationally expensive and runs slow. For many security-sensitive applications about machines, oracles f_2 do exist, but machine-learning classifiers f_1 are used popularly due to speed or efficiency.

6.4 MORE ABOUT MODELING f_1 : DECOMPOSITION OF g AND c

It is difficult to decompose an arbitrary f_1 into $g_1 \circ c_1$. However, since in our context, f_1 is a machine learning classifier, we can enumerate many possible g_1 functions to cover classic machine learning classifiers.

- Various feature selection methods are potential g_1 .
- For DNN, g_1 includes all the layers from input layer to the layer before the classification layer.
- In SVM, X_1, d_1 is decided by the chosen reproducing Hilbert kernel space.

- Regularization is another popular implicit feature extraction method. For example, ℓ_1 regularization can automatically do the feature extraction by pushing some parameters to be 0.

6.5 MORE ABOUT A.E.CONTINUITY ASSUMPTION

The a.e. continuity has a few indications,

- X is not a finite space; and $\forall x, x' \in X, \mathbb{P}(f_i(x) = f_i(x') | d_i(g_i(x), g_i(x')) < \delta_i) = 1$
- It does not mean the function f_1 is continuous in every point in its feature space X ;
- If a probability distribution admits a density, then the probability of every one-point set $\{a\}$ is zero; the same holds for finite and countable sets and the same conclusion holds for zero measure sets¹², for instance, straight lines or circle in R^n .
- The a.e. continuity follows the same property as density function: the probability of picking one-point set $\{x\}$ from the whole feature space is zero; the same holds for zero measure sets. This means: the probability of picking the discontinuous points (e.g., points on the decision boundary) is zero, because they are null sets.
- Most machine learning methods focus on $X = \mathbb{R}^p$ or space equivalent to \mathbb{R}^p (e.g., $[0, 1]^p$) (see Appendix: Section 6.8). Most machine learning methods assume f_1 is continuous a.e. (see Appendix: Section 6.7).

Definition 6.1. Suppose $(X, \mathcal{F}, \mathbb{P})$ is a probability space (for general definition, (X, Σ, μ) is a measure space), where X is the sample space, a σ -algebra \mathcal{F} is a collection of all the events and \mathbb{P} is a probability measure defined in X and \mathcal{F} . A property holds “almost everywhere” (a.e.) in X if and only if the probability measure of the set for which the property holds equals 1.

Lemma 6.2. If the a.e. continuity assumption doesn't hold, there exists a non-zero measure set \mathcal{D} , such that

$$\begin{aligned} \forall x \in \mathcal{D}, \exists x' \\ \text{s.t. } f_1(x) \neq f_1(x') \\ d_1(x, x') < \delta_1 \end{aligned} \quad (6.8)$$

Proof. Without it, for any test sample x , you can easily find a very similar sample x' (i.e. for any small δ_1 , $d_1(x, x') < \delta_1$) such that $|f_1(x) - f_1(x')| > \epsilon$. In classification problems, this means that $f_1(x) \neq f_1(x')$ (i.e. there exist very similar pair of two samples x and x' that have different labels for most $x \in X_1$). \square

The Lemma (6.2) shows that f_1 is not robust to a random noise if we don't assume f_1 is continuous.

6.6 A COUNTER-EXAMPLE OF THE CONTINUITY A.E. ASSUMPTION

A counter-example can be as follows: Suppose a predictor function $f(x) = \mathbb{1}_{p(x, y=1) > \frac{1}{2}}$ for a classification problem, where $p(x, y = 1)$ is the probability density function. Assuming the $p(x, y = 1)$ is a continuous a.e. function, we define a probability density function p_0 as:

$$p_0(x) = \begin{cases} p(x), & x \in \mathbb{R} \setminus \mathbb{Q} \\ 0, & x \in \mathbb{Q} \end{cases} \quad (6.9)$$

Notice that p_0 is still the probability density function. However, $f_0(x) = \mathbb{1}_{p_0(x, y=1) > \frac{1}{2}}$ is nowhere continuous in the set $\{x | f(x) = 1\}$. This is an extreme case, but it shows that a learned probability function might not be continuous a.e..

6.7 MOST CLASSIFIERS SATISFY THE A.E. CONTINUITY ASSUMPTION

Almost all popular machine learning classifiers satisfy the a.e. continuity assumption. For example,

- **Logistic regression for text categorization with a bag of word representation.**
A classifier on a multivariate feature representation in which each feature representing (modified) counts of a word is naturally a.e. continuous. Since $\{x' | d_1(x, x') < \delta_1, x \neq x'\} = \emptyset$ when δ_1 is small and x, x' are mostly sparse vectors. Logistic regression with a bag of word representation is a continuous a.e. predictor.

¹²Zero measure sets: also named as "Null set": https://en.wikipedia.org/wiki/Null_set

- **Support Vector Machine with continuous feature representation.**

Suppose we define (X_1, d_1) by the $d_1^2(x, x') = k(x, x) + k(x', x') - 2k(x, x')$. Then support vector machine is a linear classifier on (X_1, d_1) . Thus, the SVM prediction function is continuous a.e. with d_1 .

6.8 MORE ABOUT "BOUNDARY POINTS MATTER WHEN NOT A.E. CONTINUOUS"

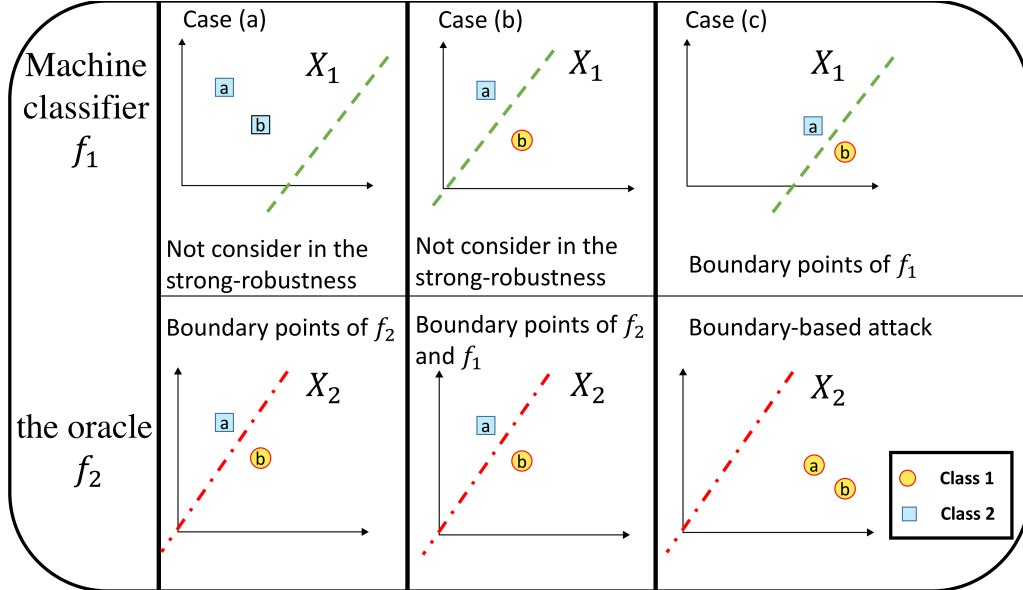


Figure 6: An example showing boundary points of f_1 and boundary points of f_2 . f_1 and f_2 are continuous a.e.. The first two columns showing boundary points of f_2 that are not considered in this paper. The third column describes “Boundary based adversarial attacks” that can only attack seed samples whose distance to the boundary of f_1 is smaller than ϵ . Essentially this attack is about those boundary points of f_1 that are treated as similar and belong to the same class by f_2 .

Most machine learning methods focus on the \mathbb{R}^n space or the space equivalent to \mathbb{R}^n (e.g., $[0, 1]^n$). For example, the sample space of image classification task intuitively is 255^p , where p is the number of features (e.g., $3 \times 224 \times 224$). However, people mostly rescale the raw image data samples into $X = [0, 1]^p$. Therefore, the sample space X for f_1 for this case is $[0, 1]^p$.

7 APPENDIX: USING METRIC SPACE AND PSEUDO METRIC SPACES TO UNDERSTAND CLASSIFIERS’ ROBUSTNESS AGAINST ADVERSARIAL SAMPLES

7.1 METRIC SPACES AND TOPOLOGICAL EQUIVALENCE OF TWO METRIC SPACES

This subsection briefly introduces the concept of metric space and topological equivalence. A metric on a set/space X is a function $d : X \times X \rightarrow [0, \infty]$ satisfying four properties: (1) non-negativity, (2) identity of indiscernibles, (3) symmetry and (4) triangle inequality. In machine learning, for example, the most widely used metric is Euclidean distance. Kernel based methods, such as SVM, kernel regression and Gaussian process, consider samples in a Reproducing kernel Hilbert space (RKHS). The metric in a RKHS is naturally defined as: $d^2(x, y) = K(x, x) + K(y, y) - 2K(x, y)$, in which $K(\cdot, \cdot)$ is a kernel function.

Now we present an important definition, namely that of “topological equivalence”, that can represent a special relationship between two metric spaces.

Definition 7.1. Topological Equivalence (Kelley, 1975)

A function or mapping $h(\cdot)$ from one topological space to another is continuous if the inverse image of any open set is open. If this continuous function is one-to-one and onto, and the inverse of the function is also continuous, then the function is called a homeomorphism and the domain of the function, in our case (X_1, d_1) , is said to be homeomorphic to the output range, e.g., here (X_2, d_2) . In other words, metric space (X_1, d_1) is topologically equivalent to the metric space (X_2, d_2) .

We can state this definition as the following equation:

$$\begin{aligned} \exists h : X_1 &\rightarrow X_2, \forall x_1, x'_1 \in X_1, \\ h(x_1) &= x_2, h(x'_1) = x'_2 \\ d_1(x_1, x'_1) &< \delta_1 \Leftrightarrow d_2(x_2, x'_2) < \delta_2 \end{aligned} \quad (7.1)$$

Here h is continuous, one-to-one and onto. δ_1 and δ_2 are two small constants.

7.2 PSEUDOMETRIC SPACES AND FINER TOPOLOGY BETWEEN TWO PSEUDOMETRIC SPACES

We have briefly reviewed the concept of metric space in Section 7.1 and proposed the related Theorem (3.2) in Section 3.2. This is partly because the concept of metric space has been widely used in many machine learning models, such as metric learning (Xing et al., 2003). Theorem (3.2) and related analysis indicate that feature spaces X_1 and X_2 (See Figure 1) are key determining factors for deciding learning model’s strong-robustness.

However, it is difficult to get the analytic form of X_2 in most applications (e.g., when an oracle f_2 is a human annotator). In fact, most previous studies (reviewed in Section 2.2) assume (X_2, d_2) equals to $(X, \|\cdot\|)$, where $\|\cdot\|$ is a norm function. Therefore, we want to extend our analysis and results from the implicit feature space X_2 to the original feature space X .

When we extend the analysis to the original space X , it is important to point out that the distance function measuring sample similarity for a learned predictor f_1 in the original space X may not be a metric. The distance function in the original feature space X for oracle f_2 may not be a metric as well. This is because the distance between two different samples in the original space X may equal to 0. Because two different samples may be projected into the same point in X_1 or X_2 . For example, a change in one pixel of background in an image does not affect the prediction of f_1 or f_2 since the g_1 and g_2 have already eliminated that (irrelevant) feature. This property contradicts the identity of indiscernibles assumption for a metric function. Therefore we need a more general concept of the distance function for performing theoretical analysis in the original space X . By using the concept of **Pseudometric Space**¹³, we derive another important theorem about strong-robustness.

Pseudometric: If a distance function $d' : X \times X \rightarrow [0, \infty]$ has the following three properties: (1) non-negativity, (2) symmetry and (3) triangle inequality, we call d' is a pseudometric or generalized metric. The space (X, d') is a pseudometric space or generalized metric space. It is worth to point out that the generalized metric space is a special case of topological space and metric space is a special case of pseudometric space.

Why Pseudometric Space: As shown in Figure 1, we can decompose a common machine learning classifier $f_1 = c_1 \circ g_1$, where $g_1 : X \rightarrow X_1$ represents the feature extraction and $c_1 : X_1 \rightarrow Y$ performs the operation of classification. Assume there exists a pseudometric $d'_1(\cdot, \cdot)$ on X and a metric $d_1(\cdot, \cdot)$ defined on X_1 ¹⁴, so that $\forall x, x' \in X$,

$$d'_1(x, x') = d_1(g_1(x), g_1(x')). \quad (7.2)$$

Since d_1 is a metric in X_1 , d'_1 fulfills the (1) non-negativity, (2) symmetry and (3) triangle inequality properties. However, d'_1 may not satisfy the identity of indiscernible property (i.e., making it not a metric). For example, suppose g_1 only selects the first three features from X . Two samples x and x' have the same value in the first three features but different values in the rest features. Clearly, $x \neq x'$, but $d'_1(x, x') = d_1(g_1(x), g_1(x')) = 0$. This shows that $d'_1(\cdot, \cdot)$ is a pseudometric but not a metric in X . Similarly, a pseudometric d'_2 for the oracle can be defined as follow:

$$d'_2(x, x') = d_2(g_2(x), g_2(x')). \quad (7.3)$$

To analyze the strong robustness problem in the original feature space X , we assume it to be a generalized metric (pseudometric) space (X, d'_1) for f_1 and a generalized metric (pseudometric)

¹³The crucial problem of the original sample space X is that it’s difficult to strictly define a metric on the original feature space.

¹⁴ $d_1(\cdot, \cdot)$ on X_1 satisfies four properties:(1) non-negativity, (2) identity of indiscernibles, (3) symmetry and (4) triangle inequality.

space (X, d'_2) for f_2 . Now we can analyze f_1 and f_2 on the same feature space X but relate to two different pseudometrics. This makes it possible to define a sufficient and necessary condition for determining the strong robustness of f_1 against adversarial perturbation.

Before introducing this condition, we need to briefly introduce the definition of topology and finer/coarser topology here:

Definition 7.2. A topology τ is a collection of open sets in a space X .

A topology τ is generated by a collection of open balls $\{B(x, \delta_1)\}$ where $x \in X$ and $B(x, \delta_1) = \{z | d(x, z) < \delta_1\}$. The collection contains $\{B(x, \delta_1)\}$, the infinite/finite number of the union of balls, and the finite number of intersection of them.

Definition 7.3. Suppose τ_1 and τ_2 are two topologies in space X . If $\tau_2 \subseteq \tau_1$, the topology τ_2 is called a coarser (weaker or smaller) topology than the topology τ_1 , and τ_1 is called a finer (stronger or larger) topology than τ_2 .

7.3 PROOFS FOR THEOREMS AND COROLLARIES

In this section, we provide the proofs for Theorem (3.2), Corollary (3.7), Theorem (3.4), and Corollary (3.6). We first prove Theorem (3.4) and Corollary (3.6). Since ‘‘topological equivalence’’ is a stronger condition than ‘‘finer topology’’, Theorem (3.2) and Corollary (3.7) are straightforward.

7.3.1 PROOF OF THEOREM (3.4) WHEN f_2 IS CONTINUOUS A.E.

Proof. Let $S_1 = \{B_1(x, \epsilon)\}$ and $S_2 = \{B_2(x, \epsilon)\}$, where $B_1(x, \epsilon) = \{y | d'_1(x, y) < \epsilon\}$ and $B_2(x, \epsilon) = \{y | d'_2(x, y) < \epsilon\}$. Then $S_1 \subset \tau_1$ and $S_2 \subset \tau_2$. In fact, τ_1 and τ_2 are generated by S_1 and S_2 . S_1 and S_2 are bases of (X, τ_1) and (X, τ_2) .

- First, we want to prove that given $\delta_2 > 0$, $\exists \delta_1 > 0$ such that if $d'_2(x, x') \leq \delta_2$, then $d'_1(x, x') \leq \delta_1$. Consider a pair of samples (x, x') and $d'_2(x, x') \leq \delta_2$. $x, x' \in B_2(x, \delta_2)$. Of course, $B_2(x, \delta_2) \in \tau_2$. Suppose the (X, d'_1) is a finer topology than (X, d'_2) . Then $B_2(x, \delta_2) \in \tau_1$. You can find $B_1(x_0, \delta_1/2) \in \tau_1$ such that $B_2(x, \delta_2) \subset B_1(x_0, \delta_1/2)$, where $\bar{B}_2(x, \delta_2)$ is the closure of $B_2(x, \delta_2)$. Therefore $d'_1(x, x') \leq \delta_1$.
Based on a.e. continuity assumption of f_1 , since $d'_1(x, x') \leq \delta_1$, $f_1(x) = f_1(x')$ a.e. . This means that $\mathbb{P}(f_1(x) = f_1(x') | d_2(g_2(x), g_2(x')) < \delta_2) = 1$, which is our definition of strong-robustness.
- Next, we want to show that if f_1 is strong-robust, then τ_1 is a finer topology than τ_2 .
Suppose f_1 is strong-robust, we need to prove that $\forall \delta_2 > 0$, $\exists \delta_1 > 0$ such that if $d'_2(x, x') \leq \delta_2$, then $d'_1(x, x') \leq \delta_1$.
Assume τ_1 is not a finer topology than τ_2 . This means there exists a $B_2(x, \delta_2)$ such that $B_2(x, \delta_2) \notin \tau_1$. Therefore $\forall \delta_1 > 0$, there exists $x' \in B_2(x, \delta_2)$ such that $d'_2(x, x') < \delta_2$ and $d'_1(x, x') > \delta_1$.
Based on a.e. continuity assumption of f_1 , $d'_1(x, x') > \delta_1$ indicates that $f_1(x) \neq f_1(x')$. This contradicts the strong-robust assumption. Thus, τ_1 is a finer topology than τ_2 . □

Proof of Theorem (3.4) when f_2 is not continuous a.e.

Proof. Let $S_1 = \{B_1(x, \epsilon)\}$ and $S_2 = \{B_2(x, \epsilon)\}$, where $B_1(x, \epsilon) = \{y | d'_1(x, y) < \epsilon\}$ and $B_2(x, \epsilon) = \{y | d'_2(x, y) < \epsilon\}$. Then $S_1 \subset \tau_1$ and $S_2 \subset \tau_2$. In fact, τ_1 and τ_2 are generated by S_1 and S_2 . S_1 and S_2 are bases of (X, τ_1) and (X, τ_2) .

- First, we want to prove that given $\delta_2 > 0$, $\exists \delta_1 > 0$ such that if $d'_2(x, x') \leq \delta_2$, then $d'_1(x, x') \leq \delta_1$. Consider a pair of samples (x, x') and $d'_2(x, x') \leq \delta_2$. $x, x' \in B_2(x, \delta_2)$. Of course, $B_2(x, \delta_2) \in \tau_2$. Suppose the (X, d'_1) is a finer topology than (X, d'_2) . Then $B_2(x, \delta_2) \in \tau_1$. You can find $B_1(x_0, \delta_1/2) \in \tau_1$ such that $B_2(x, \delta_2) \subset B_1(x_0, \delta_1/2)$, where $\bar{B}_2(x, \delta_2)$ is the closure of $B_2(x, \delta_2)$. Therefore $d'_1(x, x') \leq \delta_1$.
Based on a.e. continuity assumption of f_1 , since $d'_1(x, x') \leq \delta_1$, $f_1(x) = f_1(x')$ a.e. . This means that $\mathbb{P}(f_1(x) = f_1(x') | f_2(x) = f_2(x'), d_2(g_2(x), g_2(x')) < \delta_2) = 1$, which is our definition of strong-robustness.
- Next, we want to show that if f_1 is strong-robust, then τ_1 is a finer topology than τ_2 .
Suppose f_1 is strong-robust, we need to prove that $\forall \delta_2 > 0$, $\exists \delta_1 > 0$ such that if $d'_2(x, x') \leq \delta_2$, then $d'_1(x, x') \leq \delta_1$.

Assume τ_1 is not a finer topology than τ_2 . This means there exists a $B_2(x, \delta_2)$ such that $B_2(x, \delta_2) \notin \tau_1$. Therefore $\forall \delta_1 > 0$, there exists $x' \in B_2(x, \delta_2)$ such that $d'_2(x, x') < \delta_2$ and $d'_1(x, x') > \delta_1$. Based on a.e. continuity assumption of f_1 , $d'_1(x, x') > \delta_1$ indicates that $f_1(x) \neq f_1(x')$. This contradicts the strong-robust assumption. Thus, τ_1 is a finer topology than τ_2 . \square

7.3.2 PROOF OF THEOREM (3.5)

Proof. In Section 7.3.1, we have already proved that if the (X, d'_1) is a finer topology than (X, d'_2) , then we can have that \forall pair (x, x') ($x, x' \in X$) $d'_2(x, x') \leq \delta_2$, then $d'_1(x, x') \leq \delta_1$. Therefore,

$$\begin{aligned} & \mathbb{P}(f_1(x) = f_1(x') | f_2(x) = f_2(x'), d'_2(x, x') < \delta_2) \\ &= 1 - \mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d'_2(x, x') < \delta_2) \\ &= 1 - \mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d_1(x, x') < \delta_1, d'_2(x, x') < \delta_2) \\ &> 1 - \eta \end{aligned} \quad (7.4)$$

\square

7.3.3 PROOF OF THEOREM (3.3)

Proof. Since (X_1, d_1) and (X_2, d_2) are topologically equivalent. $\mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d_1(g_1(x), g_1(x')) < \delta_1) = \mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d_2(g_2(x), g_2(x')) < \delta_2)$. Therefore,

$$\begin{aligned} & \mathbb{P}(f_1(x) = f_1(x') | f_2(x) = f_2(x'), d_2(g_2(x), g_2(x')) < \delta_2) \\ &= 1 - \mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d_2(g_2(x), g_2(x')) < \delta_2) \\ &= 1 - \mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d_1(g_1(x), g_1(x')) < \delta_1, d_2(g_2(x), g_2(x')) < \delta_2) \\ &> 1 - \eta \end{aligned} \quad (7.5)$$

\square

7.3.4 PROOF OF THEOREM (3.2)

Proof. Since f_1 is continuous a.e., $\mathbb{P}(f_1(x) = f_1(x') | f_2(x) = f_2(x'), d_1(g_1(x), g_1(x')) < \delta_1, d_2(g_2(x), g_2(x')) < \delta_2) = 0$. Therefore, by Section 7.3.3, $\mathbb{P}(f_1(x) = f_1(x') | f_2(x) = f_2(x'), d_2(g_2(x), g_2(x')) < \delta_2) = 1$. \square

7.3.5 PROOF OF COROLLARY (3.7)

Proof. By (Kelley, 1975), we know that if d_1 and d_2 are norms in \mathbb{R}^n , (\mathbb{R}^n, d_1) and (\mathbb{R}^n, d_2) are topological equivalent. Therefore, we have the conclusion. \square

7.3.6 PROOF OF COROLLARY (3.6)

Proof. Suppose $n_1 > n_2$ and $X_2 \subset X_1$. (X, d'_2) is a finer topology than (X, d'_1) . Therefore (X, d'_1) is not a finer topology than (X, d'_2) , which indicates that f_1 is not strong-robust against adversarial samples. \square

7.4 MORE ABOUT EARLY INSIGHTS FROM TWO THEOREMS

7.4.1 MORE ABOUT g_1 MATTERS FOR THE STRONG-ROBUSTNESS AND c_1 DOES NOT

7.4.2 c_1 MATTERS FOR STRONG-ROBUSTNESS WHEN f_1 IS NOT A.E. CONTINUOUS

Based on Eq. (3.8), when f_1 is not continuous a.e., the strong-robustness of f_1 is determined to both g_1 and c_1 . Figure 9 shows an exemplar case in which X has only ten samples (i.e. $|X| = 10$). We assume the learned f_1 and the oracle f_2 derive the same feature space, i.e., $X_1 = X_2$. And we also assume f_1 performs the classification very badly because the decision boundary (by c_1) on X_1 is largely different from the decision boundary on X_2 . The probability of "adversarial samples" in this case can be calculated by using Eq. (3.8). We get $\mathbb{P}(f_1(x) \neq f_1(x') | f_2(x) = f_2(x'), d_1(g_1(x), g_1(x')) < \delta_1) = \frac{2*3}{5*2} = 0.6$.

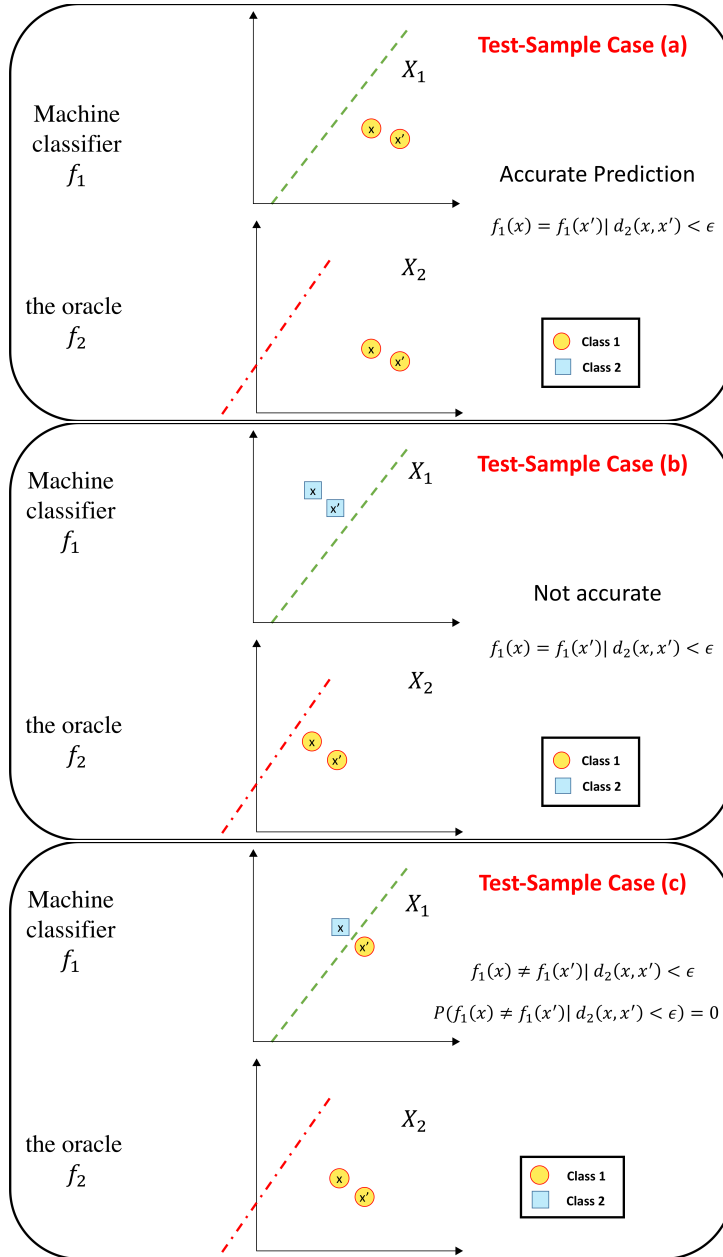


Figure 7: An example figure illustrating Table 3 Case (III) when f_1 is strong-robust. We show one case of $X_1 = X_2 = \mathbb{R}^2$ and f_1, f_2 are continuous a.e.. In terms of classification, f_1 (green boundary line) is not accurate according to f_2 (red boundary line). All pairs of test samples (x, x') can be categorized into the three cases shown in this figure. Test-case (a): f_1 and f_2 assign the same classification label (yellow circle) on x and x' . x and x' are predicted as the same class by both. Test-case (b): f_1 assigns the class of “blue square” on both x and x' . f_2 assigns the class of “yellow circle” on both x and x' . Test-case (c): f_2 assigns the class of “yellow circle” on both x and x' . However, f_1 assigns the class of “blue square” on x and assigns a different class of “yellow circle” on x' . This case has been explained in Section 2.6.

Clearly in this case, c_1 matters for the strong-robustness (when f_1 is not a.e. continuous). This figure indicates that when (1) sample space X is finite, (2) f_1 learns a wrong decision boundary and (3) the probability of test samples around f_1 's decision boundary is large, f_1 is not strong-robust against

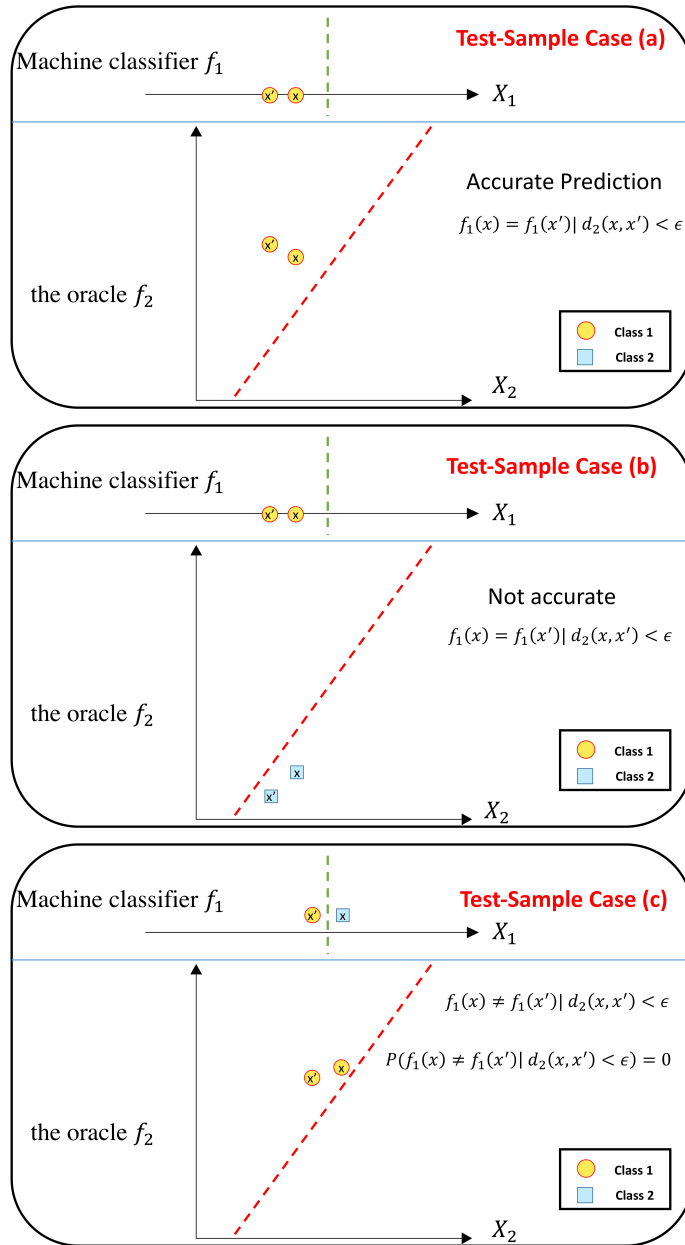


Figure 8: An example figure illustrating Table 3 Case (IV) when f_1 is strong-robust. We show one case of $1 = n_1 < n_2 = 2$, $X_1 \subset X_2$ and f_1, f_2 are continuous a.e.. In terms of classification, f_1 (green boundary line) is not accurate according to f_2 (red boundary line). All pairs of test samples (x, x') can be categorized into the three cases shown in this figure. Test-case (a): f_1 and f_2 assign the same classification label (yellow circle) on x and x' . x and x' are predicted as the same class by both. Test-case (b): f_1 assigns the class of “yellow circle” on both x and x' . f_2 assigns the class of “blue square” on both x and x' . Test-case (c): f_2 assigns the class of “yellow circle” on both x and x' . However, f_1 assigns the class of “blue square” on x and assigns a different class of “yellow circle” on x' . This case can be explained in Section 2.6.

adversarial samples. However, we want to point out that this situation is very rare for a well-trained classifier f_1 .

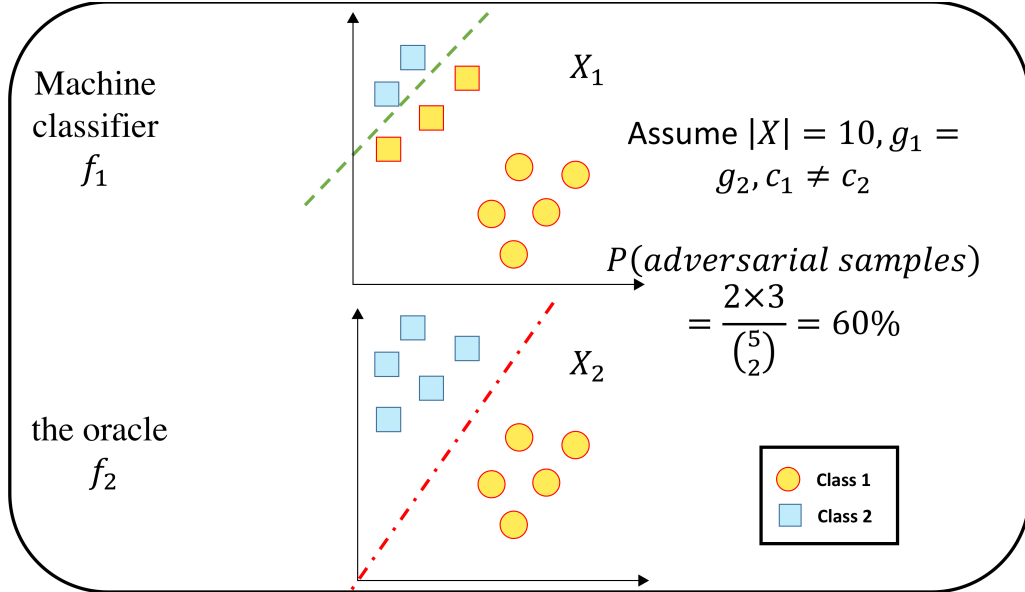


Figure 9: A counter-example showing when (1) sample space X is finite, (2) f_1 learns a wrong decision boundary and (3) the probability of test samples around f_1 's decision boundary is large, f_1 is not strong-robust against adversarial samples. However, we want to emphasize that the situation is very rare for a well-trained classifier f_1 .

8 MORE ABOUT DNNs' ROBUSTNESS AGAINST ADVERSARIAL SAMPLES

8.1 MORE ABOUT EXPERIMENTAL RESULTS OF "SIAMESE TRAINING"

Algorithm 1 Siamese Training algorithm

input Training set x , Random perturbation threshold ϵ_p , NN classifier M .

- 1: Initialize a Siamese network with weights in M .
 - 2: **for** $i = 1, N_{test}$ **do**
 - 3: Pick an example x_k , generate a random Gaussian perturbation $\|\Delta x\|_2 \leq \epsilon_p, x'_k = x_k + \Delta x$.
 - 4: Combine x_k and x'_k as the input and forward it into the network.
 - 5: Get the middle layer output of the Siamese network and pass it to the loss function.
 - 6: Do backward propagation on the network to update the weights.
 - 7: **end for**
-

Dataset and DNN model:

- **CIFAR-10:** CIFAR-10 is an image classification dataset released by (Krizhevsky & Hinton, 2009). The training set contains 50,000 32x32 color images in 10 classes, and the test set contains 10,000 32x32 color images.
- **VGG model:** We choose a VGG model (Simonyan & Zisserman, 2014) as a base DNN model. The VGG model in our experiment has 16 weight layers (55 layers in total).

We compare "Siamese training" with two baseline strategies:

- (1) original training without any extra hardening strategy,
- (2) stability training proposed in (Zheng et al., 2016).

The loss function used by stability training is :

$$L(x, x') = -\left(\sum_x f_1(x) \log \mathbb{P}(y|x; \theta) + \alpha \sum_x \mathbb{P}(f_1(x)|x; \theta) \log \mathbb{P}(f_1(x')|x'; \theta)\right) \quad (8.1)$$

The first part is the crossentropy loss on training samples and the second part is the Kullback–Leibler divergence between the original training samples and the corresponding perturbed samples by adding small random perturbations.

We implement the stability training baseline using Torch7 (Collobert et al., 2011) and choose two loss functions through “*nn.CrossEntropyCriterion()*” and “*nn.DistanceCriterion()*” in Torch7 (Collobert et al., 2011). The only hyper-parameter in this method is a regularization parameter α .

Besides, we want to emphasize that Stability training was shown to improve the model robustness against Gaussian noise in (Zheng et al., 2016). Differently, our experiments focus on testing a learning model’s robustness against "adversarial perturbation".

Four variations of Siamese Training: We implement four variations of Siamese Training.

- (1) Siamese training (G) in which the Siamese Architecture optimizes the loss function L_2 defined by Eq. (8.9) (i.e., penalizing the difference between middle-layer ($g_1(\cdot)$) outputs of (x, x'));
- (2) Siamese training used as a regularization item (G) in which the Siamese Architecture optimizes the loss function L defined by Eq. (8.8) with its L_2 defined by Eq. (8.9); See Section 8.3.3 for the connection between using Siamese training as regularization and ARCA;
- (3) Siamese training (F) in which the Siamese Architecture optimizes the loss function L_2 defined by Eq. (8.10) (i.e., penalizing the difference between middle-layer ($f_1(\cdot)$) outputs of (x, x'));
- (4) Siamese training used as a regularization item (F) in which the Siamese Architecture optimizes the loss function L defined by Eq. (8.8) with its L_2 defined by Eq. (8.10).

We choose SGD as the optimization method and Euclidean distance as the distance measure for the Siamese network. According to the result of (Zagoruyko & Komodakis, 2016), on the CIFAR-10 dataset, we train all the models for 200 epochs. The initial learning rate is set to be 0.1, and let it drop with rate 0.2 at the 60th, 120th and 160th epochs. To be fair, when comparing different hardening strategies we use the same hyper-parameters.

Evaluation Metrics:

- **Test accuracy:** We use top-1 test accuracy as the performance metric. It is defined as the number of successfully classified samples divided by the number of all test samples. The base model achieves accuracy when there’s no adversarial attack.
- **ARC (Eq. (8.4)) :** We use ARC to measure the adversarial robustness of each model. η is chosen to be 10.
- **ARCA: (Eq. (8.5)) :** We use ARCA to measure the total performance of each model.

We generate adversarial samples using the fast gradient sign method, in which the power of the adversary attack can be easily controlled. By controlling the power of fast-sign attacks, we can obtain a complete view of how the accuracy changes according to different attack powers.

In the following analysis, the attack power is defined as:

$$P = \|x - x'\|_\infty \tag{8.2}$$

For image classification tasks, we control the perturbed sample to be still in the valid input space, so that every dimension of the perturbed samples is in the range of integers between 0 and 255.

8.2 CONNECTING “SIAMESE TRAINING” TO PREVIOUS STUDIES

Similar to Siamese training (Section 4.2), multiple hardening solutions (Zheng et al., 2016; Miyato et al., 2016; Lee et al., 2015) aim to learn a better g_1 by minimizing different loss functions $L_{f_1}(x, x')$ so that when $d_2(g_2(x), g_2(x')) < \epsilon$, this loss $L_{f_1}(x, x')$ is small. This might improve the the topological equivalence or finer topology relationship. Two major variations exist among related methods: the choice of $L_{f_1}(x, x')$ and the way to generate pairs of (x, x') .

- **Choice of loss function $L_{f_1}(x, x')$:** Siamese training (G) (Section 4.2) and (Lee et al., 2015) use $L_{f_1}(x, x') = d_1(g_1(x), g_1(x'))$. Siamese training (F) chooses $L_{f_1}(x, x') = dist(f_1(x), f_1(x'))$, where $dist(\cdot, \cdot)$ is a distance function measuring the difference between $f_1(x)$ and $f_1(x')$. If f_1 is continuous a.e., when $d_1(g_1(x), g_1(x'))$ is small \rightarrow we get $dist(f_1(x), f_1(x'))$ is small. However,

Table 5: Test accuracy for different training strategies on CIFAR-10 dataset.

Attack power (Eq. (8.2))	Original model	Stability Training	Siamese with Regularization(G)	Siamese(G)	Siamese with Regularization(F)	Siamese(F)
0	93.95%	93.81%	93.71%	93.96%	94.02%	93.84%
1	78.07%	78.01%	88.49%	93.88%	88.10%	86.61%
2	61.38%	60.34%	80.42%	90.13%	81.78%	79.10%
3	50.07%	49.21%	75.30%	86.73%	77.89%	74.76%
4	42.86%	41.51%	71.15%	83.85%	75.23%	71.68%
5	37.67%	36.33%	67.82%	81.21%	72.99%	68.97%
6	33.60%	32.08%	64.46%	78.61%	70.71%	66.50%
7	29.70%	28.09%	60.64%	76.09%	68.39%	64.23%
8	26.23%	25.11%	56.93%	73.21%	65.26%	61.04%
9	23.53%	22.43%	53.03%	69.67%	61.81%	57.63%
10	20.92%	20.25%	48.78%	65.98%	57.27%	53.71%
ARC	4.9798	4.8717	7.6073	8.9332	8.1345	7.7807
ARCA	0.4253	0.4155	0.6489	0.7631	0.6953	0.6638

Table 6: Connecting "Siamese Training" to relevant hardening solutions.

	x'	as regularization ?	Loss function	On which Layers ?
Siamese Training (G)	random perturbation	Both	$\ g_1(x) - g_1(x')\ _2$	the layer before classification layer
Siamese Training (F)	random perturbation	Both	$\ f_1(x) - f_1(x')\ _2$	Classification layer
Stability training (Zheng et al., 2016)	random perturbation	YES	$KL(f_1(x), f_1(x'))$	Classification layer
(Miyato et al., 2016)	adversarial perturbation	YES	$KL(f_1(x), f_1(x'))$	Classification layer
(Lee et al., 2015)	adversarial perturbation	YES	$\ g_1(x) - g_1(x')\ _2$	the layer before classification layer

the reverse direction may not hold. Therefore, $L_{f_1}(x, x') = dist(f_1(x), f_1(x'))$ may not work for cases.

- **Generating pairs of (x, x') :** Another variation is the way of generating pairs of (x, x') so that $d_2(g_2(x), g_2(x'))$ is small. There exist two common ways. One is generating x' by adding a random (e.g. Gaussian) perturbation on x . The other one is generating the adversarial perturbation to get x' from x .

Besides, (Zheng et al., 2016) uses $L_{f_1}(x, x') = KL(f_1(x), f_1(x'))$ and uses it as a regularization term adding onto the original training loss function. Its samples x' are generated from original samples x adding a small Gaussian noise. (Miyato et al., 2016) uses the similar loss function as (Zheng et al., 2016). But (Miyato et al., 2016) uses adversarial perturbed x' from x . (Lee et al., 2015) uses $L_{f_1}(x, x') = d_1(g_1(x), g_1(x'))$ and x' s are generated x s by adding a small Gaussian noise. These studies are summarized and compared in Table 6.

8.3 A NOVEL MEASURE: ADVERSARIAL ROBUSTNESS OF CLASSIFIERS (ARC) TO QUANTIFY MODEL ROBUSTNESS AGAINST ADVERSARIAL TEST SAMPLES

Our theoretical analysis indicates that strong-robustness is a strong condition of machine learning classifiers and requires thorough understanding of oracle. Since many state-of-the-art learning models, including many DNNs, are not strong-robust, it is important to understand and quantify how far they are away from strong-robustness.

8.3.1 DEFINE ARC AND ARCA

We name such situations as "weak-robustness" and propose a quantitative measure to describe how robust a classification model is against adversarial samples. The proposed measure "Adversarial Robustness of Classifiers (ARC)" considers both the predictor f_1 and the oracle f_2 (introduced in Section 2.2). By design, a classifier (f_1)'s ARC achieves the maximum (1 since ARC is rescaled to $[0, 1]$) if and only if f_1 is strong-robust against adversarial samples and is based on the expectation of how difficult it is to generate adversarial samples.

Definition 8.1. Adversarial Robustness of Classifiers (ARC)

By adding the constraint $d_2(x, x') < \delta_2$ into Eq. (2.2) (our general definition of adversarial samples) and taking the expectation of d_2 between adversarial sample and seed sample, we define a measure quantifying the robustness of machine learning classifiers against adversarial samples.

$$\begin{aligned} \text{ARC}(f_1, f_2) &= \mathbb{E}_{x \in X} [d_2(x, x')] \\ x' &= \underset{t \in X}{\operatorname{argmin}} d_2(x, t) \\ \text{Subject to: } & f_1(x) \neq f_1(t) \\ & d_2(x, t) < \delta_2 \end{aligned} \quad (8.3)$$

Here for the case that x' doesn't exist, we assume $d_2(x, x') = \delta_2$.

Two recent studies (Moosavi-Dezfooli et al., 2015; Papernot et al., 2015b) propose two similar measures both assuming d_2 as norm functions, but do not consider the importance of an oracle. More importantly, (Papernot et al., 2015b) does not provide any computable way to calculate the measure. In (Moosavi-Dezfooli et al., 2015), the measure is normalized by the size of the test samples, while no evidence exists to show that the size of perturbation is related to the size of test samples.

The fact that previous measures neglect the oracle f_2 leads to a severe problem: the generated adversarial samples are not necessarily valid. This is because if the size of perturbation is too large, oracle f_2 may classify the perturbed sample into a different class (different from the class of the seed sample).

This motivates us to design a computable criteria to estimate Definition (8.1). For instance, for image classification tasks, we can choose $d_2 = \|\cdot\|_\infty$ as an example. Then in Eq. (8.3), to estimate of $\mathbb{E}[\|x - x'\|_\infty]$, we need to make some assumptions. Assume that there exists a threshold δ_2 , that any perturbation larger than δ_2 will change the classification of oracle f_2 . That is if $\|x - x'\|_\infty \geq \delta_2$, then $f_2(x) \neq f_2(x')$. More concretely, for image classification tasks, as the input space is discrete (with every dimension ranging from 0 to 255), ARC can be estimated by the following Eq. (8.4):

$$\begin{aligned} \text{ARC}_\infty(f_1, f_2) &= \mathbb{E}[\|x - x'\|_\infty] = \sum_{i=1}^{\delta_2-1} i \mathbb{P}(\|x - x'\|_\infty = i) \\ &\quad + \delta_2 \mathbb{P}(f_1(x) = f_1(t), \forall \|x - t\|_\infty < \delta_2). \\ x' &= \underset{t \in X}{\operatorname{argmin}} d_2(x, t) \\ \text{Subject to: } & f_1(x) \neq f_1(t) \\ & f_2(x) = f_2(t) \end{aligned} \quad (8.4)$$

Definition 8.2. Adversarial Robustness of Classifiers with Accuracy (ARCA)

As we have discussed in the Section 3.4, both accuracy and robustness are important properties in determining whether a classification model is preferred or not. Therefore we combine accuracy and ARC into the following unified measure ARCA:

$$\text{ARCA}(f_1) = \text{Accuracy}(f_1) \times \frac{\text{ARC}(f_1, f_2)}{\delta_2} \quad (8.5)$$

8.3.2 ARC AND STRONG-ROBUSTNESS

It is important to understand the relationship between strong-robustness and weak-robustness. We provide an important theorem as follows that clearly shows the weak-robustness is quantitatively related to the strong-robustness.

Theorem 8.3. f_1 is strong-robust against adversarial samples if and only if $ARC(f_1)/\delta_2 = 1$.

Proof of Theorem (8.3):

Proof. If $ARC(f_1)/\delta_2 = 1$, then based on Definition (8.1), we have that

$$\mathbb{P}(d_2(x, x') = \delta_2) = 1.$$

This indicates that

$$\mathbb{P}(f_1(x) = f_1(x') | d_2(x, x') < \delta_2) = 1, \text{ which is the exact definition of strong-robustness (Eq. (3.7)).}$$

If f_1 is strong-robust, then $\mathbb{P}(f_1(x) = f_1(x') | d_2(x, x') < \delta_2) = 1$.

Therefore $ARC(f_1) = \mathbb{E}[d_2(x, x')]$. Since $\mathbb{P}(f_1(x) \neq f_1(x') | d_2(x, x') < \delta_2) = 0$, we have that

$$\begin{aligned} ARC(f_1) &= \\ \mathbb{E}[d_2(x, x')] &= \\ \delta_2 \mathbb{P}(f_1(x) = f_1(x') | d_2(x, x') < \delta_2) &= \\ \delta_2 & \end{aligned} \tag{8.6}$$

$$ARC(f_1)/\delta_2 = 1. \quad \square$$

8.3.3 SIAMESE ARCHITECTURE CAN IMPROVE ARCA INTUITIVELY

We has shown that the Siamese architecture can be used to improve the weak-robustness against adversarial samples. Now we show a variation of using Siamese architecture can intuitively improve DNNs' ARCA. Using the definition of ARCA (defined in Eq. (8.7)), we get:

$$\begin{aligned} & \operatorname{argmax}_w ARCA(f_1(\cdot; w)) \\ &= \operatorname{argmax}_w \log(ARCA(f_1(\cdot; w))) \\ &= \operatorname{argmax}_w \log(\text{Accuracy}(f_1(\cdot; w))) + \log(ARC_\infty(f_1(\cdot; w))) \end{aligned} \tag{8.7}$$

Then Eq. (8.7) can be reformulated and generalized as the following sum of loss formulation:

$$\operatorname{argmin}_w L_1(f_1(\cdot; w)) + \alpha L_2(f_1(\cdot; w)) \tag{8.8}$$

Siamese architecture can be used to minimize two loss functions L_1 and L_2 at the same time. L_1 represents the loss function used in training DNNs to improve the accuracy, and L_2 represents the control of adversarial robustness (for instance by using Siamese training). This formulation is named as "Siamese training used as a regularization item" in our experiments.

The intuitive formulation for the second loss L_2 can include two variations:

$$L_2(f_1(\cdot; w)) = d_1(g_1(x; w), g_1(x'; w)) \tag{8.9}$$

And

$$L_2(f_1(\cdot; w)) = d_1(f_1(x; w), f_1(x'; w)) \tag{8.10}$$

We use Euclidean distance in the experiments for $d_1(\cdot, \cdot)$.