Abstract

Classification problems in security settings are usually modeled as confrontations in which an adversary tries to fool a classifier manipulating the covariates of instances to obtain a benefit. Most approaches to such problems have focused on game-theoretic ideas with strong underlying common knowledge assumptions, which are not realistic in the security realm. We provide an alternative Bayesian framework that accounts for the lack of precise knowledge about the attacker’s behavior using adversarial risk analysis. A key ingredient required by our framework is the ability to sample from the distribution of originating instances given the possibly attacked observed one. We propose a sampling procedure based on approximate Bayesian computation, in which we simulate the attacker’s problem taking into account our uncertainty about his elements. For large scale problems, we propose an alternative, scalable approach that could be used when dealing with differentiable classifiers. Within it, we move the computational load to the training phase, simulating attacks from an adversary, adapting the framework to obtain a classifier robustified against attacks.

Keywords: Classification, Bayesian Methods, Adversarial Machine Learning, Adversarial Risk Analysis, Deep Models.

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1 Introduction

Over this decade, an increasing number of processes is being automated through classification algorithms, being essential that these are robust and reliable if we are to trust key operations based on their output. State-of-the-art classifiers perform extraordinarily well on standard data, but they have been shown to be vulnerable to adversarial examples, data instances specifically targeted at fooling the algorithms (Comiter, 2019). As a fundamental hypothesis, algorithms rely on the use of independent and identically distributed (iid) data for both the training and test phases. However, security aspects in classification, which form part of the field of adversarial machine learning (AML), question such hypothesis due to the presence of adversaries ready to modify the data to obtain a benefit and, thus, making both distributions differ.

Stemming from the pioneering work in adversarial classification (AC) in Dalvi et al. (2004), the paradigm used to model the confrontation between adversaries and classification systems has been game theory, see recent reviews in Biggio and Roli (2018) and Zhou et al. (2018). As an example, the most popular attacks, including the fast gradient sign method (FGSM) (Goodfellow et al., 2014b), may be viewed from a game-theoretic perspective. Similarly, two of the most promising defence techniques, adversarial training (AT) (Madry et al., 2018), which trains the defender model with attacked samples, and adversarial logit pairing (ALP) (Kannan et al., 2018), which encourages the logits of the model to be the same for both standard and adversarial inputs, may be framed in game theoretic terms. This perspective typically entails common knowledge hypothesis (Hargreaves-Heap and Varoufakis, 2004) which, from a fundamental point of view, are not sustainable in settings such as security, as adversaries try to hide and conceal information. Recent work (Naveiro et al., 2019) presented ACRA, a novel approach for AC based on Adversarial Risk
Analysis (ARA) (Rios Insua et al., 2009). ARA makes operational the Bayesian approach to games as in Kadane and Larkey (1982) and Raiffa (1982), facilitating robust procedures to predict adversarial decisions. However, ACRA may be used only for generative classifiers (Goodfellow et al., 2016), like utility sensitive Naive Bayes classifiers (Chai et al., 2004) or deep generative classifiers based on the variational autoencoder (Kingma et al., 2014). Moreover, only binary classification problems were supported.

We present a general framework that may be used with both discriminative and generative classifiers, deal with multiple class problems and provide efficient computational schemes. First, a brief set up of the problem is provided. Next, we develop our general approach and illustrate it through a malware detection problem. We then discuss computational issues and propose an efficient approach for large scale problems which we illustrate with deep neural network classifiers in computer vision problems.

2 Basic setup

2.1 Basic notation

Consider a classifier $C$ (she) who may receive objects belonging to $k$ different types designated with a label $y_i$, $i = 1, \ldots, k$. Objects have features $x \in \mathbb{R}^d$. Uncertainty about the objects’ types is modelled through parametric distributions $p(y_i|\beta, x), i = 1, \ldots, k$. This distribution can come from a generative model, in which the feature distribution is explicitly modelled and the class distribution is obtained using Bayes formula, or from a discriminative model, in which the class distribution is directly modelled.

In classical approaches, data $D$ is used to construct a maximum likelihood estimate $\hat{\beta}$ and $p(y_i|\hat{\beta}, x)$ is employed to classify predicting the label $y_i$, given the estimate and the
test instance \( x \). \( C \) aims at maximizing expected utility (French and Rios Insua, 2000), based on classifying \( x \) to be of type \( \arg\max_{y_C} \sum_{i=1}^{k} u_C(y_C, y_i) p(y_i | \hat{\beta}, x) \), where \( u_C(y_C, y_i) \) is the utility that she perceives when an object with label \( y_i \) is classified as of type \( y_C \).

In Bayesian approaches, a prior \( p(\beta) \) is used to compute the posterior \( p(\beta | D) \) and the predictive distribution

\[
p(y_i | x, D) = \int p(y_i | \beta, x) p(\beta | D) d\beta,
\]

serves to classify based on maximum predictive expected utility

\[
\arg\max_{y_C} \sum_{i=1}^{k} u_C(y_C, y_i) p(y_i | x, D).
\]

Of particular interest in our setting will be the adoption of a 0−1 utility function, in which the classifier gets 1 for a correct classification, and 0 for an incorrect one. In this case, the decision rule is \( \arg\max_{y_C} p(y_C | x, D) \) and we aim at maximizing the probability of correct classification. From now on, we shall remove dependence on data \( D \) to lighten up the notation.

Regarding the structural form of the \( p(y_i | \beta, x) \) term, specially relevant in our developments (and in classification applications at large) are models based on a parameterized function \( f_\beta : \mathbb{R}^d \to \mathbb{R}^k \), in which the prediction is given by

\[
p(y_i | \beta, x) = \text{softmax}(f_\beta(x))[y_i], \quad \text{where} \quad \text{softmax}(x)[j] = \frac{\exp x_j}{\sum_{i=1}^{k} \exp x_i}
\]

This formulation covers a large class of models. For example, if \( f_\beta \) is linear in inputs we recover multinomial regression (McCullagh and Nelder, 1989); if we take \( f_\beta \) to be a sequence of linear transformations alternating non-linear activation functions, such as
Rectified Linear Units (ReLU), we obtain a feed-forward neural network (Goodfellow et al., 2016).

2.2 Attacks to classifiers

Consider now another agent called adversary \( A \) (he). \( A \) applies an attack \( a \) to the features \( x \) leading to \( x' = a(x) \), the actual observation received by \( C \). The attacker aims at fooling the classifier and make her misclassify objects to attain some benefit, as it happens, e.g., in fraud or spam detection. We focus on exploratory attacks, defined to have influence just over operational data, not during the training phase, and consider only integrity violations in which the adversary just modifies bad instances. Huang et al. (2011) and Barreno et al. (2006) provide taxonomies of attacks against classifiers.

Upon observing \( x' \), \( C \) needs to determine the object class. An adversary unaware classifier might be making gross mistakes as she classifies based on the received features \( x' \), instead of the actual ones. We provide two examples. Both adopt a 0–1 utility. The first one is a multiple \( (k = 10) \) class image classification problem; the second, a multiple \( (k = 4) \) class malware detection problem.

**Example 1.** The best known attacks to classification algorithms modify images in a way that alterations become imperceptible to the human eye, yet drive a model trained on millions of images to misclassify the perturbed ones (Szegedy et al., 2014). This has potentially relevant security consequences in e.g. managing autonomous driving systems (Vorobeichyk and Kantarcioglu, 2019). As an example, with a relatively simple deep convolutional neural network (CNN) model (Krizhevsky et al., 2012) we can accurately predict 99% of the handwritten digits in the MNIST data set (LeCun et al., 1998). However, if we
attack such set with FGSM (Goodfellow et al., 2014b), its accuracy gets reduced to 62%. Figure 1 provides an example of an original image and a perturbed one. To our eyes both images look like a 2. However, the CNN classifier identifies a 2 in the first case (Fig. 1a) and a 7 in the perturbed one (Fig. 1b), both with high probability.

![Original Image](image1.png) ![Perturbed Image](image2.png)

(a) Original image  
(b) Perturbed image

Figure 1: An original MNIST image identified as 2. A perturbed image identified as 7.

FGSM and related attacks in the literature, Vorobeichyk and Kantarcioglu (2019), assume that the attacker has precise knowledge of the underlying model and parameters of the involved classifier. This is debatable in most security settings.

**Example 2.** Consider a malware classification problem using a multinomial regression (MR) classifier. We test robustness against attacks to MR on a dataset containing malware and benign binaries. Malware was provided by Virus Total (Chronicle, 2018) and contains trojans, adware and virus. Benign binaries were obtained from clean copies of the Program Files folder of MS Windows 7 and 8. The proportion of malware binaries in the data is 50%. Features were extracted from binaries through: the Assembly Language Source, from which we extract registers, operation codes, API calls and keywords; and, the Portable Executable Header, providing the symbols and imports. In total, we use 76 binary features coded with
1 (0) indicating the presence (absence) of the corresponding characteristic. Additionally, a label indicates whether the binary is trojan \( (y_i = 1) \), adware \( (y_i = 2) \), virus \( (y_i = 3) \) or benign \( (y_i = 4) \). We randomly split the dataset into train and test subsets: 80%, 20%; respectively. The test subset is attacked as in Naveiro et al. (2019) allowing the attacker to undertake obfuscation attacks in at most 4 features. The accuracy attained with untainted data is 69%. On the other hand, with tainted data, we only reach accuracies of 53%, 51%, 45% and 42% when, respectively, attacking 1, 2, 3 and 4 features. Note the considerable degradation that highlights the lack of robustness to adversarial attacks of the MR model.△

3 Adversary aware classifiers

As illustrated, an adversary unaware classifier may be fooled into issuing wrong classifications potentially incurring in severe expected utility degradation. We devise strategies to mitigate this by building models of the attacks likely to be undertaken by the adversaries. We focus on Bayesian classification approaches but the ideas extend to classical ones.

3.1 The adversary aware classifier problem

Assume for a moment that the classifier knows the attack \( a \) that she has suffered and that it is invertible, in the sense that we may recover the original \( x \), designated \( a^{-1}(x') \) when convenient. Then, rather than classifying based on \( \arg\max_{y_C} \sum_{i=1}^{k} u(y_C, y_i) p(y_i|x') \), as an adversary unaware classifier would do, she should classify based on

\[
\arg\max_{y_C} \sum_{i=1}^{k} u(y_C, y_i) p(y_i|x = a^{-1}(x')).
\]
However, we do not know the attack \( a \), neither, more generally, the originating \( x \).

Suppose we model our uncertainty about the origin \( x \) of the attack through a distribution \( p(x|x') \) with support over the set \( X \) of reasonable originating features \( x \). Then, the expected utility that the classifier would get for her classification decision \( y_C \) would be

\[
\psi(y_C) = \int_X \left( \sum_{i=1}^k u(y_C, y_i) p(y_i|x = a^{-1}(x')) \right) p(x|x') dx \\
= \sum_{i=1}^k u(y_C, y_i) \left[ \int_X p(y_i|x = a^{-1}(x')) p(x|x') dx \right],
\]

then having to solve

\[
\arg \max_{y_C} \psi(y_C).
\]

Typically, we approximate the expected utilities by Monte Carlo (MC) using a sample \( \{x_n\}_{n=1}^N \) from \( p(x|x') \) so that \( \hat{\psi}(y_C) = \frac{1}{N} \sum_{i=1}^k u(y_C, y_i) \left[ \sum_{n=1}^N p(y_i|x_n) \right] \). Algorithm 1 summarises the general procedure that we later specify.

For this approach to be operational, we need to be able to estimate \( X \) and \( p(x|x') \) or, at least, sample from this distribution. Assuming that we can define a metric \( \lambda \) in the feature space, a first heuristic would be to define the set \( X \) of reasonable originating features as those \( x \) such that \( \lambda(x, x') < \rho \) for a certain threshold \( \rho \). We could then take \( p(x|x') \) as a uniform distribution over \( X \). Alternatively, we could make \( p(x|x') = \frac{h}{\lambda(x, x')} \), where \( \frac{1}{h} = \sum_{x \in X} \frac{1}{\lambda(x, x')} \), ignoring \( x' \) as possible origin. These heuristics formalize the fact that changing instances entails some cost for the adversary that probably increases with the number of features changed.

However, as shown in Ríos Insua et al. (2020), better forecasts are typically attained if we explicitly model the attacker’s behaviour using the information available about him, as
Algorithm 1 General ARA procedure for Adversarial Classification

Input: $N$, training data $D$, prior $p(\beta)$.
Output: A classification decision $y_C^*(x')$.

Training
Based on $D$ and $p(\beta)$, compute $p(\beta|D)$ and $p(y_i|x)$ for all $i$.

End Training

Operation
Read instance $x'$
Estimate $X$ and $p(x|x')$, $x \in X$
Draw sample $\{x_n\}_{n=1}^N$ from $p(x|x')$.

Find $y_C^*(x') = \arg\max_{y_C} \frac{1}{N} \sum_{i=1}^k \left( u(y_C, y_i) \left[ \sum_{n=1}^N p(y_i|x_n) \right] \right)$

End Operation
Return $y_C^*(x')$

we do next.

3.2 An Approximate Bayesian Computation sampling approach

An approach to sample from $p(x|x')$ that leverages information available about the attacker is now discussed. We call it AB-ACRA, being based on approximate Bayesian computation (ABC), Csilléry et al. (2010). As basic ingredients, it requires us to be able to generate samples from $x \sim p(x)$ and $x' \sim p(x'|x)$.

3.2.1 Basic ingredients

Estimating $p(x)$ is possible using training data, which is untainted by assumption. For this, we can use an implicit generative model, such as a generative adversarial network (Goodfellow et al., 2014a) or an energy-based model (Grathwohl et al., 2019).
On the other hand, sampling from $p(x'|x)$ entails strategic thinking, which we shall treat with the ARA methodology. Without loss of generality, assume that the attacker considers interesting for him the first $l$ classes (call them bad), the other ones being irrelevant for him (good): he is interested in modifying data associated with instances belonging to the first $l$ classes to make $C$ believe that they belong to the remaining ones. As an example, consider a fraudster who may commit $l$ types of fraud; he crafts the corresponding $x$ to make $C$ think that she has received a legitimate object of class $i$, with $i > l$. As we only consider integrity violations, we base our analysis on the decomposition

$$p(x'|x) = \sum_{i=1}^{k} p(x'|x,y_i)p(y_i|x) = \sum_{i=1}^{l} p(x'|x,y_i)p(y_i|x) + \sum_{i=l+1}^{k} \mathbb{I}(x'|x)p(y_i|x),$$

where $\mathbb{I}$ is the indicator function. We can easily generate samples from $p(y_i|x)$, as we can estimate those probabilities based on training data as in (1). Then, we can obtain samples from $p(x'|x)$ by sampling $y_i \sim p(y_i|x)$ first and, then, if $i > l$ return $x$ or sample $x' \sim p(x'|x,y_i)$ otherwise.

To sample from $p(x'|x,y_i)$, the ARA methodology helps us to model the Attacker decision problem when he has available an instance $x$ with label $y_i$. As we are not assuming common knowledge, we need to model our uncertainty about the Attacker elements. Assume that agent $A$ also aims at maximizing his expected utility when trying to confuse $C$. His utility function has the form $u_A(y_C,y_i)$, when $C$ says $y_C$ and the actual label is $y_i$. He would choose the attack (feature modification) that maximizes his expected utility by making $C$ classify instances as most beneficial as possible to him. For this, assume that
the utility that \( A \) derives from \( C \)'s decision has the following structure:

\[
u_{ji}^A := u_A(y_C = y_j, y_i) = \begin{cases} 
0, & \text{if } i \leq l \text{ and } j \leq l \\
0, & \text{if } i > l \\
u_{ji}^A 
eq 0, & \text{if } i \leq l \text{ and } j > l 
\end{cases}
\]

This reflects that the Attacker just obtains benefit when he makes the defender classify a bad instance as if it was a good one.

By transforming instance \( x \) with label \( y_i \) for \( i = 1, \ldots, l \) into instance \( x' \), the attacker would get an expected utility

\[
\sum_{c=1}^{k} u_A(y_C = y_c, y_i)p_A(y_C = c|x') = \sum_{c=l+1}^{k} u_{ci}^A p_A(y_C = c|x'), \tag{4}
\]

where \( p_A(y_C|x') \) describes the probability that \( C \) says type \( y_C \) if she observes \( x' \), from \( A \)'s perspective. The Attacker will typically be uncertain about such probability. Suppose we model it with a density \( f_A(p_A(y_C|x')) \), with mean \( p^A_c(x') \). Taking expectations in (4), the expected utility he would get is \( \sum_{c=l+1}^{k} u_{ci}^A p^A_c(x') \). Thus, the attacker would choose his action through

\[
x'(x, y_i) = \arg \max_{z \in X} \sum_{c=l+1}^{k} u_{ci}^A p^A_c(z), \tag{5}
\]

and craft object \((x, y_i)\) into \((x'(x, y_i), y_i)\).

However, we do not know \( u_A \) neither \( p^A_c \) with certitude. Suppose we model our uncertainty about these elements with, respectively, random utilities \( U_A \) and random expected probabilities \( P^A_c \), defined over an appropriate probability space. We would look for the
random optimal transformation defined by

$$X'(x, y_i) = \arg \max_{z \in \mathcal{X}} \sum_{c=l+1}^{k} U^c_A P^c_A(z),$$

and make $$p(x|x', y_i) = Pr(X'(x, y_i) = x').$$ Then, by construction, if we sample $$u_A \sim U_A$$ and $$p^c_A \sim P^c_A$$ and solve

$$x' = \arg \max_{z \in \mathcal{X}} \sum_{c=l+1}^{k} u^c_A p^c_A(z),$$

$$x'$$ would be distributed according to $$p(x'|x, y_i).$$

Of the required elements, it is relatively easy to model the random utilities $$U_A.$$ We may scale these utilities between 0 and 1 (French and Rios Insua, 2000) and use $$U_{ci} \sim Beta(\alpha_{ci}, \beta_{ci}).$$ If information about the likely values of the utilities is available, we may assess them through appropriate $$\alpha$$ and $$\beta$$ values; if information about possible perceived rankings of the utilities is available, we may introduce them as constraints and sample by rejection.

Modeling $$P^c_A(x')$$ is more delicate. It entails strategic thinking as $$C$$ needs to model her opponent’s beliefs about what classification she will adopt upon observing $$x'.$$ This could be the beginning of a hierarchy of decision making problems, as described in Rios and Rios Insua (2012) in a much simpler context. A relevant heuristic consists of modelling $$P^c_A(x')$$ using a distribution based on $$p(y_C|x')$$ with some uncertainty around it. For this, given $$x',$$ consider the set $$\mathcal{X}$$ of reasonable origins from Section 3.1. Imagine we assess a distribution $$p^*(x|x')$$ over it, for example using the metric based approach as there defined. Let $$mean_c = \sum_x p(y_C|x)p^*(x|x')$$ and, for a given variance $$var_c,$$ choose $$P^c_A(x') \sim Beta(\alpha, \beta)$$ having the above $$mean_c$$ and $$var_c,$$ for which we just make $$\alpha^c = \left(\frac{1-mean_c}{\var^c_c} - \frac{1}{mean_c}\right) mean^2_c.$$
and $\beta^c = \alpha^c \left( \frac{1}{\text{mean}_c} - 1 \right)$. In the above expression for $\text{mean}_c$, $p(y_C|x)$ would come from the estimates based on untainted data in (1); to reduce the computational cost, we could approximate $\text{mean}_c$ through $\frac{1}{M} \sum_{n=1}^{M} p(y_C|x_n)$, for a sample $\{x_n\}_{n=1}^{M}$ from $p^*(x|x')$.

### 3.2.2 AB-ACRA

Once we are able to sample from $p(x)$ and $p(x'|x)$, we need a procedure to sample from $p(x|x')$. In the discrete case\(^1\), we can use rejection sampling (Casella et al. (2004)). This entails generating $x \sim p(X)$, $\bar{x}' \sim p(X'|X = x)$, and accepting $x$ only if $\bar{x}'$ coincides with the actually observed instance $x'$. It is straightforward to prove that $x \sim p(X|X' = x')$. We can think of this procedure as generating instances $x$ and indicators $I$, where $I = 0(=1)$ if we reject (accept) the sample. Accepted instances are distributed according to

$$p(X = x|I = 1) \propto p(I = 1|X = x)p(X = x) \propto p(X' = x'|X = x)p(X = x)$$

which, using Bayes rule, coincides with the desired distribution.

When $x'$ is continuous and/or high dimensional, the acceptance rate would typically be very low, making the above approach inefficient. In such cases, we can leverage ABC techniques. This entails accepting the sample $x$ if $\phi(\bar{x}', x') < \text{TOL}$, for a given distance $\phi$ and tolerance $\text{TOL}$. The $x$ generated in this manner is distributed approximately according to $p(x|x')$. However, the probability of generating samples for which $\phi(\bar{x}', x') < \text{TOL}$ decreases as the dimensionality of $x'$ increases. A common solution replaces the acceptance criterion by $\phi(s(\bar{x}'), s(x')) < \text{TOL}$, where $s(x)$ is a set of summary statistics that capture the relevant information in $x$. The particular choice of summary statistics is problem

\(^1\)Here, for convenience, we distinguish between random variables and realizations using upper and lower cases, respectively. Thus, $X'$ refers to the actually observed instance and $X$ to the originating one.
specific. We summarise the whole procedure in Algorithm 2, which would be integrated within Algorithm 1.

**Algorithm 2** ABC scheme to sample from $p(x|x')$

**Input:** Observed instance $x'$, data model $p(x)$, $U_A$, $P_c^A$, family of statistics $s$, TOL.

**Output:** A sample approximately distributed according to $p(x|x')$.

while $\phi(s(x'), s(\tilde{x}')) > TOL$ do

- Sample $x \sim p(x)$
- Sample $y_i \sim p(y_i|x)$
  - if $i > l$ then
    - $\tilde{x}' = x$
  - else
    - Sample $u_A \sim U_A$ and $p_c^A \sim P_c^A$
    - Compute $\tilde{x}' = \arg \max_{z \in \mathcal{X}} \sum_{c=l+1}^{k} u_c^A p_c^A(z)$
  - end if
- Compute $\phi(s(x'), s(\tilde{x}'))$

end while

return $x$

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### 4 An example in multiclass malware detection

We illustrate the proposed approach with a malware detection problem\(^2\). Malware of different types is increasingly being delivered by attackers to obtain a benefit, being a current major global cyber threat (ENISA, 2019). Malware types include, among others: trojans, aimed at misleading the victim of its real intention of accessing personal information such as passwords; adware, which releases advertisements through the victim interface; or virus, that can replicate itself modifying other programs causing system failures, wasting host resources or corrupting data. It is crucial to detect the appropriate type of malware to decide

\(^2\)All code to reproduce these experiments is available at https://github.com/roinaveiro/ACRA_2.
the relevant countermeasures and mitigate its consequences. Recently, obfuscation attacks on malware binaries (You and Yim, 2010) have gained relevance as they affect critically the performance of detection algorithms as shown in Example 2. We test the performance of AB-ACRA as a defence mechanism against obfuscation attacks, based on a 0-1 utility for the Defender.

For these experiments, we use the same dataset as in Example 2. As underlying classification algorithm we deploy MR with L1 regularization. This is equivalent to performing maximum a posteriori estimation in an MR model with a Laplace prior, Park and Casella (2008). The regularization parameter was chosen using cross validation. Mean and standard deviations of accuracies in all experiments are estimated via repeated hold-out validation over ten repetitions (Kim, 2009). The accuracy of this approach on clean test data is $0.68 \pm 0.01$.

To compare AB-ACRA with raw MR on tampered data, we simulate attacks over the instances in the test set. For this purpose, we solved problem (6) for each test malware binary, removing the uncertainty that is not present from the adversary’s point of view. We restrict to attacks that involve changing at most the value of one of the features. The utility that the attacker perceives when he makes the defender misclassify a malware binary is 0.7 for all malware types. Finally, the adversary would have uncertainty about $p^*_A(x')$, as this quantity depends on the defender’s decision. We test AB-ACRA against a worst case adversary who knows the true value of $p(y_C|x_n)$ and estimates $p^*_A(x')$ through $\frac{1}{M} \sum_{n=1}^{M} p(y_C|x_n)$ for a sample $\{x_n\}_{n=1}^{M}$ from $p^*(x|x')$. We set $M = 40$. For $p^*(x|x')$ we use a uniform distribution on the set of all instances at distance 1 from the observed $x'$, using as distance $\lambda(x, x') = \sum_{i=1}^{76} |x_i - x'_i|$.

To model the uncertainty about $p^*_A(x')$ and the attacker’s utility function from the
defender’s perspective, we use beta distributions centered at the attacker’s values of probabilities and utilities, respectively, with variances chosen to guarantee that the distribution is concave in its support: they must be bounded from above by \( \min \{ \frac{\mu^2 (1 - \mu)}{1 + \mu}, \frac{\mu (1 - \mu)^2}{2 - \mu} \} \), where \( \mu \) is the corresponding mean. We set the variance to be 10% of this upper bound.

For the AB-ACRA algorithm, we used the 12 most relevant features (in terms of their coefficients having the highest posterior mode in absolute value) as summary statistics. Figure 2a compares the accuracy of ACRA and MR for different sample sizes \( N \) in Algorithm 1, and tolerance \( TOL = 2 \). As we can see, ACRA beats MR in tainted data with just 5 samples. The accuracy saturates quickly as we increase the number of samples. Thus, we get good performance with a relatively small sample size. Figure 2b plots the accuracy of ACRA against MR for different values of \( TOL \). As expected, as this parameter decreases, accuracy increases, albeit at a higher computational cost.

(a) Experiment for different number of samples. (b) Experiment for different values of tolerance.

Figure 2: Accuracy comparison LR vs AB-ACRA.

Finally, we compare AB-ACRA with tolerance 1 (this value was found to give reason-
able results for a moderate computational time), with MR and a heuristic approach that assumes that $p(x|x')$ is a uniform distribution over all possible instances at distance one from the observed $x'$. MR and the heuristic approach both obtained accuracy $0.52 \pm 0.01$, while AB-ACRA obtained $0.66 \pm 0.01$. As anticipated in Section 3.1, defences that do not model explicitly the attacker’s behavior have worse performance. However, AB-ACRA outperforms the heuristic approach and the raw MR as it explicitly models the attacker’s behaviour.

5 Large scale differentiable models

5.1 Introduction

The previous example allowed us to illustrate the general framework in a relatively simple setting with a moderate (76) number of binary features and constraints on the allowed number of changes. The scheme proposed may entail very heavy computational costs in high-dimensional settings, as sampling from $p(x|x')$ may be very costly. This approach is clearly not feasible computationally in high-dimensional domains, such as with image data.

To overcome the computational bottleneck, we shall bypass some steps from the approach in Section 3, when considering classifiers which are differentiable with respect to their parameters. These models have the benefit of being amenable to training using stochastic gradient descent (SGD) (Bottou, 2010). The use of scalable optimization methods facilitates training deep neural networks with large amounts of high-dimensional data as with text data or images, since these methods enable iterative optimization using only a mini-batch of examples at each iteration, alleviating the computational burden. In particular, our driving case will use deep neural networks with images, although the ideas
extend to differentiable models at large. Finally, instead of dealing with the attacker in the 
operation phase, as done in the previous sections, we shift to modify the training phase to 
account for future adversarial perturbations.

Essentially, with this paradigm shift, we shall be able to avoid the expensive sampling 
from \( p(x|x') \) only requiring doing it from \( p(x'|x) \) using gradient information from the de-
fender model. The crucial point is that it is easier to estimate \( p(x'|x) \) from an adversary, 
just requiring an opponent model, than to estimate \( p(x|x') \), which requires inverting the 
opponent model. Obviously, there does not exist a notion of gradient in every model and 
we would need to resort to the previous approach in those cases.

5.2 Concept

For clarity, we use 0−1 utilities, but extensions to more general utilities follow a similar 
path. We thus focus on implementing the decision rule

\[
\arg\max_y \int \int p(y_C|x, \beta)p(x|x')p(\beta|\mathcal{D})dx\,d\beta
\]

(7)
in a general scalable and robust manner.

The usual adversarial robustness definition (Katz et al., 2017) requires that \( \arg\max_y p(y|x, \beta) \approx \arg\max_y p(y|x', \beta) \), that is, for any input \( x \) and adversarial perturbation \( x' \sim p(\cdot|x, y) \) the 
predicted class should not change under an adversarial attack. On the other hand, ALP 
(Kannan et al., 2018) defences try to impose the stronger condition, \( p(y|x, \beta) \approx p(y|x', \beta) \), 
with improved robustness. In our proposal, we require the slightly stronger condition

\[
p(y, x|\beta) \approx p(y, x'|\beta).
\]

(8)
Though condition (8) may impose an extra computational burden, we provide a way to train the defender model to achieve such condition, improving robustness compared to baselines. First, to compute $p(x, y|\beta)$, as in energy-based models (Grathwohl et al., 2019) we reinterpret the logits of model (2) as in , leading to an expression for the joint probability
\[ p(x, y|\beta) = \frac{\exp(f_\beta(x, y))}{Z(\beta)}, \]
where $Z(\beta)$ is the usually intractable normalizing constant. We factor the joint distribution $p(y, x|\beta) = p(y|x, \beta)p(x|\beta)$. Then, for a sample $x \sim \mathcal{D}$ and the corresponding adversarial perturbation $x' \sim p(x'|x)$, we optimize
\[
\max_{\beta} \mathcal{L}(\beta, x, y) = \{ \log p(y|x, \beta) + \log p(y|x', \beta) - |f_\beta(x) - f_\beta(x')| - |\log p(x|\beta) - \log p(x'|\beta)| \}.
\]

A few comments are in order. The first two terms promote high predictive power for both $p(y|x, \beta)$ and $p(y|x', \beta)$. The third term encourages the logits of $x$ and $x'$ to be similar, leading to $p(y|x, \beta) \approx p(y|x', \beta)$. Finally, the last term acts as a regularizer, encouraging $p(x|\beta) \approx p(x'|\beta)$ and, with the previous term, leading to condition (8). Note that since we have a difference of the originally intractable terms, $\log p(x|\beta) - \log p(x'|\beta)$, the normalizing constant $Z(\beta)$ cancels out rendering tractable the analysis.

At the end of training, we would have $p(x|\beta) \approx p(x'|\beta)$. This implies that $p(x|x') \approx p(x'|x)$ using Bayes formula. Then, incorporating $p(y|x, \beta) \approx p(y|x', \beta)$, we can swap the original decision rule (7) by $\arg\max_{y_C} \int p(y_C|x', \beta)p(x'|x)p(\beta|\mathcal{D})dx'd\beta$. However, since the observed input $x'$ might be tainted, it is not necessary to attack it via $p(x'|x)$ anymore and just suffices to use the test time decision rule, $\arg\max_{y_C} p(y_C|x', \beta)$. To sum up, by imposing $p(x|\beta) \approx p(x'|\beta)$ during training, we obtain a robust model which has learned that starting in either $x$ or $x'$, it does not matter whether we use $p(x'|x)$ or $p(x|x')$ as we arrive at the same distribution, being simpler to sample from $p(x'|x)$. We explain how to
sample from this distribution in Section 5.3.

Note that the proposed framework is not just a mere mash-up of AT, ALP and our new regularizer, with its own computational benefits. In the next paragraphs, we use the ARA methodology to add a layer of uncertainty over the previous terms with two objectives: i) depart from standard common knowledge assumptions in adversarial classification; and ii) enhance robustness and prevent from overfitting.

5.3 Simulating attacks with ARA

With continuous data, adversarial perturbations $x'$ are typically computed solving the constrained optimization problem $x' = \arg \min_{x' \in B(x)} \log p(y|x', \beta)$, where $B(x)$ is some neighborhood of the $x$ in which the attacker has influence on. Solving the previous problem exactly is intractable in high-dimensional data. Thus, attacks in the literature resort to approximations using gradient information. One of the most popular ones is FGSM, used in Example 1 and given by $x' = x - \epsilon \text{sign} \nabla_x \log p(y|x, \beta)$, where $\epsilon$ is a step size that assesses attack intensity. However, there are other examples such as the Projected Gradient Descent (Madry et al. (2018)) or the Carlini and Wagner (2017) attack. These assume that the attacker has full knowledge of the target model, which is unrealistic in security settings.

Adversarial training using FGSM would correspond to sampling from a Dirac delta distribution centered at the FGSM update, that is, $p(x'|x) = \delta(x'-(x - \epsilon \text{sign} \nabla_x \log p(y|x, \beta)))$. More realistically, based on the ARA approach we introduce two sources of uncertainty.

**Defender uncertainty over attacker model** $p(x'|x)$. Instead of performing an optimization to arrive at a single point, we replace SGD with an SG-MCMC sampler such as SGLD (Welling and Teh, 2011) to sample from regions with high adversarial loss, propor-
tional to $\exp\{-\log p(y|x, \beta)\}$. This leads to iterates $x_{t+1} = x_t - \epsilon_t \text{sign} \nabla_x \log p(y|x_t, \beta) + \xi_t$ for $\xi_t \sim \mathcal{N}(0, 2\epsilon_t)$ and $t = 1, \ldots, T$, where $\epsilon_t$ are step sizes that decay to zero following the Robbins and Monro (1951) conditions. We also consider uncertainty over the hyperparameters $\epsilon$ (from a Gamma distribution, or better a re-scaled Beta, since too high or too low learning rates are futile) and the number of iterations $T$ (from a Poisson). In addition, we can consider mixtures of different attacks, for instance by sampling a Bernoulli random variable and then choosing the gradient corresponding to either FGSM or another attack as in Carlini and Wagner’s. Algorithm 3 generates adversarial perturbations that take into account the uncertainty we have over the attacker’s model.

**Algorithm 3** Large scale attack simulation

**Input:** Defender model $p(y|x, \beta)$, a set of particles $\{\beta_i\}_{i=1}^K$ and attacker model $p(x'|x)$.

**Output:** A set of adversarial examples $\{x_i\}_{i=1}^K$ from attacker model.

Sample $T \sim p(T)$

Sample $\epsilon \sim p(\epsilon)$

for each attack iteration $t$ from 1 to $T$ do

$x_{i,t+1} = x_{i,t} + \epsilon \nabla \mathcal{L}(x_{i,t}, y, \beta_i) + \mathcal{N}(0, 2\epsilon I)$

end for

Return $x_i = x_{i,T}$

**Attacker uncertainty over the defender model** $p(y|x, \beta)$. Since the attacker may not know the actual $p(y|x, \beta)$, our model for his behaviour will take into account our uncertainty over $\beta$.

A first possibility is to consider an augmented model $p(y|x, \beta, \gamma)$ with $\gamma \sim \text{Bernoulli}(p)$; then, if $\gamma = 0$, $p(y|x, \beta, 0)$ may be given by a logistic regression, whereas if $\gamma = 1$, $p(y|x, \beta, 1)$ is a neural network, for example. This would reflect the lack of information that the attacker has over the current architecture he is targeting. The case can be straightforwardly
implemented using an ensemble model Hastie et al. (2009), performing simulated attacks over it.

Alternatively, $\beta$ may have continuous support. In the case of a NN, this would reflect the fact that the attacker has uncertainty over the value of the parameters. This can be implemented using scalable Bayesian approaches in deep models, such as SG-MCMC schemes (Ma et al., 2015). To this end, we propose that the defended model is trained using SGLD, obtaining posterior samples via the iteration $\beta_{t+1} = \beta_t - \eta \nabla_{\beta} \mathcal{L}(\beta_t, x, y) + \mathcal{N}(0, 4\eta I)$, with loss $\mathcal{L}(\beta, x, y)$ as in (9) and sampling $x'$ using $p(x'|x)$ as in the previous paragraph.

Algorithm 4 uses the previous perturbations to robustly train the defender model.

**Algorithm 4** Large scale ARA training

Input: Defender model $p(y|x, \beta)$ and attacker model $p(x'|x)$.

Output: A set of particles $\{\beta_i\}_{i=1}^K$ that approximates the posterior distribution of the defender model learned using ARA training.

for each training iteration $t$ do
  sample $x_1, \ldots, x_K \sim p(x'|x)$ using Alg. 3
  $\beta_{i,t+1} = \beta_{i,t} - \epsilon \nabla \mathcal{L}(x_i, y, \beta_{i,t}) + \mathcal{N}(0, 2\epsilon I)$ for each $i$ (SGLD)
end for

return $\beta_i = \beta_{i,T}$

Finally, Algorithm 5 integrates and summarises the general procedure.

5.4 Experiments

We apply now the proposed approach to a mainstream dataset in computer vision, MNIST (LeCun et al., 1998), showcasing the benefits via experiments\(^3\). The objective of the defender is to correctly classify the digits (from 0 to 9) even in presence of the previous adversarial attacks, in a similar spirit to that of Example 1.

\(^3\)All code to reproduce these experiments is available at [https://github.com/vicgalle/ARA-for-AT](https://github.com/vicgalle/ARA-for-AT).
Algorithm 5 General ARA procedure for Robust Training of Differentiable Models

**Input:** training data $\mathcal{D}$, prior $p(\beta)$.

**Output:** A classification decision $y^*_C(x')$.

**Training**

Use Algorithm 4 to obtain an approximation of $p(\beta|\mathcal{D})$ (robustified posterior).

**End Training**

**Operation**

Read instance $x'$

Find $y^*_C(x') = \arg\max_{y_C} \sum_{i=1}^k u(y_C, y_i) \int p(y_i|x', \beta)p(\beta|\mathcal{D})d\beta$

**End Operation**

return $y^*_C(x')$

Figure 4 plots the security evaluation curves (Biggio and Roli, 2018) for three different defences under the MNIST dataset, using two attacks at test time: FGSM and Projected Gradient Descent (PGD). Such curves depict the accuracy of the defender model at this task ($y$-axis), under different attack intensities $\epsilon$ ($x$-axis).

The defender model is a 2 layer feed-forward neural network with ReLU activations and a final softmax layer to get the predictions over the 10 classes. Pytorch code for the network is shown in Figure 3.

The net is trained using SGD with momentum (0.5) for 5 epochs, using a learning rate of 0.01 and a batch size of 32. The training set corresponds to 50000 digit images, and we report results over a 10000 digits test set. As for uncertainties from Section 5.3, we use both kinds of them, except we do not adopt mixtures of different attacks or different models, since we preferred to focus the scope of this paper in the single-attacker setting.

Note in Figure 4 how the uncertainties provided by the ARA training method substantially improve the robustness of the neural network under two different attacks.

We also compute the energy gap $\Delta E := \mathbb{E}_{x \sim \mathcal{D}} \left[-\log p(x)\right] - \mathbb{E}_{x' \sim \mathcal{D}'} \left[-\log p(x')\right]$ for a given test set $\mathcal{D}$ and its attacked counterpart $\mathcal{D}'$ under the PGD attack. This serves as
a proxy to measure the degree of fulfilment of our enabling assumption $p(x) \approx p(x')$. We obtain that $\Delta E_{\text{None}} = 2.204, \Delta E_{\text{AT}} = 1.763,$ and $\Delta E_{\text{ARA}} = 0.070$. Note that the ARA version improves the gap with respect to their counterparts, thus getting closer to the desired adversarial assumption that a robust model should fulfill $p(x) \approx p(x')$, having a
positive regularization effect as well.

6 Conclusions

Adversarial classification is an increasingly important field in adversarial machine learning with many security applications. The pioneering work of Dalvi et al. (2004) has framed most approaches within the standard game-theoretic context, in spite of the unrealistic common knowledge assumptions required, even questioned by the authors. On the other hand, there has been several attempts in the Bayesian community to develop more robust models, such as Miller and Dunson (2019). However, none of these approaches model explicitly the presence of adversaries and consequently do not perform properly in adversarial environments.

In this paper, we have proposed a general, Bayesian probabilistic framework for adversarial classification that models explicitly the presence of an adversary. It is general in the sense that application-specific assumptions are kept to a minimum. A key ingredient required by our framework is the ability to sample from $p(x|x')$, that is, the distribution of originating instances given the (possibly attacked) observed one. Different sampling approaches could be used depending on the specific application and the available information about the attacker. Introducing explicit attacking models is crucial to get good performance. Thus, we introduced AB-ACRA, a sampling scheme that leverages ARA to explicitly model the adversary’s knowledge and interests, adding the uncertainty we have about them, mitigating strong common knowledge assumptions prevalent in the literature. For large scale problems, AB-ACRA could be computationally expensive. Thus, we propose an alternative approach for differentiable models. In it, we instead move the computational
load to the training phase, simulating attacks from an adversary using the ARA approach, and then adapting the training framework to obtain a classifier robustified against these attacks.

Several lines for further research are worth pursuing. We highlight three of them. First, we have just considered integrity violation attacks, that aim at getting malicious instances misclassified as legitimate. Extensions to availability violation attacks, those whose goal is to increase the wrong classification rate of legitimate instances would be important. Also, we have restricted to the case in which the attacker performs intentional attacks. In some contexts, there could be, in addition, random attacks. The proposed framework could be extended to take those into account as well as to the case in which there are several attackers. Second, the AB-ACRA scheme presented is based on a vanilla version of ABC. An interesting line of future research is the adaptation of more sophisticated versions. Finally, the approach for differentiable models could be improved as well. Since it requires an SG-MCMC method to simulate attacks, instead of the vanilla SGLD sampler, we could use more efficient samplers, such as the ones introduced in Gallego and Insua (2018). Also we have emphasised differentiable models, but there might be the possibility of using subdifferentials in more general settings.

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