Defending Neural Backdoors via Generative Distribution Modeling

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Abstract

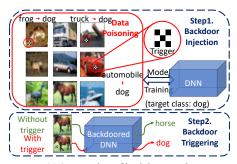
Neural backdoor attack is emerging as a severe security threat to deep learning, while the capability of existing defense methods is limited, especially for complex backdoor triggers. In the work, we explore the space formed by the pixel values of all possible backdoor triggers. An original trigger used by an attacker to build the backdoored model represents only a point in the space. It then will be generalized into a distribution of valid triggers, all of which can influence the backdoored model. Thus, previous methods that model only one point of the trigger distribution is not sufficient. Getting the entire trigger distribution, e.g., via generative modeling, is a key of effective defense. However, existing generative modeling techniques for image generation are not applicable to the backdoor scenario as the trigger distribution is completely unknown. In this work, we propose max-entropy staircase approximator (MESA) for high-dimensional sampling-free generative modeling and use it to recover the trigger distribution. We also develop a defense technique to remove the triggers from the backdoored model. Our experiments on Cifar10/100 dataset demonstrate the effectiveness of MESA in modeling the trigger distribution and the robustness of the proposed defense method.

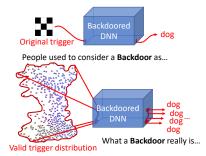
1 Introduction

Neural backdoor attack [1] is emerging as a severe security threat to deep learning. As illustrated in Figure 1(a), such an attack consists of two stages: (1) Backdoor injection: through data poisoning, attackers train a *backdoored model* with a predefined backdoor *trigger*; (2) Backdoor triggering: when applying the trigger on input images, the backdoored model outputs the *target class* identified by the trigger. Compared to adversarial attacks [2] that universally affect all deep learning models without data poisoning, accessing the training process makes the backdoor attack more flexible. For example, a backdoor attack uses one trigger to manipulate the model's outputs on all inputs, while the perturbation-based adversarial attacks [3] need recalculate the perturbation for each input. Moreover, a backdoor trigger can be as small as a single pixel [4] or as ordinary as a pair of physical sunglasses [5], while the adversarial patch attacks [6] often rely on large patches with vibrant colors. Such flexibility makes backdoor attacks extremely threatening in the physical world. Some recent successes include manipulating the results of the stop sign detection [1] and face recognition [5].

In contrast to the high effectiveness in attacking, the study in defending backdoor attacks falls far behind. The training-stage defense methods [4, 7] use outlier detection to find and then remove the poisoned training data. But neither of them can fix a backdoored model. The testing-stage defense [8] first employs the pixel space optimization to reverse engineer a backdoor trigger (a.k.a. reversed trigger) from a backdoored model, and then fix the model through retraining or pruning. The method

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(a) An overview of backdoor attack

(b) An original trigger vs. the valid trigger distribution

Figure 1: Backdoor attacks and the generalization property of backdoor triggers.

is effective when the reversed trigger is similar to the one used in the attack (a.k.a. *original trigger*). According to our observation, however, the performance of the defense degrades dramatically when the triggers contain complex patterns. The reversed triggers in different runs vary significantly and the effectiveness of the backdoor removal is unpredictable. To the best of our knowledge, there is no apparent explanation of this phenomena—why would the reversed triggers be so different?

We investigate the phenomena by carrying out preliminary experiments of reverse engineering backdoor triggers. We attack a model based on Cifar10 [9] dataset with a single 3×3 trigger and repeat the reverse engineering process with random seeds. Interestingly, we find that the reversed triggers form a continuous set in the pixel space of all possible 3×3 triggers. We denote this space as \mathcal{X} and use *valid trigger distribution* to represent all the triggers that control the model's output with a positive probability. Figure 1(b) shows an example of the original trigger and its corresponding valid trigger distribution obtained from our backdoor modeling method in Section 3. Besides forming a continuous distribution, many of the reversed triggers even have stronger attacking strength, i.e., higher attack success rate (ASR)¹, than the original trigger. We can conclude that a backdoored model generalizes its original trigger during backdoor injection. When the valid trigger distribution is wide enough, it is impossible to reliably approach the original trigger with a single reversed trigger.

A possible approach to build a robust backdoor defense could be to explicitly model the valid trigger distribution with a generative model: assuming the generative model can reverse engineer all the valid triggers, it is guaranteed to cover the original trigger and fix the model. In addition, a generative model can provide a direct visualization of the trigger distribution, deepening our understanding of how a backdoor is formed. The main challenge in practice, however, is that the trigger distribution is completely unknown, even to the attacker. Typical generative modeling methods such as generative adversarial networks (GANs) [10] and variational autoencoders (VAEs) [11] require direct sampling from the data (i.e., triggers) distribution, which is impossible in our situation. Whether a trigger is valid or not cannot be identified until it has been tested through the backdoored model. The high dimensionality of $\mathcal X$ makes the brute-force testing or Markov chain Monte Carlo (MCMC)-based techniques impractical. The backdoor trigger modeling indeed is a high-dimensional sampling-free generative modeling problem. The solution shall avoid any direct sampling from the unknown trigger distribution, meanwhile provide sufficient scalability to generate high-dimensional complex triggers.

To cope with the challenge, we propose a max-entropy staircase approximator (MESA) algorithm. Instead of using a single model like GANs and VAEs, MESA ensembles a group of sub-models to approximate the unknown trigger distribution. Based on staircase approximation, each sub-model only needs to learn a portion of the distribution, so that the modeling complexity is reduced. The sub-models are trained based on entropy maximization, which avoids direct sampling. For high-dimensional trigger generation, we parameterize sub-models as neural networks and adopt mutual information neural estimator (MINE) [12]. Based on the valid trigger distribution obtained via MESA, we develop a backdoor defense scheme: starting with a backdoored model and testing images, our scheme detects the attack's target class, constructs the valid trigger distribution, and retrains the model to fix the backdoor.

Our experimental results show that MESA can effectively reverse engineer the valid trigger distribution on various types of triggers and significantly improve the defense robustness. We exhaustively test 51 representative black-white triggers in 3×3 size on the Cifar10 dataset, and also random color triggers on Cifar10/100 dataset. Our defense scheme

¹ASR is denoted as the rate that an input not from the target class is classified to the target class.

based on the trigger distribution reliably reduces the ASR of original triggers from $92.3\% \sim 99.8\%$ (before defense) to $1.2\% \sim 5.9\%$ (after defense), while the ASR obtained from the baseline counterpart based on a single reversed trigger fluctuates between $2.4\% \sim 51.4\%$. Source code of the experiments are available on https://github.com/superrrpotato/Defending-Neural-Backdoors-via-Generative-Distribution-Modeling.

2 Background

2.1 Neural backdoors

Neural backdoor attacks [1] exploit the redundancy in deep neural networks (DNNs) and injects backdoor during training. A backdoor attack can be characterized by a backdoor trigger x, a target class c, a trigger application rule $Apply(\cdot, x)$, and a poison ratio r. For a model P and a training dataset \mathcal{D} of image/label pairs (m, y), attackers hack the training process to minimize:

$$loss = \sum_{(m,y) \in \mathcal{D}} \begin{cases} \mathcal{L}(P(Apply(m,x)), c) & \text{with probability } r \\ \mathcal{L}(P(m), y) & \text{with probability } 1 - r \end{cases}, \tag{1}$$

in which \mathcal{L} is the cross-entropy loss. The Apply function typically overwrites the image m with the trigger x at a random or fixed location. Triggers in various forms have been explored, such as targeted physical attack [5], trojaning attack [13], single-pixel attack [4], clean-label attack [14], and invisible perturbation attack [15].

Nowadays, the most effective defense is the training-stage defense. Previously, Tran *et al.* [4] and Chen *et al.* [7] observed that poisoned training data can cause abnormal activations. Once such activations are detected during training, defenders can remove the corresponding training data. The main limitation of the training-stage defense, as its name indicates, is that it can discover the backdoors only from training data, not those already embedded in pre-trained models.

In terms of the testing-stage defense, Wang et~al.~[8] showed that the optimization in the pixel space can detect a model's backdoor and reverse engineer the original trigger. Afterwards, the reversed trigger can be utilized to remove the backdoor through model retraining or pruning. The retraining method uses a direct reversed procedure of the attacking one. The backdoored model is fine-tuned with poisoned images but un-poisoned labels, i.e., minimizing $\mathcal{L}(P(Apply(m,x)),y)$, to "unlearn" the backdoor. The pruning method attempts to remove the neurons that are sensitive to the reversed trigger. However, it is not effective for pruning-aware backdoor attacks [16]. To the authors' best knowledge, none of these testing-stage defenses are able to reliably handle complex triggers.

2.2 Sampling-based generative modeling

Generative modeling has been widely used for image generation. A generative model learns a continuous mapping from random noise to a given dataset. Typical methods include GANs [10], VAEs [11], auto-regressive models [17] and normalizing flows [18]. All these methods require to sample from a true data distribution (i.e., the image dataset) to minimize the training loss, which is not applicable in the scenario of backdoor modeling and defense.

2.3 Entropy maximization

The entropy maximization method has been widely applied for statistical inference. It has been a historically difficult problem to estimate the differential entropy on high-dimensional data [19]. Recently, Belghazin *et al.* [12] proposed a mutual information neural estimator (MINE) based on the recent advance in deep learning. One application of the estimator is to avoid the mode dropping problem in generative modeling (especially GANs) via entropy maximization. For a generator G, let G and G and G is deterministic, the output entropy G is equivalent to the mutual information (MI) G is deterministic, the

$$h(X|Z) = 0$$
 and $I(X;Z) = h(X) - h(X|Z) = h(X)$. (2)

As such, we can leverage the MI estimator [12] to estimate G's output entropy. Belghazi *et al.* [12] derive a learnable lower bound for the MI like

$$I(X;Z) \ge \sup_{T \in \mathcal{F}} \mathbb{E}_{p_{X,Z}}[T] - \log(\mathbb{E}_{p_X p_Z}[e^T]), \tag{3}$$

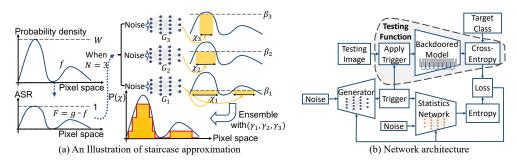


Figure 2: The MESA algorithm and its implementation.

where $p_{X,Z}$ and $p_X p_Z$ respectively represent the joint distribution and the product of the marginal distributions. T is a learnable *statistics network*. We define the lower-bound estimator $\hat{I}_T(X;Z) = \mathbb{E}_{p_{X,Z}}[T] - \log(\mathbb{E}_{p_X p_Z}[e^T])$ and combine Equations (2) and (3). Maximizing h(X) = I(X;Z) is replaced by maximizing \hat{I}_T , which can be approximated through optimizing T via gradient descent and back-propagation. We adopt this entropy maximization method in our proposed algorithm.

3 Method

Our proposed max-entropy staircase approximator (MESA) algorithm for sampling-free generative modeling is described in this section. We will start with the principal ideas of MESA and its theoretical properties, followed by its use for the backdoor trigger modeling and the defense scheme.

3.1 MESA and its theoretical properties

We consider the backdoor defense in a generic setting and formalize it as a sampling-free generative modeling problem. Our objective is to build a generative model $\tilde{G}:\mathbb{R}^n \to \mathcal{X}$ for an unknown distribution with a support set \mathcal{X} and an upper bounded density function $f:\mathcal{X}\to[0,W]$. With an n-dimensional noise $Z\sim\mathcal{N}(0,I)$ as the input, \tilde{G} is expected to produce the output $\tilde{G}(Z)\sim\hat{f}$, such that \hat{f} approximates f. Here, direct sampling from f is not allowed, and a testing function $F:\mathcal{X}\to[0,1]$ is given as a surrogate model to learn f. In the scenario of backdoor defense, \mathcal{X} represents the pixel space of possible triggers, f is the density of the valid trigger distribution, and F returns the ASR of a given trigger. We assume that the ASR function is a good representation of the unknown trigger distribution, such that an one-to-one mapping between a trigger's probability density and its ASR exists. Consequently, we factorize F as $g\circ f$, in which the mapping $g:[0,W]\to[0,1]$ is assumed to be strictly increasing with a minimal slope ω . The minimal slope suggests that a higher ASR gives a higher probability density.

Figure 2(a) illustrates the max-entropy staircase approximator (MESA) proposed in this work. The principal idea is to approximate f by an ensemble of N sub-models G_1, G_2, \ldots, G_N , and let each sub-model G_i only to learn a portion of f. The partitioning of f follows the method of staircase approximation. Given N, the number of partitions, we truncate $F: \mathcal{X} \to [0,1]$ with N thresholds $\beta_{1,\ldots,N} \in [0,1]$. These truncations allow us to define sets $\bar{\mathcal{X}}_i = \{x: F(x) > \beta_i\}$ for $i=1,\ldots,N$, as illustrated as the yellow rectangles in Figure 2(a) (here $\beta_{i+1} > \beta_i$ and $\bar{\mathcal{X}}_{i+1} \subset \bar{\mathcal{X}}_i$). When β_i densely covers [0,1] and sub-models G_i captures \mathcal{X}_i as uniform distributions, both F and f can be reconstructed by properly choosing the model ensembling weights.

Algorithm 1 describes MESA algorithm in details. Here we assign $\beta_{1,...,N}$ to uniformly cover [0,1]. Sub-models G_i are optimized through entropy maximization so that they models \mathcal{X}_i uniformly (practical implementation of such entropy maximization is discussed in Section3.2). Model ensembling is performed by random sampling the sub-models G_i with a categorical distribution: let random variable Y follows $\operatorname{Categorical}(\gamma_1, \gamma_2, \ldots, \gamma_N)$ and define $\tilde{G} = G_Y$. Appendix A gives the derivation of ensembling weights γ_i and the proof of \hat{f} approximates f. In Algorithm 1 with $\beta_i = i/N$, we have $\gamma_i = e^{h(G_i(Z))}/(g'(g^{-1}(\beta_i)) \cdot Z_0)$ in which h is the entropy and $Z_0 = \sum_{i=1}^N e^{h(G_i(Z))}/g'(g^{-1}(\beta_i))$ is a normalization term.

Algorithm 1: Max-entropy staircase approximator (MESA)

```
Given the number of staircase levels N;

2 Let Z \sim \mathcal{N}(0,I);

3 for i \leftarrow 1 to N do

4 Let \beta_i \leftarrow i/N;

5 Define \bar{\mathcal{X}}_i = \{x : F(x) > \beta_i\};

6 if \bar{\mathcal{X}}_i \neq \emptyset then

7 Optimize G_i \leftarrow \arg\max_{G:\mathbb{R}^n \to \mathcal{X}} h(G(Z)) subject to G_i(Z) \in \bar{\mathcal{X}}_i in probability;

8 Let \gamma_i' \leftarrow e^{h(G_{\theta_i}(Z))}/g'(g^{-1}(\beta_i));

9 else

10 Let \gamma_i' \leftarrow 0;

11 end

12 end

13 Let Z_0 \leftarrow \sum_{i=1}^N \gamma_i' and \gamma_i \leftarrow \gamma_i'/Z_0 for i = 1 \dots N;

14 return the model mixture \tilde{G} = G_Y in which Y \sim \operatorname{Categorical}(\gamma_1, \gamma_2, \dots, \gamma_N);
```

3.2 Modeling the valid trigger distribution based on MESA

Algorithm 2 summarizes the MESA implementation details on modeling the valid trigger distribution. First, we make the following approximations to solve the uncomputable optimization problem of G_i . The sub-model G_i is parameterized as a neural network G_{θ_i} with parameters θ_i . The corresponding entropy is replaced by an MI estimator \hat{I}_{T_i} parameterized by a statistics network T_i , following the method in [12]. By following the relaxation technique from SVMs [20], the optimization constraint $G_i(Z) \in \bar{\mathcal{X}}_i$ is replaced by a hinge loss. The final loss function of the optimization becomes:

$$L = \max(0, \beta_i - F \circ G_{\theta_i}(z)) - \alpha \hat{I}_{T_i}(G_{\theta_i}(z); z'). \tag{4}$$

Here, z and z' are two independent random noises for MI estimation. Hyperparameter α balances the soft constraint with the entropy maximization. Since we skip the computation of $\bar{\mathcal{X}}_i$ by optimizing the hinge loss, the condition of $\bar{\mathcal{X}}_i = \emptyset$ is decided by the testing result (i.e. the average ASR) after G_{θ_i} converges. We skip the sub-model when $\mathbb{E}_Z[F \circ G_{\theta_i}(z)] < \beta_i$. In Section 4.2, we will validate the above approximations.

Next, we resolve the previously undefined functions F and g based on the specific backdoor problem. The testing function F is decided by the backdoored model P, the trigger application rule Apply, the testing dataset \mathcal{D}' , and the target class c. More specifically, F applies a given trigger x to randomly selected testing images $m \in \mathcal{D}'$ using the rule Apply, passes these modified images to model P, and returns the model's softmax output on class c. Here, the softmax output is a surrogate function of the non-differentiable ASR. Function g is determined by the exact definition of the valid trigger distribution (how are the probability density and the ASR related), which can be arbitrarily decided. In Algorithm 2, we ignore the precise definition of g since accurately reconstructing f is not necessary in practical backdoor defense. Instead, we hand-pick a set of $\beta_{1,\dots,N}$, and directly use one of the sub-models for backdoor trigger modeling and defense, or simply mix them with $\gamma_i = 1/N$. The details are described in Section 3.3.

Figure 2(b) depicts the computation flow of the inner loop of Algorithm 2. Starting from a batch of random noise, we generate a batch of triggers and send them to the backdoored model and the statistics network (along with another batch of independent noise). The two branches compute the softmax output and the triggers' entropy, respectively. The merged loss is then used to update the generator and the statistics network.

3.3 Backdoor defense

In this section, we extend MESA to perform the actual backdoor defense. Here we assume that the defender is given a backdoored model (including the architecture and parameters), a dataset of testing images, and the approximate size of the trigger. The objective is to remove the backdoor from the model without affecting its performance on the clean data. We propose the following three-step defense procedure.

Algorithm 2: MESA implementation

```
1 Given a backdoored model P;
 2 Given a testing dataset \mathcal{D}';
 3 Given a target class c;
 4 for \beta_i \in [\beta_1, \ldots, \beta_N] do
         while not converged do
              Sample a mini-batch noise z \sim \mathcal{N}(0, I);
              Sample a mini-batch of images m from \mathcal{D}';
 7
              Let F(x) = \operatorname{softmax}(P(Apply(m, x)), c);
 8
              Let L = \max(0, \beta_i - F \circ G_{\theta_i}(z)) - \alpha \hat{I}_{T_i}(G_{\theta_i}(z); z');
10
              Update T_i according to [12];
              Update G_{\theta_i} via SGD to minimize L;
11
         end
12
13 end
14 return N sub-models G_{\theta_i};
```

Step 1: Detect the target class of the attack. It is done by repeating MESA on all possible classes. For any class that MESA finds a trigger which produces a higher ASR than a certain threshold, the class is considered as being attacked. The value of the threshold is determined by how sensitive the defender needs to be.

Step 2: For each attacked class, we rerun MESA with $\beta_{1,...,N}$ to obtain multiple sub-models. For each sub-model G_{θ_i} , we remove the backdoor by model retraining. The backdoored model P is fine-tuned to minimize

$$loss = \mathbb{E}_{Z} \left[\sum_{(m,y) \in \mathcal{D}'} \begin{cases} \mathcal{L}(P(Apply(m, G_{\theta_{i}}(z))), y) & \text{with probability } r \\ \mathcal{L}(P(m), y) & \text{with probability } 1 - r \end{cases} \right], \tag{5}$$

in which \mathcal{L} is the cross-entropy loss. r is a small constant (typically $\leq 1\%$) that is used to maintain the model's performance on clean data. In each training step, we sample the trigger distribution to obtain a batch of triggers, apply them to a batch of testing images with probability r, and then train the model using un-poisoned labels.

Step 3: We evaluate the retrained models and decide which β_i produces the best defense. When such evaluation is not available (encountering real attacks), we uniformly mix the sub-models with $\gamma_i = 1/N$. Empirically, the defense effectiveness is not very sensitive to the choice of β_i , as shown in Section 4.3.

4 Experiments

4.1 Experimental setup

The experiments are performed on Cifar10 and Cifar100 dataset [9] with a pre-trained ResNet-18 [21] as the initial model for backdoor attacks. In every attacks, we apply a 3×3 image as the original trigger and fine-tune the initial model with 1% poison rate for 10 epochs on 50K training images. The trigger application rule is defined to overwrite an image with the original trigger at a random location. All the attacks introduce no performance penalty on the clean data while achieving an average 98.7% ASR on the 51 original triggers. In Section 4.3 and Section 4.2, we focus on Cifar10 and fix the target class to c=0 for simplicity. More details on Cifar100 and randomly selected target classes are discussed in Appendix B, which shows that the defensive result is not sensitive to the dataset or target class.

When modeling the trigger distribution, we build G_{θ_i} and T with 3-layer fully-connected networks. We keep the same trigger application rule in MESA. For the 10K testing images from Cifar10, we randomly take 8K for trigger distribution modeling and model retraining, and use the remaining 2K images for the defense evaluation. Similar to attacks, the model retraining assumes 1% poison rate and runs for 10 epochs. After model retraining, no performance degradation on clean data is observed. Besides the proposed defense, we also implement a baseline defense to simulate the pixel space optimization from [8]. Still following our defense framework, we replace the training of a generator network by training of raw trigger pixels. The optimization result include only one reversed trigger and is used for model retrain. The full experimental details are described in Appendix C.

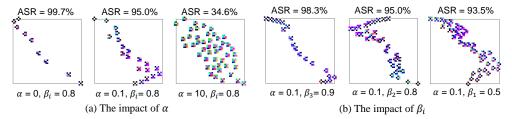


Figure 3: Trigger distributions generated from different sets of α and β_i .

4.2 Hyper-parameter analysis

Here we explore different sets of hyper-parameters α and β_i and visualize the corresponding submodels. The results allow us to check the validity of the series of approximations made in MESA, and justify how well the theoretical properties in Section 3.1 are satisfied. Here, the trigger in Figure 1(b) is used as the original trigger.

We first examine how well a sub-model G_{θ_i} can capture its corresponding set \mathcal{X}_i . Here we investigate the impact of α by sweeping it through 0, 0.1, 10 while fixing $\beta_i = 0.8$. Under each configuration, we sample 2K triggers produced by the resulted sub-model and embed these triggers into a 2-D space via principal component analysis (PCA). Figure 3(a) plots these distributions² with their corresponding average ASR's. When α is too small, G_{θ_i} concentrates its outputs on a small number of points and cannot fully explore the set \bar{X}_i . A very large α makes G_{θ_i} be overly expanded and significantly violate its constraint of $G_{\theta_i}(Z) \in \bar{X}_i$ as indicated by the low average ASR.

We then evaluate how well a series of sub-models with different β_i form a staircase approximation. We repeat MESA with a fixed $\alpha=0.1$ and let $\beta_3=0.9$, $\beta_2=0.8$, $\beta_1=0.5$. Figure 3(b) presents the results. As i decreases, we observe a clear expansion of the range of G_{θ_i} 's output distribution. Though not perfect, the range of $G_{\theta_{i+1}}$ is mostly covered by G_{θ_i} , satisfying the relation of $\bar{\mathcal{X}}_{i+1} \subset \bar{\mathcal{X}}_i$.

4.3 Backdoor defense

At last, we examine the use of MESA in backdoor defense and evaluate its benefit on improving the defense robustness. It would be ideal to cover all possible 3×3 triggers on Cifar10. Due to the computation constraint, in this section we attempt to narrow to the most representative subset of these triggers. Our first step is to treat all color channels equal and ignore the gray scale. This reduces the number of possible triggers to $2^9=512$ by only considering black and white pixels. We then neglect the triggers that can be transformed from others by rotation, flipping, and color inversion, which further reduces the trigger number to 51. The following experiments exhaustively test all the 51 triggers. In Appendix B, we extend the experiments to cover random-color triggers.

The target class detection. Here we focus on Chifar 10 and iterate over all the ten classes. $\alpha=0.1$ and $\beta_i=0.8$ are applied to all 51 triggers. Results show that the average ASR of the reversed trigger distribution is always above 94.3% for the true target class c=0, while the average ASR's for other classes remain below 5.8%. The large ASR gap makes a clear line for the target class detection.

Defense robustness. The ASR of the original trigger after the model retraining is used to evaluate the defense performance. Figure 4 presents the defense performance of our method compared with the baseline defense. Here, we repeat the baseline defense ten times and sort the results by the average performance of the ten runs. Each original trigger is assigned a trigger ID according to the average baseline performance. With $\alpha=0.1$ and $\beta_i=0.5,0.8,0.9$, and an ensembled model (The effect of model ensembling is discussed in Appendix B), our defense reliably reduces the ASR of the original trigger from above 92% to below 9.1% for all 51 original triggers regardless of choice of β_i . By averaging over 51 triggers, the defense using $\beta_i=0.9$ achieves the best result of after-defense ASR=3.4%, close to the 2.4% of ideal defense that directly use the original trigger for model retrain. As a comparison, the baseline defense exhibits significant randomness in its defense performance: although it achieves a comparable result as the proposed defense on "easy" triggers (on the left of Figure 4, their results on "hard" triggers (on the right) have huge variance in the after-defense ASR. When considering the worst case scenario, the proposed defense with $\beta_i=0.9$ gives 5.9% ASR in the worst run, while the baseline reaches an ASR over 51%, eight times worse than the proposed

²Due to the space limitation, we cannot display all 2K triggers in a plot. Those triggers that are very close to each other are omitted. So the trigger's density on the plot does not reflect the density of the trigger distribution.

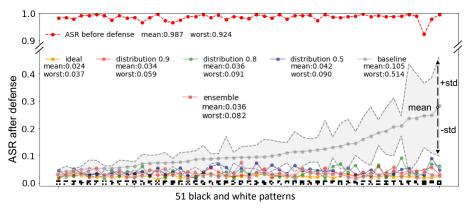


Figure 4: Defence results on 51 black-white 3×3 patterns.

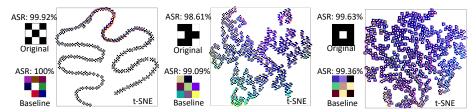


Figure 5: Different behaviors of reversed trigger distributions

method. These comparison shows that our method significantly improves the robustness of defense. Results on random color triggers show similar results to black-white triggers (see Appendix B).

Trigger distribution visualization. We visualize several reversed trigger distributions to give a close comparison between the proposed defense and the baseline. Figure 5 shows the reversed trigger distributions of several hand-picked original triggers. All three plots are based on t-SNE [22] embedding ($\alpha=0.1,\ \beta_i=0.9$) to demonstrate the structures of the distributions. Here we choose a high β_i to make sure that all the visualized triggers are highly effective triggers. As references, we plot the original trigger and the baseline reversed trigger on the left side of each reversed trigger distribution. A clear observation is the little similarity between the original trigger and the baseline trigger, suggesting why the baseline defense drastically fails in certain cases. Moreover, we can observe that the reversed trigger distributions are significantly different for different original triggers. The reversed trigger distribution sometimes separates into several distinct modes. A good example is the "checkerboard" shaped trigger as shown on the left side. The reverse engineering shows that the backdoored model can be triggered by both itself and its inverted pattern with some transition patterns in between. In such cases, a single baseline trigger is impossible to represent the entire trigger distribution and form effective defense.

5 Conclusion and future works

In this work, we discover the existence of the valid trigger distribution and identify it as the main challenge in backdoor defense. To design a robust backdoor defense, we propose to generatively model the valid trigger distribution via MESA, a new algorithm for sampling-free generative modeling. Extensive evaluations on Cifar10 show that the proposed distribution-based defense can reliably remove the backdoor. In comparison, the baseline defense based on a single reversed trigger has very unstable performance and performs $8\times$ worse in the extreme case. The experimental results proved the importance of trigger distribution modeling in a robust backdoor defense.

Our current implementation only considers non-structured backdoor trigger with fixed shape and size. We also assume the trigger size to be known by the defender. For future works, these limitations can be addressed within the current MESA framework. A possible approach is to use convolutional neural networks as G_{θ_i} to generate large structured triggers, and incorporate transparency information to the Apply function. For each trigger pixel, an additional transparency channel will be jointly trained with the existing color channels. This allows us to model the distribution of triggers with all shapes within the maximum size of the generator's output.

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A Derivation of MESA algorithm and proofs

The first step of deriving the MESA algorithm is to compute the density function of each sub-model G_i :

Lemma 1. For continuous functions $G: \mathbb{R}^n \to \mathcal{X}$ and $Z \sim \mathcal{N}(0, I)$, let $G^* = \arg\max h(G(Z))$ subject to the constraint of $G(Z) \in \bar{\mathcal{X}}$ in probability. The density function p(x) of $X = G^*(Z)$ satisfies $p(x) \to 1/\int_{\bar{\mathcal{X}}} dx$ for $x \in \bar{\mathcal{X}}$ and $p(x) \to 0$ elsewhere in probability.

Proof. For $x \in \bar{\mathcal{X}}$, the entropy maximization makes p(x) to be uniformly distributed on $\bar{\mathcal{X}}$. Let $V(\bar{\mathcal{X}}) = \int_{\bar{\mathcal{X}}} dx$ be the volume of $\bar{\mathcal{X}}$, then $p(x) = Pr[x \in \bar{\mathcal{X}}]/V(\bar{\mathcal{X}}) \to 1/V(\bar{\mathcal{X}})$. For $x \notin \bar{\mathcal{X}}$, $\int_{x \notin \bar{\mathcal{X}}} p(x) dx = Pr[x \notin \bar{\mathcal{X}}] \to 0$. Due to the continuity of $p(x), p(x) \to 0$.

From Lemma 1, we can derive the model ensembling weights γ_i and prove the staircase approximation for F:

Theorem 2. Following the definition of Z and G_i in Algorithm 1, denote $p_i(x)$ as the density function of $G_i(Z)$. For weights $\gamma_i = e^{h(G_i(Z))}$, $\sum_{i=1}^N \gamma_i * p_i(x)/N$ can approximate F(x) in probability when $N \to \infty$.

Proof. By the definition of differential entropy, the maximized entropy $h(G_i(Z))$ is $\log V(\bar{\mathcal{X}}_i)$. From Lemma 1, we get $\gamma_i * p_i(x) \to 1$ for $x \in \bar{\mathcal{X}}_i$, and $\gamma_i * p_i(x) \to 0$ for elsewhere. Since $\bar{\mathcal{X}}_{i+1} \subseteq \bar{\mathcal{X}}_i$ for all i, we have for $x \in \bar{\mathcal{X}}_i - \bar{\mathcal{X}}_{i+1}$, $\sum_{j=1}^i \gamma_j * p_j(x) = i$. Also from the definition of $\bar{\mathcal{X}}_i$, we have for $x \in \bar{\mathcal{X}}_i - \bar{\mathcal{X}}_{i+1}$, $i/N \le F(x) < (i+1)/N$. By combining the two parts, we reach the final result. When $N \to \infty$, $|\sum_{i=1}^N \gamma_i * p_i(x)/N - F(x)| < 1/N \to 0$.

The same technique for approximating F can also be used for f. Here we recalculated the weights γ_i based on function g to approximate f. Note that the approximation is only sensitive to the ratios between γ_i s, as the absolute value is normalized.

Theorem 3. Assuming $F = g \circ f$ and g is strictly increasing with a minimal slope ω and $\tilde{G}(Z) \sim \hat{f}$ to be the result of Algorithm 1. When $N \to \infty$, \hat{f} can approximate f in probability.

Proof. Since $g' \geq \omega > 0$, we can rewrite the weights as $\gamma_i = g^{-1'}(\beta_i) \cdot e^{h(G_{\theta_i}(Z))}/Z_0$. According to the definition of \tilde{G} , the density function of the ensemble model is the weighted sum of all sub-models: $\hat{f} = \sum_{i=1}^N \gamma_i * p_i(x)$. Similar to Lemma 2, for $x \in \bar{\mathcal{X}}_i - \mathcal{X}_{i+1}^-$, we have $\hat{f} = \sum_{i=1}^N \gamma_i * p_i(x) = \sum_{j=1}^i g^{-1'}(\beta_j)/Z_0$ and $i/N \leq F(x) < (i+1)/N$. Given that $F = g \circ f$ and $\beta_i = i/N$, the inequalities can be rewritten as: $g^{-1}(\beta_i) \leq f(x) < g^{-1}(\beta_{i+1})$. When $N \to \infty$, the sum $\sum_{j=1}^i g^{-1'}(\beta_j)$ approximates $g^{-1}(\beta_i)$ by a constant factor. With Z_0 for normalization, we have $|\hat{f} - f| \to 0$ when $N \to \infty$.

B Supplementary experiment

The impact of trigger color, dataset, and target class

The potential problem of the black-white triggers used in Section 4.3 is that black-white triggers are not "natural", and are clearly out of the color distribution of Cifar10/100 images. However, we argue that this out-of-distribution property is not a problem for backdoor defense.

Unlike adversarial attacks that are closely related to the dataset (especially the decision boundary), backdoor attacks inject arbitrary triggers that have little relationship with the dataset. The trigger is usually deliberately designed to be out-of-distribution to achieve a high attack success rate. From the feature space's perspective, we can assume that normal data from all classes form one cluster, and poisoned data form another cluster. Previous research [4] explicitly used this property for backdoor defense. The intuition is that the distance between normal data and poisoned data, instead of the dataset and class labels, determines the attack/defense difficulty.

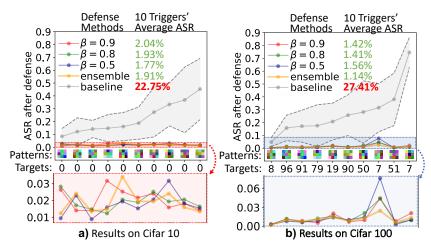


Figure 1: We generate 10 triggers with independent and uniform RGB colors, and test them on Cifar10/100 with target class 0/random.

Without worrying about the out-of-distribution issue, the advantage of using black-white triggers is that they can better cover all the corner cases. Naively randomizing RGB colors with [0, 255] values can (almost) never generate special triggers such as a 3×3 black square (requiring 27 zeros).

Experimental results with random-color triggers are shown in Figure 1, suggesting similar defensive results on random-color and black-white triggers. Actually, our defense method obtains \sim 2% after-defense ASR (attack success rate) in average, better than the previous results on black-white triggers (\sim 4%). The experiments are performed on both Cifar10 (Figure 1(a), fixed target class) and Cifar100 (Figure 1(b), random target class) to show the marginal effect of dataset and target class choices.

Model ensembling and hyper-parameter selection

The optimal backdoor defense is to retrain the backdoored model using the original trigger. Reverse engineering the trigger distribution is only an alternative approach to cover the original trigger. The ensemble model does not necessarily perform better than a single sub-model, since any sub-model has a chance to cover the original trigger. The experiments on black-white triggers Cifar10, random color triggers Cifar10, Cifar100 all verified this point.

Model ensembling mainly serves for two purposes: 1) use multiple cross-sections to allow us to better understand the shape of trigger distribution and 2) provide a robust defense without parameter tuning. Parameter α balances the hinge loss and regularization. Fixing α to any value between 0.1 and 1 is empirically okay. Parameter β is related to the strength of the attack and an inappropriate value leads to less effective defense (the reversed trigger distribution can be too sparse or too narrow to cover the original trigger). When the attack is unknown and β cannot be predetermined, an ensemble model provides a robust defense without tuning β (see yellow lines in Figure 1).

C Detailed experiment setup

Main experiments

The Cifar10 dataset [9] is a well-known image dataset consists of 10 classes images with the size of 32×32 pixels. The whole dataset can be found at https://www.cs.toronto.edu/~kriz/cifar.html. In our experiment, we use the whole 50,000 training set images for backdoor attack and the whole 10,000 testing-set images for defense. In the defense part, we randomly pick 80% images (8,000 images) to search the trigger's distribution using our algorithm. We use the remaining 20% images (2,000 images) to test our defense results. All of the accuracy results reported in the paper are evaluated on the testing set. Both the training set and the testing set are normalized to have zero mean and variance one. All the experiment are done using a single TITAN RTX GPU. The original Cifar10 model is a ResNet-18 model [21] build following https://github.com/kuangliu/pytorch-cifar's instruction and reaching 95.0% accuracy.

During attack, we use stochastic gradient descent (SGD) [23] with momentum = 0.9, $learning\ rate = 0.001$ [24]to fine-tune the original model 10 more epochs with $batch\ size = 128$ and $poison\ ratio = 0.01$ for all of the 51 triggers and generate 51 backdoored models.

The step by step defense experiment includes:

- 1) Search distribution. The generator is a three-layer perceptron with $input\ dimension=64$, $hidden\ layer=512$. A batch normalization layer and a Leaky ReLu layer ($negative\ slope=0.2$) are followed by both input layer and hidden layer. The input noise follows uniform distribution. The $output\ layer=27$ is used to generate a 3×3 pixels with 3 channels trigger's pattern. Together with Generator, we have a Statistic Network to estimate entropy. The Statistic Network has two inputs. One input is the output of Generator, the other input is a uniform distribution noise (keep same with the Generator's input distribution). Each of them goes through a linear layer and transforms to a vector with 512 dimensions. Then the Statistic Network adds them together (with bias), following by two linear layers ($512\times512,512\times1$), and generates an output. Each linear layer in Statistic Network follows with a leaky ReLu layer ($negative\ slope=0.2$). When searching the backdoor distribution, we always train our Generator and Statistic Network 50 epochs using Adam optimizer [25] with $learning\ rate=0.0002$.
- 2) Use our generator to defend the backdoor attack. We defend the backdoored model through retraining using the same parameter as we attack it (SGD, momentum = 0.9, $learning\ rate = 0.001$, $10\ epochs,\ batch\ size = 128$ and $poison\ ratio = 0.01$). We apply model ensemble defense using all of the three models with $\beta = 0.9, 0.8, 0.5$. During 10 rounds defense, we sample the three models 4, 3, 3, times respectively to generate 10 different triggers in total .
- 3) Compare with baseline and ideal case. Baseline follows pixel space optimization. The initial trigger's pattern is generated from uniform distribution. Using cross entropy loss, SGD optimizer, momentum = 0.9, $learning\ rate = 0.1$, we search the trigger's pattern for 5 epochs. For each backdoored model, we search 10 patterns totally and calculate their mean and standard deviation of defense performance as our baseline. The ideal case uses the original trigger's pattern to perform defense, so it does not require extra search parameters. The defence parameters for both baseline and ideal cases are the same as the parameters that are used in attack (SGD, momentum = 0.9, $learning\ rate = 0.001$, 10 epochs, $batch\ size = 128$ and $poison\ ratio = 0.01$).

When plotting Figure. 5, we sample 2000 points from our Generator, and using t-SNE provided by sckit-learn [26] (init='pca', random_state=0). When plotting Figure. 3, we sample 128 points from our Generator and using PCA provided by sckit-learn (decomposition.TruncatedSVD). The minimum distance is set to 6e-3 so as to prevent results from overlap.

Supplementary experiments To further test the performance of our method on a larger dataset, with different color triggers, and different target class, we keep the experimental environment as close to the previous one as possible. The differences between supplementary experiments and the main experiments are:

- Instead of always attacking class 0 on Cifar10, we randomly select 10 classes to attack on Cifar100
- Instead of using only black and white triggers, we generate 10 triggers with independent and uniform RGB colors on both Cifar10 and Cifar100
- Instead of setting the generator's $hidden\ layer=512$ on Cifar10, we set $hidden\ layer=2048$ on Cifar100.
- The original Cifar100 model is a ResNet-18 model build following https://github.com/weiaicunzai/pytorch-cifar100's instruction and reaching 76.23% accuracy.

We keep other settings unchanged.