LEARNING TO DEFENSE BY LEARNING TO ATTACK

Anonymous authors
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ABSTRACT

Adversarial training provides a principled approach for training robust neural networks. From an optimization perspective, the adversarial training is essentially solving a minimax robust optimization problem. The outer minimization is trying to learn a robust classifier, while the inner maximization is trying to generate adversarial samples. Unfortunately, such a minimax problem is very difficult to solve due to the lack of convex-concave structure. This work proposes a new adversarial training method based on a generic learning-to-learn (L2L) framework. Specifically, instead of applying the existing hand-designed algorithms for the inner problem, we learn an optimizer, which is parametrized as a convolutional neural network. At the same time, a robust classifier is learned to defense the adversarial attack generated by the learned optimizer. Our experiments over CIFAR-10 and CIFAR-100 datasets demonstrate that the L2L outperforms existing adversarial training methods in both classification accuracy and computational efficiency. Moreover, our L2L framework can be extended to the generative adversarial imitation learning and stabilize the training.

1 INTRODUCTION

This decade has witnessed great breakthroughs in deep learning in a variety of applications, such as computer vision (Taigman et al., 2014; Girshick et al., 2014; He et al., 2016; Liu et al., 2017). Recent studies (Szegedy et al., 2013), however, show that most of these deep learning models are very vulnerable to adversarial attacks. Specifically, by injecting a small perturbation to a normal sample, one can obtain an adversarial example. Although the adversarial example is semantically indistinguishable from the normal one, it can fool deep learning models and undermine the security of deep learning, causing reliability problems in autonomous driving, biometric authentication, etc.

Researchers have devoted many efforts to studying efficient adversarial attack and defense (Szegedy et al., 2013; Goodfellow et al., 2014b; Nguyen et al., 2015; Zheng et al., 2016; Madry et al., 2017; Carlini and Wagner, 2017). There is a growing body of work on generating adversarial examples, e.g., fast gradient sign method (FGSM, Goodfellow et al. (2014b)), projected gradient method (PGM, Kurakin et al. (2016)), Carlini-Wagner (CW, Paszke et al. (2017)) etc. As for defense, Goodfellow et al. (2014b) propose to robustify the network by adversarial training, which trains over the adversarial examples and still requires the network to output the correct label. Further, Madry et al. (2017) formalize the adversarial training as the following minimax optimization problem:

$$\min_{\boldsymbol{\theta}} \ \frac{1}{n}\sum_{i=1}^{n}\left[\max_{\boldsymbol{\delta}_i\in\mathcal{B}} \ell(f(\boldsymbol{x}_i+\boldsymbol{\delta}_i;\boldsymbol{\theta}), y_i)\right], \tag{1}$$

where $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \subset \mathbb{R}^d \times \mathcal{Y}$ are n pairs of input feature and the corresponding label, ℓ denotes a loss function, $f(\cdot;\boldsymbol{\theta})$ denotes the neural network with parameter $\boldsymbol{\theta}$, and $\boldsymbol{\delta}_i \in \mathcal{B}$ denotes the perturbation for x_i in constraint $\mathcal{B}$. The existing literature on the optimization also refers to $\boldsymbol{\theta}$ as the primal variable and $\boldsymbol{\delta}_i$'s as the dual variables. Different from the well-studied convex-concave problem[1], problem (1) is very challenging since ℓ is nonconvex in $\boldsymbol{\theta}$ and nonconcave in $\boldsymbol{\delta}$. As a result, they may be many equilibria, and majority of them are unstable. In the existing optimization literature, there is no algorithm to converge to a stable equilibrium with theoretical guarantees. Empirically, the existing primal-dual algorithms perform poorly for solving (1).

Minimax formulation (1) naturally provides us with a unified perspective on prior works of adversarial training. Such a minimax problem consists of two optimization problems, an inner maximization problem and an outer minimization problem: The inner problem targets on finding an optimal attack

[1]Loss function $\ell(\boldsymbol{\theta};\boldsymbol{\delta})$ is convex in primal variable $\boldsymbol{\theta}$ and concave in dual variable $\boldsymbol{\delta}$.

for a given data point $(\boldsymbol{x}, y)$ that maximizes the loss, which essentially is the adversarial attack; The outer problem aims to find a $\boldsymbol{\theta}$ so that the loss given by the inner problem is minimized.

For solving (1), Goodfellow et al. (2014b) propose to use FGSM to solve the inner problem. Kurakin et al. (2016) then find that FGSM with true label suffers from a "label leaking" effect, which can ruin the adversarial training. Madry et al. (2017) further suggest to solve the inner problem by PGM and obtain a better result than FGSM, since FGSM essentially is one iteration PGM. However, adversarial training needs to find a $\boldsymbol{\delta}_i$ for each $(\boldsymbol{x}_i, y_i)$, thus the dimension of the overall search space for all data is substantial, which makes the computation expensive.

Instead, we propose a new learning-to-learn (L2L) framework that provides a more principled and *efficient* way for adversarial training. Specifically, we parameterize the optimizer of the inner maximization problem by a neural network denoted by $g(\mathcal{A}(\boldsymbol{x}, y, \boldsymbol{\theta}); \boldsymbol{\phi})$, where $\mathcal{A}(\boldsymbol{x}, y, \boldsymbol{\theta})$ denotes the input of the optimizer g. We also call the optimizer as the attacker network. Since the neural network is very powerful in function approximation, our parameterization ensures that g is able to yield strong adversarial perturbations. Under our framework, instead of directly solving $\boldsymbol{\delta}_i$, we update the parameter $\boldsymbol{\phi}$ of g. Our training procedure becomes updating the parameters of two neural networks, which is very similar to Generative Adversarial Network (GAN, Goodfellow et al. (2014a)). The proposed L2L is a generic framework and can be applied to other minimax optimization problems, e.g., generative adversarial imitation learning, which is studied in Section 4.

Different from the hand-designed methods that compute the adversarial perturbation for each individual sample using gradients from backpropagation, our methods generate the perturbations for all samples through the shared attacker g. This enables g to learn potential common structures of the perturbations. Therefore, our method is capable of yielding strong perturbations and accelerating the training process. Furthermore, L2L framework is very *flexible*: we can either choose different input $\mathcal{A}(\boldsymbol{x}, y, \boldsymbol{\theta})$, or use different attacker architectures. For example, we can include gradient information in $\mathcal{A}(\boldsymbol{x}, y, \boldsymbol{\theta})$ and use a recurrent neural network (RNN) to mimic multi-step gradient-type methods. Instead of simply computing the high order information with finite difference approximation or multiple gradients, by parameterizing the algorithm as a neural network, our proposed methods can capture this information in a much smarter way (Finn et al., 2017). Our experiments demonstrate that our proposed methods not only *outperform* existing adversarial training methods, e.g., PGM training, but also enjoy the computational efficiency over CIFAR-10 and CIFAR-100 datasets (Krizhevsky and Hinton, 2009).

The research on L2L has a long history (Schmidhuber, 1987; 1992; 1993; Younger et al., 2001; Hochreiter et al., 2001; Andrychowicz et al., 2016). The basic idea is that one first models the updating formula of complicated optimization algorithms in a parametric form, and then uses some simple algorithms, e.g., stochastic gradient algorithm to learn the parameter of the optimizer. Among existing works, Hochreiter et al. (2001) propose a system allowing the output of backpropagation from one network to feed into an additional learning network, with both networks trained jointly; Based on this, Andrychowicz et al. (2016) further show that the design of an optimization algorithm can be cast as a learning problem. Specifically, they use long short-term memory RNNs to model the algorithm and allow the RNNs to exploit structure in the problems of interest in an automatic way, which is undoubtedly one of the most popular methods for learning-to-learn.

However, there are two major drawbacks of the existing L2L methods: **(1)** It requires a large amount of datasets (or a large number of tasks in multi-task learning) to guarantee the learned optimizer to generalize, which significantly limits their applicability (most of the related works only consider the image encoding as the motivating application); **(2)** The number of layers/iterations in RNN for modeling algorithms cannot be large to avoid significant computational burden in backpropagation.

Our contribution is that we fill the blank of the learning-to-learn framework in solving minimax problem, and our proposed methods do not suffer from the aforementioned drawbacks: **(1)** The attacker network g with a different $\boldsymbol{\phi}$ essentially generates a different task/dataset. Therefore, for adversarial training, we have sufficiently many tasks for learning-to-learn; **(2)** The inner problem does not need a large scale RNN, and we use a convolutional neural network (CNN) or a length-two RNN (sequence of length 2) as our attacker network, which eases the computation.

Our work is also related to GAN and dual-embedding (Goodfellow et al., 2014a; Dai et al., 2016). All solve minimax problems and share some common ground. We discuss these works in Section 5.

Notations. Given $a \in \mathbb{R}$, denote $(a)_+$ as $\max(a, 0)$. Given $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$, denote x_i as the i-th element of $\boldsymbol{x}$, $||\boldsymbol{x}||_\infty = \max_i |x_i|$ as ℓ_∞-norm of $\boldsymbol{x}$, and $\boldsymbol{x} \circ \boldsymbol{y} = [x_1 y_1, \cdots, x_d y_d]^\top$ as element-wise product.

2 METHOD

This paper focuses on ℓ_∞-norm attack. We define the ℓ_∞-ball with center $\mathbf{0}$ and radius ϵ by $\mathcal{B}(\epsilon) = \{\boldsymbol{\delta} \in \mathbb{R}^d : ||\boldsymbol{\delta}||_\infty \leq \epsilon\}$ and the corresponding projection as follows:

$$\Pi_{\mathcal{B}(\epsilon)}(\boldsymbol{\delta}) = \mathrm{sign}(\boldsymbol{\delta}) \circ \max(|\boldsymbol{\delta}|, \epsilon),$$

where sign and max are element-wise operators.

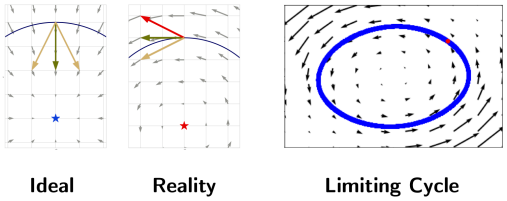


Figure 1: *Illustration for the hardness of problem* (1). *A wrong descent direction leads to a limiting cycle and algorithms fail to converge.*

2.1 ADVERSARIAL TRAINING

The goal of adversarial training is to robustify neural networks. Recall that from a robust optimization perspective, given n samples $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$, where x_i is the i-th feature vector and y_i is the corresponding label, adversarial training is reformulated as the following optimization problem (1):

$$\min_{\boldsymbol{\theta}} \ \frac{1}{n} \sum_{i=1}^n \left[\max_{\boldsymbol{\delta}_i \in \mathcal{B}} \ell(f(\boldsymbol{x}_i + \boldsymbol{\delta}_i; \boldsymbol{\theta}), y_i) \right],$$

where f denotes the network with parameter $\boldsymbol{\theta}$, ℓ denotes a loss function, and ϵ is maximum perturbation magnitude.

We first demonstrate the hardness of solving problem (1). Ideally, we want to obtain the optimal solution for the inner problem

$$\boldsymbol{\delta}_i^* := \mathrm{argmax}_{\boldsymbol{\delta}_i \in \mathcal{B}} \ell(f(\boldsymbol{x}_i + \boldsymbol{\delta}_i; \boldsymbol{\theta}), y_i).$$

However, note that the loss function $\ell(f(\boldsymbol{x}_i + \boldsymbol{\delta}_i; \boldsymbol{\theta}), y_i)$ is highly nonconcave in $\boldsymbol{\delta}_i$. Therefore, in reality the $\boldsymbol{\delta}_i$ we obtained is very unlikely to be the optimum $\boldsymbol{\delta}_i^*$. This then often leads to a highly unreliable or even completely wrong search direction, e.g.,

$$\langle \nabla_{\boldsymbol{\theta}} \ell(f(\boldsymbol{x}_i + \boldsymbol{\delta}_i; \boldsymbol{\theta}), y_i), \nabla_{\boldsymbol{\theta}} \ell(f(\boldsymbol{x}_i + \boldsymbol{\delta}_i^*; \boldsymbol{\theta}), y_i) \rangle < 0,$$

which may further results in a limiting cycle shown in Figure 1. This becomes even worse when sample noises exist.

In the existing literature, the standard pipeline of adversarial training is shown in Algorithm 1. Since the step of generating adversarial perturbation $\boldsymbol{\delta}_i$ in Algorithm 1 is intractable, most adversarial training methods adopt hand-designed algorithms. For example, Kurakin et al. (2016) propose to solve the inner problem approximately by first order methods such as PGM. Specifically, PGM iteratively updates the adversarial perturbation by projected sign gradient ascent method for each sample: Given one sample $(\boldsymbol{x}_i, y_i)$, at the t-th iteration, PGM takes

Algorithm 1 *Standard pipeline of adversarial training*

Input: $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$: clean data, α: learning rate, N: number of epochs, ϵ: maximum perturbation magnitude.
for $t \leftarrow 1$ *to* N **do**
  Sample a minibatch $\mathcal{M}_t$
  for i *in* $\mathcal{M}_t$ **do**
    $\boldsymbol{\delta}_i \leftarrow \mathrm{argmax}_{\boldsymbol{\delta}_i \in \mathcal{B}(\epsilon)} \ell(f(\boldsymbol{x}_i + \boldsymbol{\delta}_i; \boldsymbol{\theta}), y_i)$
    Generate adversarial perturbation for $(\boldsymbol{x}_i, y_i)$
  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \frac{1}{|\mathcal{M}_t|} \sum_{i \in \mathcal{M}_t} \nabla_{\boldsymbol{\theta}} \ell(f(\boldsymbol{x}_i + \boldsymbol{\delta}_i; \boldsymbol{\theta}), y_i)$
  Update $\boldsymbol{\theta}$ over adversarial data $\{(\boldsymbol{x}_i + \boldsymbol{\delta}_i, y_i)\}_{i \in \mathcal{M}_t}$

$$\boldsymbol{\delta}_i^t \leftarrow \Pi_{\mathcal{B}(\epsilon)} \left(\boldsymbol{\delta}_i^{t-1} + \eta \cdot \mathrm{sign} \left(\nabla_{\boldsymbol{x}} \ell(f(\widetilde{\boldsymbol{x}}_i^t; \boldsymbol{\theta}), y) \right) \right), \tag{2}$$

where $\widetilde{\boldsymbol{x}}_i^t = \boldsymbol{x}_i + \boldsymbol{\delta}_i^{t-1}$, η is the learning rate, T is a pre-defined total number of iterations, and $\boldsymbol{\delta}_i^0 = \mathbf{0}$, $t = 1, \cdots, T$. Finally PGM takes $\boldsymbol{\delta}_i = \boldsymbol{\delta}_i^T$. Note that FGSM essentially is one-iteration PGM. Besides, some works adopt other optimization methods, such as momentum gradient method (Dong et al., 2018), and L-BFGS (Tabacof and Valle, 2016). However, except for FGSM, all require numerous queries for gradients through backpropagation, which is computationally expensive.

2.2 LEARNING TO DEFENSE BY LEARNING TO ATTACK (L2L)

Since the objective function is nonconvex-nonconcave, there is no guarantee for hand-designed methods to perform well. Instead, we propose to learn an optimizer for the inner problem. Specifically, we parameterize the attacker by a Neural Network $g(\mathcal{A}(\boldsymbol{x}, y, \boldsymbol{\theta}); \boldsymbol{\phi})$, where $\mathcal{A}(\boldsymbol{x}, y, \boldsymbol{\theta})$, the input of the network g, summaries the information of data and neural network $f(\cdot; \boldsymbol{\theta})$. We then convert problem (1) to

$$\min_{\boldsymbol{\theta}} \frac{1}{n} \sum_{i=1}^{n} \left[\ell(f(\boldsymbol{x}_i + g(\mathcal{A}(\boldsymbol{x}_i, y_i, \boldsymbol{\theta}); \boldsymbol{\phi}^*); \boldsymbol{\theta}), y_i)\right], \tag{3}$$

where $\boldsymbol{\phi}^*$ is defined as the solution to the following optimization problem:

$$\boldsymbol{\phi}^* \in \operatorname*{argmax}_{\boldsymbol{\phi}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(\boldsymbol{x}_i + g(\mathcal{A}(\boldsymbol{x}_i, y_i, \boldsymbol{\theta}); \boldsymbol{\phi}); \boldsymbol{\theta}), y_i) \quad \text{subject to} \quad g(\mathcal{A}(\boldsymbol{x}, y, \boldsymbol{\theta}); \boldsymbol{\phi}) \in \mathcal{B}(\epsilon).$$

Solving problem (3) naturally consists of two stages. In the first stage, the classifier f aims to fit over all perturbed data; While in the second stage, given a certain f obtained in the first stage, the attacker network g targets on generating optimal perturbations under constraints $\boldsymbol{\delta}_i$'s $\in \mathcal{B}(\epsilon)$.

Since $\boldsymbol{\delta}_i = g(\mathcal{A}(\boldsymbol{x}_i, y_i; \boldsymbol{\theta}); \boldsymbol{\phi})$, constraints can be simply handled by a $\tanh$ activation function in the last layer of g. Specifically, because the magnitude of $\tanh$ output is bounded by 1, after we rescale the output by ϵ, the output of g automatically satisfies the constraints.

This framework is very flexible. We can choose $\mathcal{A}(\boldsymbol{x}, y, \boldsymbol{\theta})$ as the input and mimic multi-step gradient algorithms shown in Figure 2. Here we provide the following three examples:

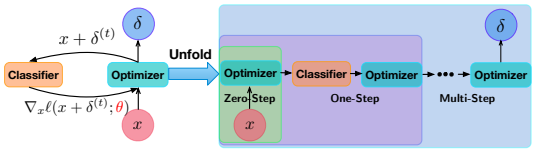


Figure 2: *An illustration of L2L. We learn a neural network to model the algorithm for generating adversarial attack.*

Naive Attacker Network. This is the simplest example among our methods, taking the original image $\boldsymbol{x}_i$ as the input, i.e.,

$$\mathcal{A}(\boldsymbol{x}_i, y_i, \boldsymbol{\theta}) = \boldsymbol{x}_i \quad \text{and} \quad \boldsymbol{\delta}_i = g(\boldsymbol{x}_i; \boldsymbol{\phi}).$$

Under this setting, L2L training is similar to GAN training. The major difference is that the generator in GAN yields synthetic data by transforming random noises, while the naive attacker network generates perturbations by transforming training samples.

Gradient Attacker Network. Motivated by hand-designed methods, e.g., FGSM, we design an attacker which takes the gradient information into computation. Specifically, we concatenate image $\boldsymbol{x}_i$ and gradient $\nabla_{\boldsymbol{x}} \ell(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$ from backpropagation as the input of g, i.e.,

$$\mathcal{A}(\boldsymbol{x}_i, y_i, \boldsymbol{\theta}) = \left[\boldsymbol{x}_i, \nabla_{\boldsymbol{x}} \ell(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)\right]$$
$$\text{and} \quad \boldsymbol{\delta}_i = g\big(\boldsymbol{x}_i, \nabla_{\boldsymbol{x}} \ell(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i); \boldsymbol{\phi}\big).$$

Since more information is provided, we expect the attacker network to be more efficient to learn and yield more powerful perturbations.

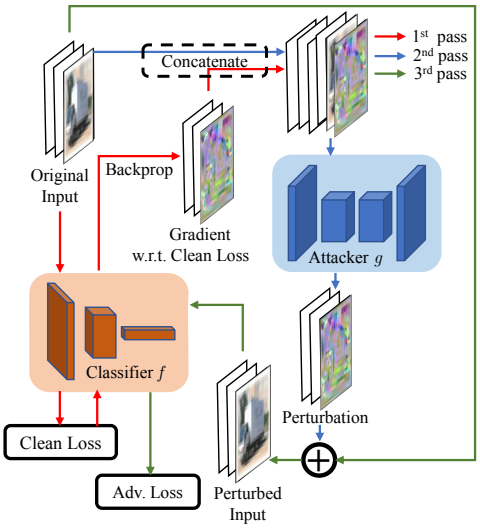


Figure 3: *The architecture of L2L adversarial training with gradient attacker network.*

Multi-Step Gradient Attacker Network. We adapt the RNN to mimic a multi-step gradient update. Specifically, we use the gradient attacker network as the cell of RNN sharing the same parameter $\boldsymbol{\phi}$. As we mentioned earlier, the number of layers/iterations in the RNN for modeling algorithms cannot be very large so as to avoid significant computational burden in backpropagation. In this paper, we focus on a length-two RNN to mimic a two-step gradient update. The corresponding perturbation becomes:

$$\boldsymbol{\delta}_i = \Pi_{\mathcal{B}(\epsilon)}\big(\boldsymbol{\delta}_i^{(0)} + g\big(\widetilde{\boldsymbol{x}}_i, \nabla_{\boldsymbol{x}} \ell(f(\widetilde{\boldsymbol{x}}_i, y_i; \boldsymbol{\theta}); \boldsymbol{\phi})\big)\big),$$

where $\widetilde{\boldsymbol{x}}_i = \boldsymbol{x}_i + \boldsymbol{\delta}_i^{(0)}$ and $\boldsymbol{\delta}_i^{(0)} = g\big(\boldsymbol{x}_i, \nabla_{\boldsymbol{x}} \ell(f(\boldsymbol{x}_i, y_i; \boldsymbol{\theta}); \boldsymbol{\phi}\big)$.

Taking gradient attacker network as an example, Figure 3 illustrates how L2L works and jointly trains two networks: The first forward pass is used to obtain gradient of the classification loss over clean data; The second forward pass is used to generate perturbation $\boldsymbol{\delta}_i$ by attacker g; The third forward pass is used to calculate the adversarial loss ℓ in (3). Since our gradient attacker network only needs one backpropagation to query gradient, it amortizes the adversarial training cost, which leads to better computational efficiency. Moreover, L2L may adapt to the underlying optimization problem and yield better solution for the inner problem. The corresponding procedure of L2L is shown in Algorithm 2.

Algorithm 2 *Learning-to-learn-based adversarial training with gradient attacker network*

Input: $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$: clean data, α_1, α_2: learning rates, N: number of epochs, ϵ: maximum perturbation magnitude.
for $t \leftarrow 1$ *to* N **do**
  Sample a minibatch $\mathcal{M}_t$
  for i *in* $\mathcal{M}_t$ **do**
    $\boldsymbol{u}_i \leftarrow \nabla_{\boldsymbol{x}} \ell(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$
    $\boldsymbol{\delta}_i \leftarrow g(\boldsymbol{x}_i, \boldsymbol{u}_i; \boldsymbol{\phi})$
    Generate perturbation by g
  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha_1 \frac{1}{|\mathcal{M}_t|} \sum_{i \in \mathcal{M}_t} \nabla_{\boldsymbol{\theta}} \ell(f(\boldsymbol{x}_i + \boldsymbol{\delta}_i; \boldsymbol{\theta}), y_i)$
  Update $\boldsymbol{\theta}$ over adversarial data $\{(\boldsymbol{x}_i + \boldsymbol{\delta}_i, y_i)\}_{i \in \mathcal{M}_t}$
  $\boldsymbol{\phi} \leftarrow \boldsymbol{\phi} + \alpha_2 \frac{1}{|\mathcal{M}_t|} \sum_{i \in \mathcal{M}_t} \nabla_{\boldsymbol{\phi}} \ell(f(\boldsymbol{x}_i + \boldsymbol{\delta}_i \boldsymbol{\theta}), y_i)$
  Update $\boldsymbol{\phi}$ over adversarial data $\{(\boldsymbol{x}_i + \boldsymbol{\delta}_i, y_i)\}_{i \in \mathcal{M}_t}$

3 EXPERIMENTS

To demonstrate the effectiveness and computational efficiency of our methods, we compare our methods with PGM training over CIFAR-10 and CIFAR-100 datasets. All experiments are done in PyTorch with one NVIDIA 2080 Ti GPU.

For simplicity, we denote Plain Net as the classifier network trained over clean data only, PGM Net as the classifiers with PGM training, and Naive L2L, Grad L2L, and 2-Step L2L as classifiers using L2L training with corresponding attacker networks.

Classifier Network. All experiments adopt a 34-layer wide residual network (WRN-34-10, Zagoruyko and Komodakis (2016)) implemented by Zhang et al. (2019) as the classifier network. For each method, we train the classifier network from scratch. For Plain Nets, we adapt the same training procedure as Zagoruyko and Komodakis (2016). We use cross entropy as the loss function.

Attacker Network. Table 1 presents the architecture of our attacker network[2]. The ResBlocks use the same structure as the generator proposed in Miyato et al. (2018). The detailed structure of ResBlocks is provided in Appendix B. Batch normalization (BN) and activations, e.g., ReLU and $\tanh$, are applied when specified. The $\tanh$ function easily makes the output of attacker satisfy the constraints.

Table 1: *Attacker network architecture: k, c, s, p denote the kernel size, output channels, stride and padding parameters of convolutional layers, respectively.*

Conv:	$[k = 3 \times 3, c = 64, s = 1, p = 1]$, BN+ReLU
ResBlock:	$[k = 3 \times 3, c = 128, s = 1, p = 1]$
ResBlock:	$[k = 3 \times 3, c = 256, s = 1, p = 1]$
ResBlock:	$[k = 3 \times 3, c = 128, s = 1, p = 1]$
Conv:	$[k = 3 \times 3, c = 3, s = 1, p = 1]$, $\tanh$

White-box and Black-box. We compare different methods under both white-box and black-box settings. Under the white-box setting, attackers can access all parameters of target models and generate adversarial examples based on the models; whereas under the black-box setting, accessing parameters is prohibited. Therefore, we adopt the standard transfer attack method from Liu et al. (2016). Due to the space limit, we leave results of the black-box setting in Appendix A.

Robust Evaluation. We evaluate the robustness of the networks by PGM, CW, and 2-Step L2L attacker with the maximum perturbation magnitude $\epsilon = 0.03$ (after rescaling the pixels to $[0, 1]$) over CIFAR-10 and CIFAR-100. For PGM attack, we use 20, 40, and 100-iteration PGM with a perturbation step size $\eta = 0.003$. For CW attack, we adopt the implementation from Paszke et al. (2017), and the maximum number of iterations as 100. For each method, we repeat 5 runs with different random initial seeds and report the *worst result*.

L2L. To update classifier's parameter $\boldsymbol{\theta}$, we use the SGD algorithm with Polyak's momentum (parameter 0.9, Liu et al. (2018)) and weight decay (parameter 2×10^{-4}, Krogh and Hertz (1992)); To

[2]We provide another architecture in the Appendix B.

update the attacker's parameter ϕ, we use the Adam optimizer (parameter $[0.9, 0.999]$, Kingma and Ba (2014)) and weight decay (parameter 2×10^{-4}) so that it adaptively balances the inner and outer optimization. In addition, we train the whole network for 100 epochs and set the initial learning rate for SGD as 0.1, the learning rate decay parameter as 0.1 with decay schedule [30,60,90], and the initial learning rate for Adam optimizer as 0.001 without learning rate decay.

PGM Adversarial Training. For CIFAR-10, we directly report the result from Madry et al. (2017) as the baseline; For CIFAR-100, we train a PGM Net as a baseline. To update the parameter $\boldsymbol{\theta}$, we use the same configuration of SGD algorithm in L2L. Moreover, we adopt the setting from Madry et al. (2017), that is, we first use 10-iteration PGM with the perturbation step size 0.007 in (2) to generate the adversarial samples, and then train the PGM Net over these samples.

Table 2: Results of different defense methods under white-box setting.

Defense Method	Attack	Dataset	Clean Accuracy	Robust Accuracy
Zheng et al. (2016)	PGM-20	CIFAR10	94.64%	0.15%
Kurakin et al. (2016)	PGM-20	CIFAR10	85.25%	45.89%
Madry et al. (2017)	PGM-20	CIFAR10	87.30%	47.04%
Naive L2L	PGM-20	CIFAR10	94.53%	0.01%
Grad L2L	PGM-20	CIFAR10	85.84%	51.17%
2-Step L2L	PGM-20	CIFAR10	85.35%	54.32%
Grad L2L	PGM-100	CIFAR10	85.84%	47.72%
2-Step L2L	PGM-100	CIFAR10	85.35%	52.12%
Grad L2L	CW	CIFAR10	85.84%	53.5%
2-Step L2L	CW	CIFAR10	85.35%	57.07%
PGM Net	PGM-20	CIFAR100	62.68%	23.75%
Grad L2L	PGM-20	CIFAR100	62.18%	28.67%
2-Step L2L	PGM-20	CIFAR100	60.95%	31.03%
PGM Net	PGM-100	CIFAR100	62.68%	22.06%
Grad L2L	PGM-100	CIFAR100	62.18%	26.69%
2-Step L2L	PGM-100	CIFAR100	60.95	29.75%
PGM Net	CW	CIFAR100	62.68%	25.95%
Grad L2L	CW	CIFAR100	62.18%	29.65%
2-Step L2L	CW	CIFAR100	60.95%	32.28%

Table 3: *Running time for one epoch over CIFAR-10 (1st Row) and CIFAR-100 (2nd Row). (Unit: s)*

Plain Net	PGM Net	Naive L2L	Grad L2L	2-Step L2L
106.5 ± 1.5	1310.8 ± 14.2	293.7 ± 3.1	617.5 ± 6.1	805.1 ± 8.1
106.9 ± 1.4	1354.8 ± 14.1	310.0 ± 2.9	623.1 ± 6.3	824.7 ± 8.4

Experiment Results. Table 2 shows the results of all methods over CIFAR-10 and CIFAR-100 under the white-box setting. As can be seen, without gradient information, Naive L2L is vulnerable to the PGM attacks. However, when the attacker utilizes the gradient information, Grad L2L and 2-Step L2L *significantly outperform* the PGM Net over CIFAR-10 and CIFAR-100, with a small loss for the clean accuracy. In addition, Table 3 shows the one epoch running time of all methods over CIFAR-10 and CIFAR-100. As can be seen, Grad L2L and 2-Step L2L is much faster than PGM Net. By further comparing the accuracy of Grad/2-Step L2L and PGM Net in Table 2, we find that L2L enjoys computational efficiency. In addition, Figure 4 presents the robust accuracy against the number of iterations (fixed perturbation magnitude $\epsilon = 0.031$) and the perturbation magnitude (fixed number of iterations $T = 10$). As can be seen, 2-Step L2L is much more robust than the PGM Net.

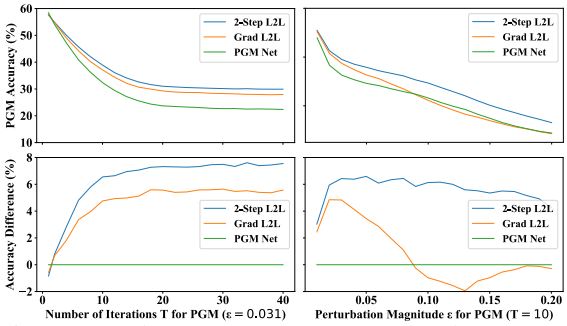
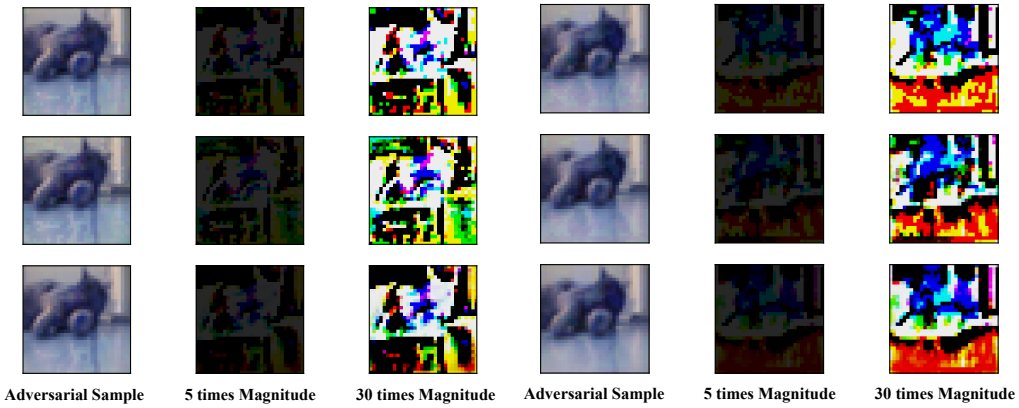


Figure 4: *Robust accuracy against perturbation magnitudes and number of iterations of PGM over CIFAR-100. Top two figures show the absolute accuracy over adversarial samples; the bottom two show the difference accuracy (PGM Net as baseline).*

Visualization of Adversarial Examples. Figure 5 provides an illustrative example of the adversarial perturbations generated by FGSM, PGM-20 and 2-Step L2L attacker for a *cat* over CIFAR-10.

As can be seen, the attacks for these two networks are very different. Moreover, the perturbation generated by the 2-Step L2L attacker is much more smooth than the FGSM and PGM. In this example, 2-Step L2L labels all adversarial samples correctly; whereas the PGM Net is fooled by the PGM-20 attack and misclassifies it as a *dog*.



(a) Adversarial samples from 2-Step L2L. (b) Adversarial samples from PGM Net.

Figure 5: *An illustrative examples of FGSM (Top), PGM-20 (Mid), and 2-Step L2L (Bottom) perturbations for a cat under PGM Net, and 2-Step L2L with perturbation magnitude* 0.031.

4 Extension: Generative Adversarial Imitation Learning

Our proposed L2L is a *generic* framework and can be applied to a *broad* class of minimax optimization problems. Here, we investigate the generative adversarial imitation learning (GAIL, Ho and Ermon (2016)). GAIL aims to learn a policy from expert's behavior, by recovering the expert's cost function and extracting a policy from the recovered cost function, which can also be formulated as a minimax optimization problem. We then show that under L2L framework, we stabilize the GAIL training by replacing the inner optimizer with a neural network.

Original GAIL. GAIL solves the following minimax optimization problem:

$$\min_{\theta_\pi} \max_{\theta_{\mathrm{D}}} \mathbb{E}_{(s,a)\sim\pi(s;\theta_\pi)}[\log(D(s,a;\theta_{\mathrm{D}}))] + \mathbb{E}_{(\widetilde{s},\widetilde{a})\sim\pi_{\mathrm{E}}}[\log(1-D(\widetilde{s},\widetilde{a};\theta_{\mathrm{D}}))] - \lambda H(\pi), \tag{4}$$

where $\pi(\cdot;\theta_\pi)$ is the trained policy parameterized by θ_π, π_{E} denotes the expert policy, π_{E}, $D(\cdot,\cdot;\theta_{\mathrm{D}})$ is the discriminator parameterized by θ_{D}, $\lambda H(\pi)$ denotes a entropy regularizer with tuning parameter λ, (s,a) and $(\widetilde{s},\widetilde{a})$ denote the state-action for the trained policy and expert policy, respectively. By optimizing 4, the discriminator D distinguishes the state-action (s,a) generated from the learned policy π with the sampled trajectories $(\widetilde{s},\widetilde{a})$ generated from some expert policy π_E. In the original GAIL training, for each iteration, we update the parameter of D, θ_{D}, by stochastic gradient ascend and then update θ_π by the trust region policy optimization (TRPO, Schulman et al. (2015)).

GAIL with L2L. Similar to the adversarial training with L2L, we apply our L2L framework to GAIL by parameterizing the inner optimizer as a neural network $U(;\theta_{\mathrm{U}})$ with parameter θ_{U}. Its input contains two parts: parameter θ_{D} and the gradient of loss function with respect to θ_{D}:

$$g_{\mathrm{D}}(\theta_{\mathrm{D}},\theta_\pi) = \mathbb{E}_{s,a\sim\pi(s;\theta_\pi)}[\nabla_{\theta_{\mathrm{D}}}\log(D(s,a;\theta_{\mathrm{D}}))] + \mathbb{E}_{\widetilde{s},\widetilde{a}\sim\pi_E}[\nabla_{\theta_{\mathrm{D}}}\log(1-D(\widetilde{s},\widetilde{a};\theta_{\mathrm{D}}))].$$

In practice, we use a minibatch (several sample trajectories) to estimate $g_{\mathrm{D}}(\theta_{\mathrm{D}},\theta_\pi)$, denoted as $\widehat{g}_{\mathrm{D}}(\theta_{\mathrm{D}},\theta_\pi)$. Specifically, at the t-th iteration, we first calculate $\widehat{g}_{\mathrm{D}}^t = \widehat{g}_{\mathrm{D}}(\theta_{\mathrm{D}}^t,\theta_\pi^t)$ and then update $\theta_{\mathrm{D}}^{t+1} = U(\theta_{\mathrm{D}}^t,\widehat{g}_{\mathrm{D}}^t;\theta_{\mathrm{U}}^t)$. Next, we update θ_{U} by gradient ascend based on the sample estimate of

$$\mathbb{E}_{s,a\sim\pi(s;\theta_\pi^t)}[\nabla_{\theta_{\mathrm{U}}}\log(D(s,a;U(\theta_{\mathrm{D}}^t,\widehat{g}_{\mathrm{D}}^t;\theta_{\mathrm{U}}^t)))] + \mathbb{E}_{\widetilde{s},\widetilde{a}\sim\pi_{\mathrm{E}}}[\nabla_{\theta_{\mathrm{U}}}\log(1-D(\widetilde{s},\widetilde{a};U(\theta_{\mathrm{D}}^t,\widehat{g}_{\mathrm{D}}^t;\theta_{\mathrm{U}}^t)))].$$

The detailed algorithm is presented in Appendix C.

Experiments. We compare the performance between the original GAIL and GAIL with L2L on two simulated environments: CartPole and Mountain Car (Brockman et al., 2016). As can be seen in Figure 6, we find that GAIL has a sudden performance drop after training for a long time. We

conjecture that is because the discriminator overfits the expert trajectories and converges to a bad optimum, which is not generalizable. On the other hand, GAIL with L2L is much more stable. It is very important to real applications of GAIL, since in real-world environment the actual reward is often not accessible. If we simply train GAIL for a long time, it may converge to the bad optima. We, however, have no clue whether there is a sudden performance drop. With the help of L2L, we can stabilize the training and obtain a much more reliable algorithm for real-world applications.

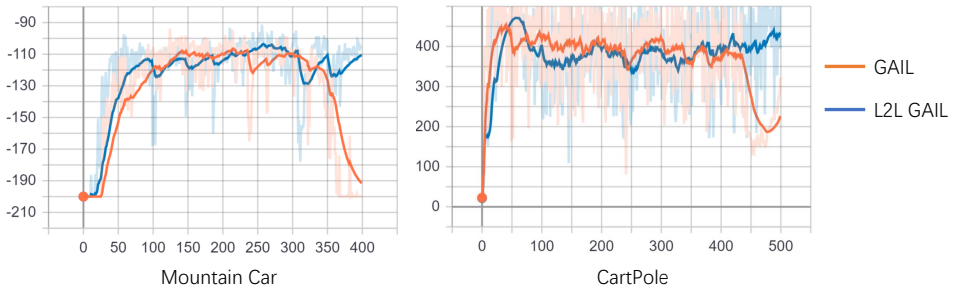


Figure 6: *Reward vs. iteration of the trained policy using original GAIL and L2L GAIL.*

5 Discussions

We emphasize the benefits of our L2L approach and discuss several closely related works.

Benefits of our neural network approach in adversarial training: **(1)** Since the neural network has been known to be powerful in function approximation, Our attacker network g can yield strong adversarial perturbations. Since they are generated by the same attacker, the attacker g essentially learns some common structures across all samples; **(2)** The attacker networks in our experiments are actually *overparametrized*, which has been conjectured to ease the training of deep neural networks. We believe that similar phenomena happen to our attacker network, and ease the adversarial training.

Closely related works:

• By leveraging the Fenchel duality and feature embedding technique, Dai et al. (2016) convert a learning conditional distribution problem to a minimax problem , which is similar to naive attacker network. Both approaches, however, lack the primal information. In contrast, gradient attacker network considers the gradient information of primal variables, and achieves good results.

• Goodfellow et al. (2014a) propose the GAN, which is very similar to our L2L framework. Both GAN and L2L contain one generator network and one classifier network, and jointly train these two networks. There are two major difference between GAN and our framework: (1) GAN aims to transform the random noises to the synthetic data which is similar to the training examples, while ours targets on transforming the training examples to the adversarial examples for robustifying the classifier; (2) Our generator network does not only take the training examples (analogous to the random noise in GAN) as the input, but also exploits the gradient information of the objective function, since it essentially represents an optimization algorithm. The training procedure of these two, however, are quite similar. We adopt some tricks from GAN training to our framework to stabilize the training process. For example, in Grad L2L training over SVHN, we adopt the two-time scale trick (Heusel et al., 2017).

• There are some other works simply combining the GAN framework and adversarial training together. For example, Baluja and Fischer (2017) and Xiao et al. (2018) propose some ad hoc GAN-based methods to robustify neural networks. Specifically, for generating adversarial examples, they only take training examples as the input of the generator, which lacks the information of the outer mimnimization problem. Instead, our proposed L2L methods (e.g., Grad L2L, 2-step L2L) connect outer and inner problems by delivering the gradient information of the objective function to the generator. This is a very important reason for our performance gain on the benchmark datasets. As a result, the aforementioned GAN-based methods are only robust to simple attacks, e.g., FGSM, on simple data sets, e.g., MNIST, but fail for strong attacks, e.g., PGM and CW, on complicated data sets, e.g. CIFAR, where our L2L methods achieve significantly better performance.

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Appendix

A BLACK-BOX ATTACK

Under the black-box setting, we first train a surrogate model with the same architecture of the target model but a different random seed, and then attackers generate adversarial examples to attack the target model by querying gradients from the surrogate model.

The black-box attack highly relies on the transferability, which is the property that the adversarial examples of one model are likely to fool others. However, the transferred attack is very unstable, and often has a large variation in its effectiveness. Therefore, results of the black-box setting might not be reliable and effective. Thus we only present one result here to demonstrate the robustness of different models.

Table 4: *Results of the black-box setting over CIFAR-10. We evaluate L2L methods with slim attacker networks.*

Surrogate	Plain Net		FGSM Net		PGM Net	
	FGSM	PGM10	FGSM	PGM10	FGSM	PGM10
Plain Net	40.03	5.60	74.42	75.25	67.37	65.92
FGSM Net	79.20	85.02	**89.90**	80.40	64.28	63.89
PGM Net	83.80	84.73	84.33	85.29	67.05	65.54
Naive L2L	45.52	25.95	83.99	77.94	68.14	67.13
Grad L2L	**86.10**	86.87	87.93	**88.01**	**71.15**	**69.95**
2-Step L2L	85.83	**87.10**	86.51	87.60	70.58	69.38

Table 5: Experiments under the black-box setting over CIFAR-100. Note that here we only evaluate L2L methods using the slim attacker network.

Surrogate	Plain Net		FGSM Net		PGM Net	
	FGSM	PGM10	FGSM	PGM10	FGSM	PGM10
Plain Net	21.04	9.04	50.57	54.06	40.06	41.30
FGSM Net	42.87	50.73	**61.68**	44.70	39.34	40.08
PGM Net	56.63	58.34	56.99	57.97	40.19	39.87
Naive L2L	20.97	10.47	50.36	54.07	38.63	39.91
Grad L2L	57.63	59.62	59.18	**61.26**	41.71	41.15
2-Step L2L	**58.66**	**59.31**	58.92	59.46	**45.80**	**45.31**

Table 6: Experiments under the black-box setting on SVHN. Note that here we only evaluate L2L methods using the wide attacker network.

Surrogate	Plain Net		FGSM Net		PGM Net	
	FGSM	PGM10	FGSM	PGM10	FGSM	PGM10
Plain Net	21.72	6.94	41.81	33.13	56.77	49.41
FGSM Net	57.36	51.54	56.25	38.11	55.99	48.96
PGM Net	**81.04**	**81.52**	**78.66**	80.42	54.85	49.21
Naive L2L	73.02	42.14	78.11	59.79	**85.31**	**61.08**
Grad L2L	71.74	74.31	77.19	80.70	71.99	58.71
2-Step L2L	65.78	74.07	76.13	**82.80**	61.69	54.13

B SLIM NETWORK

Table 7 presents the other architecture we used in the L2L. In this network, the second convolutional layer uses downsampling, while the second last deconvolutional layer uses upsampling. Therefore, this network is computationally cheap, due to the downsampling. However, it loses some information of input. Inspired by residual learning in He et al. (2016), we use a skip layer connection to ease the training of this network. Specifically, the last layer takes the concatenation of $\mathcal{A}(\boldsymbol{x}, y, \boldsymbol{\theta})$ and the output of the second last layer as input.

Table 7: *Attacker Network Architecture.*

Conv:	$[k = 3 \times 3, c = 128, s = 1, p = 1]$, BN+ReLU
ResBlocks:	[channel = 256]
ResBlocks:	[channel = 128], BN
DeConv:	$[k = 4 \times 4, c = 16, s = 2, p = 1]$, BN+ReLU
Conv:	$[k = 3 \times 3, c = 3, s = 1, p = 1]$, tanh

Figure 7 presents the architecture of ResBlocks. PReLU is a special type of Leaky ReLU with a learnable slope parameter.

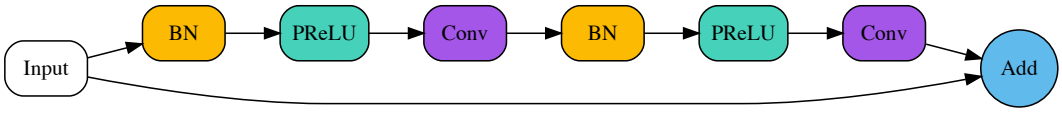

Figure 7: *An illustration example for the architecture of ResBlocks.*

Table 8 shows the results of L2L with the architecture shown in Table 7.

Table 8: *Results of L2L with the other attacker network under white-box setting over CIFAR.*

	CIFAR-10				**CIFAR-100**			
	Clean	FGSM	PGM10	CW	Clean	FGSM	PGM10	CW
Naive L2L	94.41	28.44	0.01	0.00	75.27	8.47	0.05	0.00
Grad L2L	85.31	57.44	53.42	42.72	60.60	26.58	27.77	23.14
2-Step L2L	75.36	60.19	46.42	40.82	60.23	25.92	20.63	22.70

C GENERATIVE ADVERSARIAL IMITATION LEARNING

C.1 ALGORITHMS

Algorithm 3 *Learning-to-learn-based generative adversarial imitation learning*

Input: Expert trajectories $(\widetilde{s}, \widetilde{a} \sim \pi_E(\widetilde{s}))$, initial policy, discriminator and updater parameters $\theta_\pi, \theta_{\mathrm{D}}, \theta_{\mathrm{U}}$.

for $t \leftarrow 1$ *to* N **do**

Sample trajectories $(s, a \sim \pi(a; \theta_\pi))$

Compute gradient:

$g_{\mathrm{D}}^t \leftarrow \frac{1}{|(s,a)|} \sum_{(s,a)} [\nabla_{\theta_{\mathrm{D}}} \log(D(s, a; \theta_{\mathrm{D}}^t))] + \frac{1}{|(\widetilde{s},\widetilde{a})|} \sum_{(\widetilde{s},\widetilde{a})} [\nabla_{\theta_{\mathrm{D}}} \log(1 - D(\widetilde{s}, \widetilde{a}; \theta_{\mathrm{D}}^t))]$

Update the discriminator parameters:

$\theta_{\mathrm{D}}^{t+1} = U(\theta_{\mathrm{D}}^t, g_{\mathrm{D}}^t; \theta_{\mathrm{U}}^t)$.

Update the updater parameters θ_{U} by minimizing:

$\frac{1}{|(s,a)|} \sum_{(s,a)} [\log(D(s, a; U(\theta_{\mathrm{D}}^t, g_{\mathrm{D}}^t; \theta_{\mathrm{U}}^t)))] + \frac{1}{|(\widetilde{s},\widetilde{a})|} \sum_{(\widetilde{s},\widetilde{a})} [\log(1 - D(\widetilde{s}, \widetilde{a}; U(\theta_{\mathrm{D}}^t, g_{\mathrm{D}}^t; \theta_{\mathrm{U}}^t)))]$.

Update the policy parameters θ_π by a policy step using the TRPO rule (Ho and Ermon (2016))

C.2 EXPERIMENT SETTING

Updater Architecture We use simple 3-layer perceptron with a skip layer as our updater. The number hidden units are ($2m \to 8m \to 4m \to m$), where m is the dimension of θ_{D} that depends on the original task. For the first and the second layer, we use PReLu as the activation function, while the last layer has no activation function. Finally we add the output to θ_{D} in the original input as the updated parameter for the discriminator network.

Hyperparameter Settings For all baselines we exactly follows the setting in Ho and Ermon (2016), except that we use a 2-layer discriminator with number of hidden units ($(s, a) \to 64 \to 32 \to 1$) using tanh as the activation. We use the same neural network architecture for π and the same optimizer configuration. The expert trajectories are obtained by an expert trained using TRPO. For L2L based GAIL, we also use Adam optimizer to update the θ_{U} with the same configuration as updating θ_{D} in original GAIL.