Adversarial Purification with the Manifold Hypothesis

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Abstract

In this work, we formulate a novel framework for adversarial robustness using the manifold hypothesis. This framework provides sufficient conditions for defending against adversarial examples. We develop an adversarial purification method with this framework. Our method combines manifold learning with variational inference to provide adversarial robustness without the need for expensive adversarial training. Experimentally, our approach can provide adversarial robustness even if attackers are aware of the existence of the defense. In addition, our method can also serve as a test-time defense mechanism for variational autoencoders. Code is available at: https://github.com/GoL2022/AdvPFY.

Introduction

State-of-the-art neural network models are known to be vulnerable to adversarial examples. With small perturbations, adversarial examples can completely change predictions of neural networks (Szegedy et al. 2014). Defense methods are then designed to produce robust models towards adversarial attacks. Common defense methods for adversarial attacks include adversarial training (Madry et al. 2018), certified robustness (Wong and Kolter 2018), etc. Recently, adversarial purification has drawn increasing attention (Croce et al. 2022), which purifies adversarial examples during test time and thus requires fewer training resources.

Existing adversarial purification methods achieve superior performance when attackers are not aware of the existence of the defense; however, their performance drops significantly when attackers create defense-aware or adaptive attacks (Croce et al. 2022). Besides, most of them are empirical with limited theoretical justifications. Differently, we adapt ideas from the certified robustness and build an adversarial purification method with a theoretical foundation.

Specifically, our adversarial purification method is based on the assumption that high-dimensional images lie on low-dimensional manifolds (the manifold hypothesis). Compared with low-dimensional data, high-dimensional data are more vulnerable to adversarial examples (Goodfellow, Shlens, and Szegedy 2015). Thus, we transform the adversarial robustness problem from a high-dimensional image domain to a low-dimensional image manifold domain.

Related Work

Adversarial Training. Adversarial training is one of the most effective adversarial defense methods which incorporates adversarial examples into the training set (Goodfellow, Shlens, and Szegedy 2015; Madry et al. 2018). Such a
method could degrade classification accuracy on clean data (Tsipras et al. 2019; Pang et al. 2022). To reduce the degradation in clean classification accuracy, TRADES (Zhang et al. 2019) is proposed to balance the trade-off between clean and robust accuracy. Recent works also study the effects of different hyperparameters (Pang et al. 2021; Huang et al. 2022a; Rice, Wong, and Kolter 2020) and data augmentation (Rebuffi et al. 2021; Sehwag et al. 2022; Zhao et al. 2020) to reduce robust overfitting and avoid the decrease of model’s robust accuracy. Besides the standard adversarial training, others also study the adversarial training on manifolds (Stutz, Hein, and Schiele 2019; Lin et al. 2020; Zhou, Liang, and Chen 2020; Patel et al. 2020). In this work, we introduce a novel defense without adversarial training.

### Adversarial Purification and Test-time Defense

As an alternative to adversarial training, adversarial purification aims to shift adversarial examples back to the representations of clean examples. Some efforts perform adversarial purification using GAN-based models (Samangouei, Kabbab, and Chellappa 2018), energy-based models (Grathwohl et al. 2020; Yoon, Hwang, and Lee 2021; Hill, Mitchell, and Zhu 2021), autoencoders (Hwang et al. 2019; Yin, Zhang, and Zuo 2022; Willetts et al. 2021; Gong et al. 2022; Meng and Chen 2017), augmentations, self-supervised learning (Pérez et al. 2021; Shi, Holtz, and Mitchell 2021; Ma et al. 2021), PixelCNN (Song et al. 2018) etc. Prior efforts (Athalye, Carlini, and Wagner 2018; Croce et al. 2022) have shown that methods such as Defense-GAN, PixelDefend (PixelCNN), SOAP (self-supervised), autoencoder-based purification are vulnerable to the Backward Pass Differentiable Approximation (BPDA) attacks (Athalye, Carlini, and Wagner 2018). Recently, diffusion-based adversarial purification methods have been studied (Nie et al. 2022; Xiao et al. 2022) and show adversarial robustness against adaptive attacks such as BPDA. Lee and Kim (2023), however, observe that the robustness of diffusion-based purification drops significantly when evaluated with the surrogate gradient designed for diffusion models. Similar to adversarial purification, existing test-time defense techniques (Nayak, Rawal, and Chakraborty 2022; Huang et al. 2022b) are also vulnerable to adaptive white-box attacks. In this work, we present a novel defense combining manifold learning and variational inference which achieves better performance compared with prior works and greater robustness on adaptive white-box attacks.

### Methodology

In this section, we introduce an adversarial purification method with the manifold hypothesis. We first define sufficient conditions (in theory) to quantify the robustness of predictions. Then, we use variational inference to approximate such conditions in implementation and achieve adversarial robustness without adversarial training.

Let $D_{XY}$ be a set of clean images and their labels where each image-label pair is defined as $(x, y)$. The manifold hypothesis states that many real-world high-dimensional data $x \in \mathbb{R}^n$ lies on a low-dimensional manifold $M$ diffeomorphic to $\mathbb{R}^m$ with $m \ll n$. We define an encoder function $f : \mathbb{R}^n \to \mathbb{R}^m$ and a decoder function $f^\dagger : \mathbb{R}^m \to \mathbb{R}^n$ to form an autoencoder, where $f$ maps data point $x \in \mathbb{R}^n$ to point $f(x) \in \mathbb{R}^m$. For $x \in M$, $f^\dagger$ and $f$ are approximate inverses. See Yang et al. (2023) for notation details.

### Problem Formulation

Let $L = \{1, \ldots, c\}$ be a discrete label set of $c$ classes and $h : \mathbb{R}^m \to L$ be a classifier of the latent space. Given an image-label pair $(x, y) \in D_{XY}$, the encoder maps the image $x$ to a lower-dimensional vector $z = f(x) \in \mathbb{R}^m$ and the functions $f$ and $h$ form a classifier of the image space $y_{\text{pred}} = h(z) = (h \circ f)(x)$. Generally, the classifier predicts labels consistent with the ground truth labels such that $y_{\text{pred}} = y$. However, during adversarial attacks, the adversary can generate a small adversarial perturbation $\delta_{\text{adv}}$ such that $(h \circ f)(x) \neq (h \circ f)(x + \delta_{\text{adv}})$. Thus, our purification framework aims to find a purified signal $\epsilon_{\text{pyf}} \in \mathbb{R}^n$ such that $(h \circ f)(x) = (h \circ f)(x + \delta_{\text{adv}} + \epsilon_{\text{pyf}}) = y$. However, it is challenging to achieve $\epsilon_{\text{pyf}} = -\delta_{\text{adv}}$ because $\delta_{\text{adv}}$ is unknown. Thus, we aim to seek an alternative approach to estimate the purified signal $\epsilon_{\text{pyf}}$ and defend against attacks.

### Theoretical Foundation for Adversarial Robustness

The adversarial perturbation is usually $\ell_p$-bounded where $p \in \{0, 2, \infty\}$. We define the $\ell_p$-norm of a vector $a = [a_1, \ldots, a_n]^T$ as $||a||_p$, and a classifier of the image space as $G : \mathbb{R}^n \to L$. We follow Bastani et al. (2016); Leino, Wang, and Fredrikson (2021) to define the local robustness.

**Definition 1** (Locally robust image classifier) Given an image-label pair $(x, y) \in D_{XY}$, a classifier $G$ is $(x, y, \tau)$-robust with respect to $\ell_p$-norm if for every $\eta \in \mathbb{R}^n$ with $||\eta||_p \leq \tau$, $y = G(x) = G(x + \eta)$. Human vision is robust up to a certain perturbation. For example, given a clean MNIST image $x$ with pixel values in $[0, 1]$, if $||\eta||_\infty \leq 85/255$, we assign $(x + \eta)$ and $x$ to the same class (Madry et al. 2018). We use $\rho_H(x, y)$ to represent the maximum perturbation budget for static human vision interpretations given an image-label pair $(x, y)$. Exact $\rho_H(x, y)$ is often a large value but difficult to estimate. We use it to represent the upper bound of achievable robustness.

**Definition 2** (Human-level image classifier) For every image-label pair $(x_i, y_i) \in D_{XY}$, if a classifier $G_R$ is $(x_i, y_i, \tau_i)$-robust and $\tau_i \equiv \rho_H(x_i, y_i)$ where $\rho_H(\cdot, \cdot)$ represents the maximum perturbation budget for static human vision interpretations, we define such a classifier as a human-level image classifier.

The human-level image classifier $G_R$ is an ideal classifier that is comparable to human. To construct such $G_R$, we need a robust feature extractor $f_R$ of the image space and a robust classifier $H_R$ of the feature space to form $G_R = H_R \circ f_R$. However, it is a challenge to construct a robust $f_R$ due to the high-dimensional image space. Therefore, we aim to find an alternative solution to enhance the robustness of $h \circ f$ against adversarial attacks by enforcing the semantic consistency between the decoder $f^\dagger$ and the classifier $h$. Both functions ($f^\dagger$ and $h$) take inputs from a lower dimensional space (compared with the encoder); thus, they are more reliable (Goodfellow, Shlens, and Szegedy 2015).
We define a semantically consistent classifier on the manifold as $h_S : \mathbb{R}^m \to \mathcal{L}$, which yields a class prediction $h_S(z)$ given a latent vector $z \in \mathbb{R}^m$.

**Definition 3 (Semantically consistent classifier on the manifold $\mathcal{M}$)** A semantically consistent classifier $h_S$ on the manifold $\mathcal{M}$ satisfies the following condition: for all $z \in \mathbb{R}^m$, $h_S(z) = (G_R \circ F)(z)$.

A classifier (on the manifold) is a semantically consistent classifier if its predictions are consistent with the semantic interpretations of the images reconstructed by the decoder. While this definition uses the human-level image classifier $G_R$, we can use the Bayesian method to approximate $h_S$ without using $G_R$ in experiment. Below, we provide the sufficient conditions of adversarial robustness for $h_S \circ f$ given an input $x$, where the encoder $f$ is not adversarially robust.

**Proposition 1** Let $(x, y)$ be an image-label pair from $\mathcal{P}_{X,Y}$ and the human-level image classifier $G_R$ be $(x, y, \tau)$-robust. If the encoder $f$ and the decoder $F$ are approximately invertible for the given $x$ such that the reconstruction error $||x - (F^\dagger \circ f)(x)||_p \leq \kappa \leq \tau$ (sufficient condition), then there exists a function $F : \mathbb{R}^n \to \mathbb{R}^n$ such that $(h_S \circ f \circ F)$ is $(x, y, \tau - \kappa)$-robust. (See Yang et al. (2023) for proof.)

Our framework requires semantic consistency between the classifier on the manifold and the decoder on the manifold. Despite that the classifiers and decoders (on the manifold) have a low input dimension, it is still difficult to achieve high semantic consistency between them. Meanwhile, the human-level image classifier $G_R$ is not available. Thus, we assume that predictions and reconstructions from high data density regions of $p(z|x)$ are more likely to be semantically consistent (Zhou 2022). Next, we introduce a practical implementation of adversarial purification based on our framework. The implementation includes two stages: (1) enforce consistency during training and (2) test-time purification of adversarial examples, see Figure 2.

**Semantic Consistency with the ELBO**

Exact inference of $p(z|x)$ is often intractable, we, therefore, use variational inference to approximate the posterior $p(z|x)$ with a different distribution $q(z|x)$. We define two parameters $\theta$ and $\phi$ which parameterize the distributions $p_\theta(x|z)$ and $q_\phi(z|x)$. When the evidence lower bound (ELBO) is maximized, $q_\phi(z|x)$ is considered to be a reasonable approximation of $p(z|x)$. To enforce the semantic consistency between the classifier and the decoder, we force the latent vector $z$ inferred from the $q_\phi(z|x)$ to contain the class label information of the input $x$. We define a one-hot label vector as $y = [y_1, y_2, \ldots, y_c]^T$, where $c$ is the number of classes and $y_i = 1$ if the image label is $i$ otherwise it is zero. A classification head parametrized by $\psi$ is represented as $h_\psi(z) = [h_1(z), h_2(z), \ldots, h_c(z)]^T$ and the cross-entropy classification loss is $-\mathbb{E}_{x \sim q_\phi(z|x)}[y^T \log h_\psi(z)]$ where $\log(\cdot)$ is an element-wise function for a vector. We assume the classification loss is no greater than a threshold $\omega$ and the training objective can then be written as

$$
\max_{\theta, \phi} \mathbb{E}_{x \sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}[q_\phi(z|x)\|p(z)] \tag{1}
$$

ELBO (lower bound of $\log p_\theta(x)$)

$$
\text{s.t. } -\mathbb{E}_{x \sim q_\phi(z|x)}[y^T \log h_\psi(z)] \leq \omega. \tag{2}
$$

**Figure 2**: Two-stage pipeline: (a) jointly training for semantic consistency between the decoder and the classifier and (b) iterative updates of $e_{py}$ to purify $x_{adv}$ in inference.

Our conditions indicate that higher reconstruction quality could lead to stronger robustness. Meanwhile, our method can certify robustness up to $\frac{\kappa}{2}$ (reconstruction error $\kappa = 0$) when a human-level image classifier can certify robustness up to $\tau$. The insight is that adding a purified signal on top of an adversarial example could change the image semantic, see Figure 5(c). Our framework is based on the triangle inequality and can be extended to other distance metrics.
We use the Lagrange multiplier with KKT conditions to optimize this objective as
\[
\max_{\theta, \phi, \psi} \text{ELBO} + \lambda \mathbb{E}_{x \sim q_\phi(z|x)}[y^T \log h_\psi(z)],
\]
where \( \lambda \) is a trade-off term to balance the two loss terms.

We follow Kingma and Welling (2014) to define the prior \( p(x) = \mathcal{N}(0, I) \) and the posterior (encoder) \( q_\phi(z|x) \) by using a normal distribution with diagonal covariance. Given an input vector \( x \), an encoder model parameterized by \( \phi \) is used to model the posterior distribution \( q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \text{diag}(\sigma^2_\phi(x))) \). The model predicts the mean vector \( \mu_\phi(x) = [\mu_1(x), \mu_2(x), \ldots, \mu_m(x)]^T \) and the diagonal covariance \( \sigma^2_\phi(x) = [\sigma^2_{\phi_1}(x), \ldots, \sigma^2_{\phi_m}(x)]^T \). We define \( \rho_\theta(x|z) = (1/\beta) \exp(-\gamma \|x - f_\theta(z)\|^2) \), where \( \gamma \) controls the variance, \( \beta \) is a normalization constant, and \( f_\theta \) is a decoder parameterized by \( \theta \), which maps data from the latent space to the image space. The illustrated network optimizing over Eq. (3) is provided in Figure 2(a).

Adversarial Attack and Purification

We mainly focus on the white-box attacks here. During inference time, the attackers can create adversarial perturbations on the classification head. Given a clean image \( x \), an adversarial example can be crafted as \( x_{\text{adv}} = x + \delta_{\text{adv}} \) with
\[
\delta_{\text{adv}} = \arg \max_{\delta \in \mathcal{C}_{\text{adv}}} -\mathbb{E}_{z \sim q_\phi(z|x+\delta)}[y^T \log h_\psi(z)],
\]
where \( \mathcal{C}_{\text{adv}} = \{ \delta \in \mathbb{R}^n | x + \delta \in [0, 1]^n \text{ and } \|\delta\|_p \leq \delta_{\text{th}} \} \) is the feasible set for \( \delta_{\text{th}} \)-bounded perturbations.

To avoid changing the semantic interpretation of the image, we need to estimate the purified signal with a \( \ell_p \)-norm no greater than a threshold value \( \epsilon_{\text{th}} \). The purified signal also needs to project the sample to a high-density region of the manifold with a small reconstruction loss. The ELBO contains \( \ell_2 \) reconstruction loss (relaxation from \( \ell_p \)-metric), and it can be applied to maximize the posterior \( q_\phi(z|x) \). Therefore, we present a defense method that optimizes the ELBO during the test time to degrade the effects of the attacks. Given an adversarial example \( x_{\text{adv}} \), a purified sample can be obtained by \( x_{\text{py}} = x_{\text{adv}} + \epsilon_{\text{py}} \) with
\[
\epsilon_{\text{py}} = \arg \max_{\epsilon \in \mathcal{C}_{\text{py}}} \mathbb{E}_{z \sim q_\phi(z)}[\log \hat{p}_\theta(\epsilon)] - D_{KL}[\hat{q}_\phi(\epsilon)||p(z)],
\]
where \( \hat{p}_\theta(\epsilon) \overset{\triangle}{=} p_\theta(x_{\text{adv}} + \epsilon|z), \hat{q}_\phi(\epsilon) \overset{\triangle}{=} q_\phi(z|x_{\text{adv}} + \epsilon) \) and \( \mathcal{C}_{\text{py}} = \{ \epsilon \in \mathbb{R}^n | x_{\text{adv}} + \epsilon \in [0, 1]^n \text{ and } \|\epsilon\|_p \leq \epsilon_{\text{th}} \} \) is a feasible set for purification. Compared with training a model to produce the purified signal \( \epsilon_{\text{py}} = \mathcal{S}(x) \), the test-time optimization of the ELBO is more efficient.

We focus on \( \ell_\infty \)-bounded purified vectors while our method is effective for both \( \ell_2 \) and \( \ell_\infty \) attacks in our experiments. We define \( \alpha \) as the learning rate and \( \text{Proj}_\epsilon \) as the projection operator which projects a data point back to its feasible region when it is out of the region. We use a clipping function as the projection operator to ensure \( \|x_{\text{py}} - x\|_\infty = \|\epsilon_{\text{py}}\|_\infty \leq \epsilon_{\text{th}} \) and \( x_{\text{py}} = x + \epsilon_{\text{py}} \in [0, 1]^n \). We use a clipping function as the projection operator to ensure \( \|x_{\text{py}} - x\|_\infty = \|\epsilon_{\text{py}}\|_\infty \leq \epsilon_{\text{th}} \) and \( x_{\text{py}} = x + \epsilon_{\text{py}} \in [0, 1]^n \).

Algorithm 1: Test-time Purification

Input: \( x_{\text{adv}} \): input (adv) data; \( \alpha \): learning rate; \( T \): number of purification iterations; \( \epsilon_{\text{th}} \): purification budget.

Output: \( x_{\text{py}} \): purified data; \( s \): purification score.

1. procedure PURIFY\((x, \alpha, T, \epsilon_{\text{th}})\)
2. \( \epsilon_{\text{py}} \leftarrow \mathcal{U}(-\epsilon_{\text{th}}, \epsilon_{\text{th}}) \) \( \triangleright \) random initialization
3. for \( t = 1, 2, \ldots, T \) do
4. \( \epsilon_{\text{py}} \leftarrow \epsilon_{\text{py}} + \alpha \cdot \text{sign}(\nabla_{\epsilon_{\text{py}}} \mathcal{F}(x_{\text{adv}} + \epsilon_{\text{py}})) \)
5. \( \epsilon_{\text{py}} \leftarrow \min(\max(\epsilon_{\text{py}} - \epsilon_{\text{th}}, \epsilon_{\text{th}})) \)
6. \( \epsilon_{\text{py}} \leftarrow \min(\max(\epsilon_{\text{py}} + \epsilon_{\text{py}}, 0), 1) \) - \( x_{\text{adv}} \)
7. \( x_{\text{py}} \leftarrow x_{\text{adv}} + \epsilon_{\text{py}} \) \( \triangleright \) purified data
8. \( s \leftarrow \mathcal{F}(x_{\text{py}}) \) \( \triangleright \) purification score
9. return \( x_{\text{py}}, s \)

Figure 3: (a) 2D trajectories of Fashion-MNIST. (b) Input and reconstructed image pairs on clean (top), adversarial (middle), and purified (bottom) examples with model predictions (numerical index) and failure cases (in box).

and iterative purification given adversarial example \( x_{\text{adv}} \) as
\[
\epsilon_{t+1} = \text{Proj}_\epsilon \left( \epsilon_t + \alpha \cdot \text{sgn}(\nabla_{\epsilon} \mathcal{F}(x_{\text{adv}} + \epsilon; \theta, \phi)) \right),
\]
where the element-wise sign function \( \text{sgn}(x) = x/\|x\| \) if \( x \) is non-zero otherwise it is zero. A detailed procedure is provided in Figure 2(b) and Algorithm 1.

The test-time optimization of the ELBO projects adversarial examples back to their feasible regions with a high posterior \( q(z|x) \) (regions where decoders and classifiers have strong semantic consistency) and a small reconstruction error (defend against adversarial attacks). To better demonstrate the process, we build a classification model in a 2-dimensional latent space (Figure 3 (a)) on Fashion-MNIST and show examples of clean, attack, and purified trajectories in Figure 3. Correspondingly, adversarial attacks are likely to push latent vectors to abnormal regions which cause abnormal reconstructions (Lemma 1). Through the test-time optimization over the ELBO, the latent vectors can be brought back to their original regions (Theorem 1).

If attackers are aware of the existence of purification, they could take advantage of this knowledge to create adaptive attacks. A straightforward formulation is to perform the multi-
objective attacks with a trade-off term $\lambda_\alpha$ to balance the classification loss $\mathcal{H}(x, y; \theta, \psi)$ and the purification objective $\mathcal{F}(x; \theta, \phi)$ (Mao et al. 2021; Shi, Holtz, and Mishne 2021). The adversarial perturbation of the multi-objective attacks is

$$\delta_{\text{adv}} = \arg \max_{\delta \in \mathcal{C}_{\text{adv}}} \mathcal{H}(x + \delta, y; \theta, \psi) + \lambda_\alpha \mathcal{F}(x + \delta; \theta, \phi). \quad (8)$$

Another popular adaptive attack is the BPDA attack (Athalye, Carlini, and Wagner 2018). Consider a purification process as $x_{\text{pfy}} = F(x)$ and a classifier as $G(x_{\text{pfy}}) = (G \circ F)(x)$. The BPDA attack uses an approximation $\nabla_x F(x) \approx I$ (identity) to estimate the gradient as $\nabla_x G(F(x))|_{x=x} \approx \nabla_x G(F(x))|_{x=x}$. Many adversarial purification methods are vulnerable to the BPDA attack (Athalye, Carlini, and Wagner 2018; Croce et al. 2022). We show that even if attackers are aware of the defense, our method can still achieve effective robustness to this white-box adaptive attacks.

## Experiments

We first evaluate our method on MNIST (LeCun, Cortes, and Burges 2010), Fashion-MNIST (Xiao, Rasul, and Vollgraf 2017), SVHN (Netzer et al. 2011), and CIFAR-10 (Krizhevsky and Hinton 2009), followed by CIFAR-100 (Krizhevsky and Hinton 2009) and CelebA (64 × 64 and 128 × 128) for gender classification (Liu et al. 2015). See Yang et al. (2023) for the dataset details.

### Model Architectures and Hyperparameters

We use three types of models (encoders) in our experiments: (1) tiny ResNet with standard training (for ablation study), (2) ResNet-50 with standard training (He et al. 2016) (for comparison with benchmark), and (3) PreActResNet-18 with adversarial training (Rebuffi et al. 2021) (to study the impact on adversarially trained models). We use several residual blocks to construct decoders and use linear layers for classification. We empirically set the weight of the classification loss ($\lambda$ in Eq. (3)) to 8. See Yang et al. (2023) for details.

### Adversarial Attacks

We evaluate our method on standard adversarial attacks and adaptive attacks (multi-objective and BPDA). All attacks are untargeted. For standard adversarial attacks (Eq. (4)), we use Foolbox (Rauber, Brendel, and Bethge 2017) to generate the PGD $(\ell_\infty)$ attacks (Madry et al. 2018). We use Croce and Hein (2020) for the AutoAttack $(\ell_\infty, \ell_2)$. For the adaptive attacks, we use Torchattacks (Kim 2020) for the BPDA-PGD/APGD $(\ell_\infty)$ attacks (Athalye, Carlini, and Wagner 2018), and standard PGD $(\ell_\infty)$ for the multi-objective attacks. For MNIST and Fashion-MNIST, we report the attack hyperparameters and numerical results in Yang et al. (2023). For SVHN, CIFAR-10/100, and CelebA, we set the $\ell_\infty$ attack budget $\epsilon_{th}$ to $8/255$ and the $\ell_2$ attack budget to 0.5. We run 100 iterations with step size $2/255$ for PGD $(\ell_\infty)$ and 50 iterations with step size $2/255$ for the BPDA attack.

We also evaluate our ResNet-50 (CIFAR-10) model on the RayS (blackbox) attack (Chen and Gu 2020), the FGSM $(\ell_\infty)$ attack (Goodfellow, Shlens, and Szegedy 2015) and the C&W $(\ell_2)$ attack (Carlini and Wagner 2017) in Yang et al. (2023) and our defense is effective for these attacks.

### Test-time Purification

Key hyperparameters and experimental details are provided below, and only the $\ell_\infty$-bounded purification is considered in this work. We initialize the purified signal $\epsilon_{pfy}$ by sampling from an uniform distribution $u(-\epsilon_{th}, \epsilon_{th})$, where $\epsilon_{th}$ is the purification budget. We run purification 16 times in parallel with different initializations and select the signal with the best purification score measured by the reconstruction loss or the ELBO. Step size $\alpha$ is alternated between $\{1/255, 2/255\}$ for each run. For SVHN, CIFAR-10/100, and CelebA, we set the $\ell_\infty$-purification budget $\epsilon_{th}$ to $8/255$ with 32 iterations. Despite the aforementioned hyperparameters, our method also works on other hyperparameter settings as shown in Figure 7.

### Baselines

We compare our VAE-Classifier (V-CLF) with the standard autoencoders, denoted by Standard-AE-Classifier (S-CLF), by replacing the ELBO with reconstruction loss. One should note that the classifiers of the Standard-AE-Classifier may not have consistency with their decoders. See Yang et al. (2023) for details.

### Objectives of Test-time Purification

The autoencoders are
trained with the reconstruction loss and the ELBO respectively. The Standard-AE-Classifier can only minimize the reconstruction loss during inference while the VAE-Classifier can optimize both the reconstruction loss and the ELBO during inference. We use “TP (R)” to represent the test-time optimization of the reconstruction loss and “TP (E)” for the test-time optimization of the ELBO.

**Inference Time.** We evaluate our method on an NVIDIA Tesla P100 GPU in PyTorch. For ResNet-50 with a batch size of 256 on CIFAR-10, the average run time per batch for 32 purification steps is 17.65s. Following the standard in (Croce et al. 2022), our method is roughly $10^2 \times$. To reduce the inference time, one can adapt APGD (adaptive learning rate and momentum) during purification.

**Experiment Results**

**Standard Adversarial Attacks.** For the standard adversarial attacks, only the classification heads are attacked. We observe that, for MNIST, Fashion-MNIST, and SVHN, the standard adversarial attacks of the VAE-Classifier create abnormal reconstructed images while this is not applied to the Standard-AE-Classifier. It indicates that the classifiers and the decoders of the VAE-Classifier are strongly consistent. Figure 4 shows various sample predictions and reconstructions on clean, attack, and purified images from the VAE-Classifier. For clean images, the VAE-Classifier models achieve qualified reconstruction and predictions. For adversarial examples, the VAE-Classifier models generate abnormal reconstructions which are correlated with abnormal predictions from the classifiers (implied by Lemma 1). In other words, if the prediction of an adversarial example is 2, the digit on the reconstructed image may look like 2 as well. If we can estimate the purified vectors by minimizing the errors between inputs and reconstructions, the attacks could be defended (implied by Theorem 1). In our experiments, the predictions and reconstructions of adversarial examples become normal after using the test-time optimization (ELBO).

Figure 5 shows various sample predictions and reconstructions from the VAE-Classifier on CIFAR-10 and CelebA. The results are slightly different from those on MNIST, Fashion-MNIST, and SVHN: in Figures 5(a)-(b), although the reconstructed images are more blurry compared with MNIST, Fashion-MNIST, and SVHN, the VAE-Classifier is still robust under adversarial attacks. Distribution of the negative ELBO for clean, attack, and purified examples are shown in Figure 6.

We use tiny ResNet backbones for ablation study between the Standard-AE-Classifier and the VAE-Classifier. Classification accuracy of CIFAR-10 and SVHN is provided in Table 1 (see Yang et al. (2023) for results on MNIST and Fashion-MNIST). According to our results, optimizing the ELBO during the test time is more effective than only optimizing the reconstruction loss. Table 2 shows test-time purification (CIFAR-10) with larger backbones such as ResNet-50 (standard training) and PreActResNet-18 (adversarial training). With our defense, the robust accuracy of ResNet-50 on CIFAR-10 increases by more than 50%. Our method can also be applied to adversarially trained models (PreActResNet-18) to further increase their robust accuracy.

**Multi-objective Attacks.** We evaluate our method with the multi-objective attacks on CIFAR-10 and provide accuracy with respect to trade-off term $\lambda_\alpha$ of Eq. (8) in Figure 7(a). We observe that the classification accuracy of adversarial examples increases as the trade-off term increases while impacts on our defense are not significant. Thus, our defense is robust to the multi-objective attacks. We show some multi-objective adversarial examples in Yang et al. (2023).

**Backward Pass Differentiable Approximation (BPDA).** We apply PGD and APGD to optimize the objective of the BPDA attacks. We highlight the minimum classification accuracy of CIFAR-10 and SVHN with respect to trade-off term $\lambda_\alpha$. We apply PGD and APGD to optimize the objective of the BPDA attacks. We report the minimum accuracy.

| Arch. | Method | Clean | PGD | AA-$\ell_\infty$ | AA-$\ell_2$ | BPDA |
|-------|--------|-------|-----|------------------|-------------|------|
| R50   | V-CLF  | 94.82 | 23.84 | 0.04            | 63.09       | 63.16 | 57.15 |
|       | TP (E) | 85.12 |       |                 |             | 63.16 |      |
| PR18  | V-CLF  | 87.35 | 61.08 | 58.65           |             |      |      |
|       | TP (E) | 85.14 |       |                 |             | 63.73 | 60.52 |

Table 2: VAE-Classifier with ResNet-50 (R50) and adversarially trained PreActResNet-18 (PR18) on CIFAR-10. We set $\ell_\infty = 8/255$. See Yang et al. (2023) for more results.

Figure 6: Illustration of negative ELBOs. Adversarial attacks yield higher negative ELBOs while our purification reverses the ELBO shifts. Compared with MNIST, diverse backgrounds of CIFAR-10 lead to less obvious ELBO shifts.

| Method | Clean | PGD | AA-$\ell_\infty$ | AA-$\ell_2$ | BPDA |
|--------|-------|-----|------------------|-------------|------|
| S-CLF  | 94.00 | 0.00 | 0.00             | 1.67        |      |
| TP (R) | 93.03 | 40.83 | 44.82           | 59.93       | 7.65 |
| V-CLF  | 95.27 | 16.01 | 0.33             | 6.61        |      |
| TP (R) | 90.66 | 72.44 | 73.92           | 79.15       | 66.68 |
| TP (E) | 86.29 | 72.72 | 73.47           | 76.21       | 64.70 |

Table 1: Classification accuracy on SVHN and CIFAR-10 with $\ell_\infty = 8/255$ and $\ell_2 = 0.5$. “S-CLF”: Standard-AE-Classifier, “V-CLF”: VAE-Classifier, “TP (R)”: Test-time minimization of the reconstruction loss, “TP (E)”: Test-time minimization of the negative ELBO, and “AA”: AutoAttack. We evaluate the model with both BPDA-(PGD/APGD) and report the minimum accuracy.
### Table 3: Benchmark on SVHN and CIFAR-10 with $\ell_\infty = 8/255$. Accuracy is directly reported from the respective paper except for the adaptive attack which is reported from Lee and Kim (2023) for diffusion-based purification and Athalye et al. (2018); Croce et al. (2022) for BPDA. Numbers in bold are the minimum/robust accuracy. “*”: adversarially trained models. “-”: missing from the references, “St.A”: strongest standard attacks and “Adap.A”: strongest adaptive attacks. “WR”: Wide-ResNet. “PR”: PreActResNet. Other works follow different evaluation standards, and we compare with them in Yang et al. (2023). We achieve robust performance without adversarial training.

| Method       | SVHN       | CIFAR-10    |
|--------------|------------|-------------|
| Semi-SL*     | 94.00      | 58.50       |
| PR18*        | 61.00      | 45.00       |
| WR28* (Rebuffi et al. 2021) | 61.09 | 53.58 |
| WR28 (Lee and Kim 2023) | - | 49.65 |
| ResNet-Tiny (ours) | 72.72 | 64.70 |
| WRN28 (Shi et al. 2021) | 53.58 | 3.70 |
| ResNet (Song et al. 2018) | 46.00 | 9.00 |
| WR28 (Hill et al. 2021) | 78.91 | 54.90 |
| WR28 (Yoon et al. 2021) | 85.45 | 33.70 |
| PR18 (Mao et al. 2021) | 34.40 | - |
| WR34* (Zhang et al. 2019) | 53.08 | - |
| WR70* (Wang et al. 2023) | 70.69 | - |
| WR70* (Rebuffi et al. 2021) | 66.56 | - |
| PR18* (Rebuffi et al. 2021) | 58.50 | - |
| WR70 (Nie et al. 2022) | 71.29 | 51.13 |
| WR70 (Lee and Kim 2023) | 70.31 | 56.88 |
| ResNet50 (ours) | 63.09 | 57.15 |

Table 4: Classification accuracy on CIFAR-100 and CelebA (size: ClbA-$x^2$) using the VAE-Classifer with $\ell_\infty = 8/255$.

| Dataset   | V-CLF | +TP (E) |
|-----------|-------|---------|
| CIFAR100  | 72.37 | 26.13   |
| ClbA-64   | 97.86 | 93.91   |
| ClbA-128  | 97.78 | 93.91   |

**Conclusion**

We formulate a novel adversarial purification framework via manifold learning and variational inference. Our test-time purification is evaluated with several attacks and shows its adversarial robustness for non-adversarially trained models. Even if attackers are aware of our defense method, we can still achieve competitive adversarial robustness. Our method is also capable of being combined with adversarially trained models to further increase their adversarial robustness.

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