ENERGY-BASED TEST SAMPLE ADAPTATION FOR DOMAIN GENERALIZATION

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ABSTRACT

In this paper, we propose energy-based sample adaptation at test time for domain generalization. Where previous works adapt their models to target domains, we adapt the unseen target samples to source-trained models. To this end, we design a discriminative energy-based model, which is trained on source domains to jointly model the conditional distribution for classification and data distribution for sample adaptation. The model is optimized to simultaneously learn a classifier and an energy function. To adapt target samples to source distributions, we iteratively update the samples by energy minimization with stochastic gradient Langevin dynamics. Moreover, to preserve the categorical information in the sample during adaptation, we introduce a categorical latent variable into the energy-based model. The latent variable is learned from the original sample before adaptation by variational inference and fixed as a condition to guide the sample update. Experiments on six benchmarks for classification of images and microblog threads demonstrate the effectiveness of our proposal.

1 INTRODUCTION

Deep neural networks are vulnerable to domain shifts and suffer from lack of generalization on test samples that do not resemble the ones in the training distribution (Recht et al., 2019; Zhou et al., 2021; Krueger et al., 2021). To deal with the domain shifts, domain generalization has been proposed (Muandet et al., 2013; Gulrajani & Lopez-Paz, 2020; Cha et al., 2021). Domain generalization strives to learn a model exclusively on source domains in order to generalize well on unseen target domains. The major challenge stems from the large domain shifts and the unavailability of any target domain data during training.

To address the problem, domain invariant learning has been widely studied, e.g., (Motiian et al., 2017; Zhao et al., 2020; Nguyen et al., 2021), based on the assumption that invariant representations obtained on source domains are also valid for unseen target domains. However, since the target data is inaccessible during training, it is likely an "adaptivity gap" (Dubey et al., 2021) exists between representations from the source and target domains. Therefore, recent works try to adapt the classification model with target samples at *test time* by further fine-tuning model parameters (Sun et al., 2020; Wang et al., 2021) or by introducing an extra network module for adaptation (Dubey et al., 2021). Rather than adapting the model to target domains, Xiao et al. (Xiao et al., 2022) adapt the classifier for each sample at test time. Nevertheless, a single sample would not be able to adjust the whole model due to the large number of model parameters and the limited information contained in the sample. This makes it challenging for their method to handle large domain gaps. Instead, we propose to adapt each target sample to the source distributions, which does not require any fine-tuning or parameter updates of the source model.

In this paper, we propose energy-based test sample adaptation for domain generalization. The method is motivated by the fact that energy-based models (Hinton, 2002; LeCun et al., 2006; Song & Kingma, 2021) flexibly model complex data distributions and allow for efficient sampling from the modeled distribution by Langevin dynamics (Du & Mordatch, 2019; Welling & Teh, 2011). Specifically, we define a new discriminative energy-based model as the composition of a classifier and a neural-network-based energy function in the data space, which are trained simultaneously on the source domains. The trained model iteratively updates the representation of each target sample by gradient descent of energy minimization through Langevin dynamics, which eventually adapts the sample to

the source data distribution. The adapted target samples are then predicted by the classifier that is simultaneously trained in the discriminative energy-based model.

Since Langevin dynamics tends to draw samples randomly from the distribution modeled by the energy function, it cannot guarantee category equivalence. In order to maintain the category information of the target samples during adaptation and promote better classification performance, we further introduce a categorical latent variable in our energy-based model. Our model learns the latent variable to explicitly carry categorical information by variational inference in the classification model. We utilize the latent variable as conditional categorical attributes like in compositional generation (Du et al., 2020a; Nie et al., 2021) to guide the sample adaptation to preserve the categorical information of the original sample. At inference time, we simply ensemble the predictions obtained by adapting the unseen target sample to each source domain as the final domain generalization result.

We conduct experiments on six benchmarks for classification of images and microblog threads to demonstrate the promise and effectiveness of our method for domain generalization.

2 METHODOLOGY

In domain generalization, we are provided source and target domains as non-overlapping distributions on the joint space $\mathcal{X} \times \mathcal{Y}$, where $\mathcal{X}$ and $\mathcal{Y}$ denote the input and label space, respectively. Given a dataset with S source domains $\mathcal{D}_s = \{D_s^i\}_{i=1}^S$ and T target domains $\mathcal{D}_t = \{D_t^i\}_{i=1}^T$, a model is trained only on $\mathcal{D}_s$ and required to generalize well on $\mathcal{D}_t$. Under the homogeneous domain generalization settings of Zhou et al. (2021), that we follow in our work, the label space is shared across domains.

In this work, we propose energy-based test sample adaptation, which adapts target samples to source distributions to tackle the domain gap between target and source distributions. The rationale behind our model is that adapting the target samples to the source data distributions is able to improve the prediction of the target data with source models by reducing the domain shifts, as shown in Figure 1 (left). In this section, we first provide a preliminary on energy-based models and then present our energy-based test sample adaptation.

2.1 ENERGY-BASED MODEL PRELIMINARY

Energy-based models (LeCun et al., 2006) represent any probability distribution $p(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^D$ as $p_\theta(\mathbf{x}) = \frac{\exp(-E_\theta(\mathbf{x}))}{Z_\theta}$, where $E_\theta(\mathbf{x}) : \mathbb{R}^D \to \mathbb{R}$ is known as the energy function that maps each input sample to a scalar and $Z_\theta = \int \exp(-E_\theta(\mathbf{x}))d\mathbf{x}$ denotes the partition function. However, Z_θ is usually intractable since it computes the integration over the entire input space of $\mathbf{x}$. Thus, we cannot train the parameter θ of the energy-based model by directly maximizing the log-likelihood $\log p_\theta(\mathbf{x}) = -E_\theta(x) - \log Z_\theta$. Nevertheless, the log-likelihood has the derivative (Du & Mordatch, 2019; Song & Kingma, 2021) :

$$\frac{\partial \log p_\theta(\mathbf{x})}{\partial \theta} = \mathbb{E}_{p_d(\mathbf{x})}\Big[-\frac{\partial E_\theta(\mathbf{x})}{\partial \theta}\Big] + \mathbb{E}_{p_\theta(\mathbf{x})}\Big[\frac{\partial E_\theta(\mathbf{x})}{\partial \theta}\Big], \tag{1}$$

where the first expectation term is taken over the data distribution $p_d(\mathbf{x})$ and the second one is over the model distribution $p_\theta(\mathbf{x})$.

The objective function in eq. (1) encourages To do so, we need to draw samples from $p_\theta(\mathbf{x})$, which is challenging and usually approximated by MCMC methods (Hinton, 2002). An effective MCMC method used in recent works (Du & Mordatch, 2019; Nijkamp et al., 2019; Xiao et al., 2021b; Grathwohl et al., 2020) is Stochastic Gradient Langevin Dynamics (Welling & Teh, 2011), which simulates samples by

$$\mathbf{x}^{i+1} = \mathbf{x}^i - \frac{\lambda}{2}\frac{\partial E_\theta(\mathbf{x}^i)}{\partial \mathbf{x}^i} + \epsilon, \quad s.t., \quad \epsilon \sim \mathcal{N}(0, \lambda) \tag{2}$$

where λ denotes the step-size and $\mathbf{x}^0$ is drawn from the initial distribution $p_0(\mathbf{x})$, which is usually a uniform distribution (Du & Mordatch, 2019; Grathwohl et al., 2020).

Actually, maximizing $\log p_\theta(\mathbf{x})$ is equivalent to minimizing the KL divergence $\mathbb{D}_{\mathrm{KL}}(p_d(\mathbf{x})||p_\theta(\mathbf{x}))$ (Song & Kingma, 2021), which is alternatively achieved in (Hinton, 2002) by minimizing contrastive

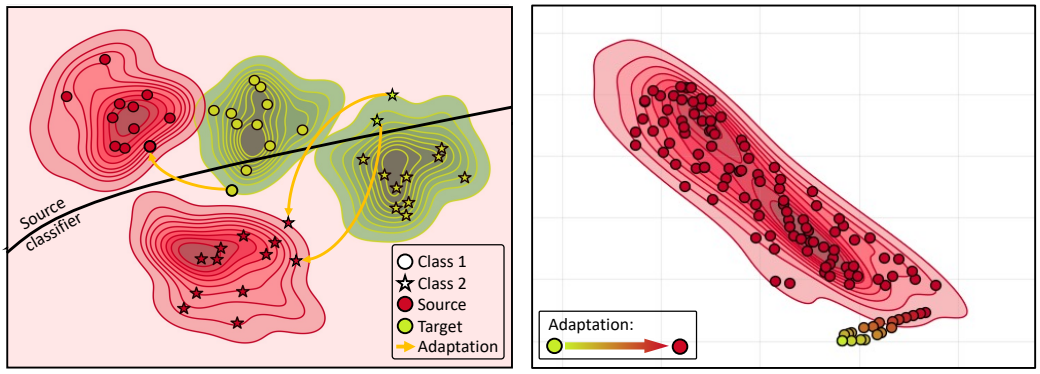

Figure 1: **Illustration of the proposed energy-based model.** It aims to adapt the target samples to the source distributions, which can be more accurately classified by the source domain classifier (left). With Langevin dynamics, each target sample is adapted iteratively to the source data distributions, which are represented as the gradient colors from green to red (right). Best viewed in color.

divergence:

$$\mathbb{D}_{\mathrm{KL}}(p_d(\mathbf{x})||p_\theta(\mathbf{x})) - \mathbb{D}_{\mathrm{KL}}(q_\theta(\mathbf{x})||p_\theta(\mathbf{x})), \tag{3}$$

where $q_\theta(\mathbf{x}) = \prod_\theta^t p_d(\mathbf{x})$, representing t sequential MCMC transitions starting from $p(\mathbf{x})$ (Du et al., 2021) and minimizing eq. (3) is achieved by minimizing:

$$\mathbb{E}_{p_d(\mathbf{x})}[E_\theta(\mathbf{x})] - \mathbb{E}_{\mathrm{stop_grad}(\mathrm{q}_\theta(\mathbf{x}))}[E_\theta(\mathbf{x})] + \mathbb{E}_{q_\theta(\mathbf{x})}[E_{\mathrm{stop_grad}(\theta)}(\mathbf{x})] + \mathbb{E}_{q_\theta(\mathbf{x})}[\mathrm{log} q_\theta(\mathbf{x})]. \tag{4}$$

Eq. (4) avoids drawing samples from the model distribution $p_\theta(\mathbf{x})$, which often requires an exponentially long time for MCMC sampling (Du et al., 2021). Intuitively, $q_\theta(\mathbf{x})$ is closer to $p_\theta(\mathbf{x})$ than $p_d(\mathbf{x})$, which guarantees that $\mathbb{D}_{\mathrm{KL}}(p_d(\mathbf{x})||p_\theta(\mathbf{x})) \geq \mathbb{D}_{\mathrm{KL}}(q_\theta(\mathbf{x})||p_\theta(\mathbf{x}))$ and eq. (3) can only be zero when $p_\theta(\mathbf{x}) = p_d(\mathbf{x})$.

2.2 Energy-based test sample adaptation

We propose energy-based test sample adaption to tackle the domain gap between source and target data distributions. This is inspired by the fact that Langevin dynamics simulates samples of the distribution expressed by the energy-based model through gradient-based updates, with no restriction on the sample initialization if the sampling steps are sufficient (Welling & Teh, 2011; Du & Mordatch, 2019). We leverage this property to conduct test sample adaptation with Langevin dynamics by setting the target sample as the initialization and updating it iteratively. With the energy-based model of the source data distribution, as shown in Figure 1 (right), target samples are gradually updated towards the source domain and with sufficient update steps, the target sample will eventually be adapted to the source distribution.

Discriminative energy-based model. We propose the discriminative energy-based model $p_{\theta,\phi}(\mathbf{x}, \mathbf{y})$ on the source domain, which is constructed by a classification model and an energy function in the data space. Different from the regular energy-based models that generate data samples from uniform noise, our goal is to promote the discriminative task, i.e., the conditional distribution $p(\mathbf{y}|\mathbf{x})$, which is preferred to be jointly modeled with the data distributions $p(\mathbf{x})$. Thus, the proposed energy-based model is defined on the joint space of $\mathcal{X} \times \mathcal{Y}$ to consider both the classification task and energy function. Formally, the discriminative energy-based model of a source domain is formulated as:

$$p_{\theta,\phi}(\mathbf{x}, \mathbf{y}) = p_\phi(\mathbf{y}|\mathbf{x}) \frac{\exp(-E_\theta(\mathbf{x}))}{Z_{\theta,\phi}}, \tag{5}$$

where $p_\phi(\mathbf{y}|\mathbf{x})$ denotes the classification model and $E_\theta(\mathbf{x})$ is an energy function, which is nowadays implemented with neural networks. eq. (5) enables the energy-based model to jointly model the data distribution and the conditional distribution on the source domains. An unseen target sample $\mathbf{x}_t$ is iteratively adapted to the data distribution of the source domain D_s by Langevin dynamics update with the energy function $E_\theta(\mathbf{x})$ and predicted by the classification model $p_\phi(\mathbf{y}|\mathbf{x})$.

The model parameters θ and ϕ can be jointly optimized following eq. (3) by minimizing:

$$\mathbb{D}_{\mathrm{KL}}(p_d(\mathbf{x}, \mathbf{y})||p_{\theta,\phi}(\mathbf{x}, \mathbf{y})) - \mathbb{D}_{\mathrm{KL}}(q_{\theta,\phi}(\mathbf{x}, \mathbf{y})||p_{\theta,\phi}(\mathbf{x}, \mathbf{y})), \tag{6}$$

which is derived as:

$$\begin{aligned}\mathcal{L} = &- \mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\left[\log p_\phi(\mathbf{y}|\mathbf{x})\right] + \mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\left[E_\theta(\mathbf{x})\right] - \mathbb{E}_{\mathrm{stop_grad}(\mathrm{q}_{\theta,\phi}(\mathbf{x},\mathbf{y}))}\left[E_\theta(\mathbf{x})\right] \\ &+ \mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\left[E_{\mathrm{stop_grad}(\theta)}(\mathbf{x}) - \log p_{\mathrm{stop_grad}(\phi)}(\mathbf{y}|\mathbf{x})\right],\end{aligned} \tag{7}$$

where $p_d(\mathbf{x},\mathbf{y})$ denotes the real data distribution and $q_{\theta,\phi}(\mathbf{x},\mathbf{y}) = \prod_\theta^t p(\mathbf{x},\mathbf{y})$ denotes t sequential MCMC samplings from the distribution expressed by the energy-based model similar to eq. (4) (Du et al., 2021). We provide the detailed derivation in Appendix A.

In eq. (7), the first term encourages to learn a discriminative classifier on the source domain. The second and third terms train the energy function to model the data distribution of the source domain by assigning low energy on the real samples and high energy on the samples from the model distribution. The fourth term minimizes the energy and maximizes the prediction log-likelihood of the samples from the model distribution.

Notably, different from the first three terms that directly supervise the model parameters θ and ϕ, the fourth term imposes the supervision on the adaptation procedure. We stop the gradients of the energy function E_θ and classifier ϕ while updating the parameters by back-propagating the gradients of the adapted samples from the model distribution $q_{\theta,\phi}(\mathbf{x},\mathbf{y})$ similar to Du et al. (2021). Since the adaptation is achieved by updating $\mathbf{x}$ with a variation $-\frac{\partial E_\theta(\mathbf{x})}{\partial \mathbf{x}}$ in Langevin dynamics (eq. 2), the gradients of the updated $\mathbf{x}$ can be back-propagated through the variation to update the parameters θ, whose gradients is calculated by $-\frac{\partial E_\theta(\mathbf{x})}{\partial \theta \partial \mathbf{x}}$.

Essentially, the last term trains the model θ to provide a variation for each sample that encourages its adapted version to be both discriminative on the source domain classifier and low energy on the energy function. Intuitively, it supervises the model to learn the ability to preserve categorical information during adaptation and find a faster way to minimize the energy.

Label-preserving adaptation with categorical latent variable. Since the ultimate goal is to correctly classify target domain samples, it is necessary to maintain the categorical information in the target sample during the iterative adaptation process. Eq. (7) contains a supervision term that encourages the adapted target samples to be discriminative for the source classification models. However, as the energy function E_θ operates only in the $\mathcal{X}$ space and the sampling process of Langevin dynamics tends to result in random samples from the sampled distribution that are independent of the starting point, there is no categorical information considered during the adaptation procedure.

To achieve label-preserving adaptation, we introduce a categorical latent variable $\mathbf{z}$ into the energy function to guide the adaptation of target samples to preserve the category information. With the latent variable, the energy function E_θ is defined in the joint space of $\mathcal{X} \times \mathcal{Z}$. The categorical information contained in $\mathbf{z}$ will be explicitly incorporated into the iterative adaptation. To do so, we define the energy-based model with the categorical latent variable as:

$$p_{\theta,\phi}(\mathbf{x},\mathbf{y}) = \int p_{\theta,\phi}(\mathbf{x},\mathbf{y},\mathbf{z})d\mathbf{z} = \int p_\phi(\mathbf{y}|\mathbf{z},\mathbf{x})p_\phi(\mathbf{z}|\mathbf{x})\frac{\exp(-E_\theta(\mathbf{x}|\mathbf{z}))}{Z_{\theta,\phi}}d\mathbf{z}, \tag{8}$$

where ϕ denotes the parameters of the classification model that predicts $\mathbf{z}$ and $\mathbf{y}$ and E_θ denotes the energy function that models the distribution of $\mathbf{x}$ considering the information of latent variable $\mathbf{z}$. $\mathbf{z}$ is trained to contain sufficient categorical information of $\mathbf{x}$ and serves as the conditional attributes that guide the adapted samples $\mathbf{x}$ preserving the categorical information. Once obtained from the original input $\mathbf{x}$, $\mathbf{z}$ is fixed and taken as the input of the energy function together with the updated $\mathbf{x}$ in each iteration. Intuitively, when $\mathbf{x}$ is updated from the target domain to the source domain via Langevin dynamics, $\mathbf{z}$ helps it preserve the classification information contained in the original $\mathbf{x}$, without introducing additional information.

To learn the latent variable $\mathbf{z}$ with more categorical information, we estimate $\mathbf{z}$ by variational inference and design a variational posterior $q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})$, where $\mathbf{d}_\mathbf{x}$ is the average representation of samples from the same category as $\mathbf{x}$ on the source domain. Therefore, $q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})$ can be treated as a probabilistic prototypical representation of a class. By incorporating $q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})$ into eq. (8), we obtain the lower bound of the log-likelihood:

$$\log p_{\theta,\phi}(\mathbf{x},\mathbf{y}) \geq \mathbb{E}_{q_\phi}[\log p_\phi(\mathbf{y}|\mathbf{z},\mathbf{x}) - E_\theta(\mathbf{x},\mathbf{z}) - \log Z_{\theta,\phi}] + \mathbb{D}_{\mathrm{KL}}[q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})||p_\phi(\mathbf{z}|\mathbf{x})]. \tag{9}$$

Note that in eq. (9), the categorical latent variable $\mathbf{z}$ is incorporated into both the classification model $p_\phi(\mathbf{y}|\mathbf{z},\mathbf{x})$ and the energy function $E_\theta(\mathbf{x}|\mathbf{z})$. The energy function contains both data information

and categorical information. During the Langevin dynamics update for sample adaptation, the latent variable provides categorical information in each iteration, which enables the adapted target samples to be discriminative.

By incorporating eq. (9) into eq. (6), we derive the objective function with the categorical latent variable as:

$$\begin{aligned}\mathcal{L}_f = &\mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\Big[\mathbb{E}_{q_\phi(\mathbf{z})}[-\log p_\phi(\mathbf{y}|\mathbf{z},\mathbf{x})] + \mathbb{D}_{\mathrm{KL}}[q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})||p_\phi(\mathbf{z}|\mathbf{x})]\Big] + \mathbb{E}_{q_\phi(\mathbf{z})}\Big[\mathbb{E}_{p_d(\mathbf{x})}[E_\theta(\mathbf{x}|\mathbf{z})] \\ &- \mathbb{E}_{\mathrm{stop_grad}(\mathrm{q}_\theta(\mathbf{x}))}[E_\theta(\mathbf{x},\mathbf{z})]\Big] + \mathbb{E}_{q_\theta(\mathbf{x})}\Big[\mathbb{E}_{q_{\mathrm{stop_grad}(\phi)}(\mathbf{z})}\big[E_{\mathrm{stop_grad}(\theta)}(\mathbf{x},\mathbf{z}) \\ &- \log p_{\mathrm{stop_grad}(\phi)}(\mathbf{y}|\mathbf{z},\mathbf{x})\big] - \mathbb{D}_{\mathrm{KL}}[q_{\mathrm{stop_grad}(\phi)}(\mathbf{z}|\mathbf{d}_\mathbf{x})||p_{\mathrm{stop_grad}(\phi)}(\mathbf{z}|\mathbf{x})]\Big],\end{aligned} \tag{10}$$

where $p_d(\mathbf{x})$ and $q_\theta(\mathbf{x})$ denote the data distribution and the t sequential MCMC samplings from the energy-based distribution of the source domain D_s. Similar to eq. (7), the first term trains the classification model on the source data. The second term trains the energy function to model the source data distribution. The last term is conducted on the adapted samples to supervise the adaptation procedure. The complete derivation is provided in Appendix A.

Ensemble inference. Since the target data is inaccessible during training, we train the specific parameters θ and ϕ to model each source distribution by adapting the samples from other source domains to the current source distribution. In each iteration, we train the energy-based model θ^i of one randomly selected source domain D_s^i. The adapted samples generated by samples $\mathbf{x}^j, \mathbf{x}^k$ from the other source domains D_s^j, D_s^k are used as the negative samples while $\mathbf{x}^i$ as the positive samples to train the energy-based model. During inference, the target sample is adapted to each source distribution with the specific energy function and predicted by the specific classifier. After that, we combine the predictions of all source domain models to obtain the final prediction:

$$p(\mathbf{y}_t) = \frac{1}{S}\sum_{i=1}^{S}\frac{1}{N}\sum_{n=1}^{N} p_{\phi^i}(\mathbf{y}|\mathbf{z}^n,\mathbf{x}) \qquad \mathbf{z}^n \sim p(\mathbf{z}^n|\mathbf{x}_t), \mathbf{x} \sim p_{\theta^i}(\mathbf{x}). \tag{11}$$

Here ϕ^i and θ^i denote the domain specific classification model and energy function of domain D_s^i. Note that since the labels of the $\mathbf{x}^t$ are unknown, $\mathbf{d}_{\mathbf{x}^t}$ in eq. (10) is not available during inference. Therefore, we draw $\mathbf{z}^n$ from the prior distribution $p(\mathbf{z}^n|\mathbf{x}_t)$, where $\mathbf{x}_t$ is the original target sample without any adaptation. With fixed $\mathbf{z}^n$, $\mathbf{x} \sim p_{\theta^i}(\mathbf{x})$ are drawn by Langevin dynamics as in eq. (2) with the target samples $\mathbf{x}^t$ as the initialization sample. $p_{\theta^i}(\mathbf{x})$ denotes the distributions modeled by the energy function $E_{\theta^i}(\mathbf{x}|\mathbf{z}^n)$. Moreover, to be efficient, the feature extractor is shared by all source domains and only the energy functions and classifiers are domain specific. We deploy the energy-based model on feature representations rather than on raw images, which leads to lighter neural networks for domain specific energy functions and classification models. We provide the training and inference algorithms in Appendix B.

3 EXPERIMENTS

Datasets. We conduct our experiments on five widely used datasets for domain generalization, **PACS** (Li et al., 2017), **Office-Home** (Venkateswara et al., 2017), **DomainNet** (Peng et al., 2019), and **Rotated MNIST and Fashion-MNIST**. Since we conduct the energy-based distribution on the feature space, our method can also handle other data formats. Therefore, we also evaluate the method on **PHEME** (Zubiaga et al., 2016), which is a dataset for natural language processing. PACS consists of 9,991 images of seven classes from four domains, i.e., *photo*, *art-painting*, *cartoon* and *sketch*. We use the same training and validation split as (Li et al., 2017) and follow their "leave-one-out" protocol. Office-Home also contains four domains, i.e., *art*, *clipart*, *product* and *real-world*, which totally have 15,500 images of 65 categories. DomainNet is more challenging since it has six domains i.e., *clipart*, *infograph*, *painting*, *quickdraw*, *real*, *sketch*, with 586,575 examples of 345 classes. We use the same experimental protocol as PACS. We utilize the Rotated MNIST and Fashion-MNIST dataset by following the settings in Piratla et al. (Piratla et al., 2020). PHEME is a dataset for rumour detection. There are a total of 5,802 tweets labelled as rumourous or non-rumourous from 5 different events, i.e., *Charlie Hebdo*, *Ferguson*, *German Wings*, *Ottawa Shooting*, and *Sydney Siege*. Same as PACS, we evaluate our methods on PHEME also by the "leave-one-out" protocol.

Table 1: **Benefit of energy-based test sample adaptation.** Experiments on PACS using a ResNet-18 averaged over five runs. Optimized by eq. (7), our model improves after adaptation. With the latent variable (eq. 10) performance improves further, both before and after adaptation.

	Adaptation	**Photo**	**Art-painting**	**Cartoon**	**Sketch**	*Mean*
Without latent variable (eq. 7)	✗	94.73 ±0.22	78.66 ±0.59	78.24 ±0.71	78.34 ±0.62	82.49 ±0.26
	✓	94.59 ±0.16	80.45 ±0.52	79.98 ±0.51	**79.23** ±0.32	83.51 ±0.30
With latent variable (eq. 10)	✗	95.12 ±0.41	79.79 ±0.64	79.15 ±0.37	**79.28** ±0.82	83.33 ±0.43
	✓	**96.05** ±0.37	**82.28** ±0.31	**81.55** ±0.65	**79.81** ±0.41	**84.92** ±0.59

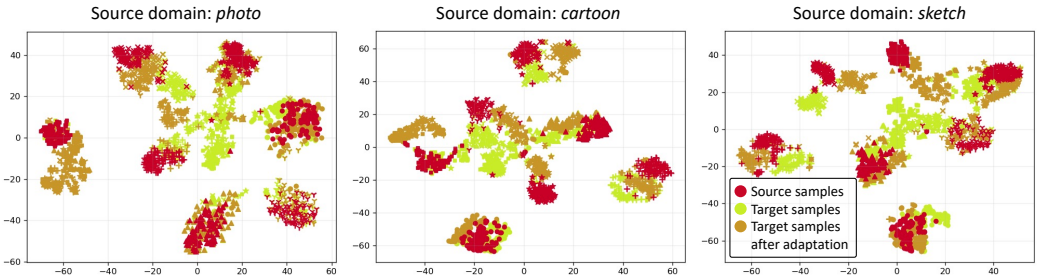

Figure 2: **Benefit of energy-based test sample adaptation.** Different shapes denote different classes. From left to right: adaptation to the source domains *photo*, *cartoon*, and *sketch* of samples from the target domain *art-painting*. After adaptation, the target samples (●) are more close to the source data (●) than before (●), demonstrating the effectiveness of our method. Best viewed in color.

Implementation details. We evaluate on PACS and Office-Home with both a ResNet-18 and ResNet-50 (He et al., 2016) backbone and on DomainNet with a ResNet-50. The backbones are pretrained on ImageNet (Deng et al., 2009). On PHEME we conduct the experiments based on a pretrained DistilBERT (Sanh et al., 2019), following (Wright & Augenstein, 2020). The hyperparameters and other details are provided in Appendix C.

Benefit of energy-based test sample adaptation. We first investigate the effectiveness of our energy-based test sample adaptation in Table 1. Before adaptation, we evaluate the target samples directly by the classification model of each source domain and ensemble the predictions. After the adaptation to the source distributions, the performance of the target samples improves, especially on the *art-painting* and *cartoon* domains, demonstrating the benefit of the iterative adaptation by our energy-based model. The results of models with latent variable, i.e., trained by eq. (10), are shown in the last two rows. With the latent variable, the performance is improved both before and after adaptation, which shows the benefit of incorporating the latent variable into the classification model. The performance improvement after adaptation is also more prominent than without the latent variable, demonstrating the effectiveness of incorporating the latent variable into the energy function and Langevin dynamics. Figure 2 visualizes the source domain features and the target domain features both before and after the adaptation to each individual source domain.

Effectiveness of iterative test sample adaptation by Langevin dynamics. We also visualize the iterative adaptation of the target samples in Figure 3. In each subfigure, the target and source samples have the same label. The visualization shows that the target samples gradually approach the source data distributions during the iterative adaptation by Langevin dynamics. After adaptation, the predictions of the target samples on the source domain classifier also become more accurate. For instance, in Figure 3 (a), the target sample of the *house* category is predicted incorrectly, with a probability of *house* being only 0.02%. After adaptation, the probability becomes 99.7%, which is predicted correctly. More visualizations, including several failure cases, are provided in Appendix D.

Benefit for larger domain gaps. To show the benefit of our proposal for domain generalization scenarios with large gaps, we conduct experiments on rotated MNIST and Fashion MNIST. The results are shown in Figure 4. The models are trained on source domains with rotation angles from 15° to 75°, 30° to 60°, and 30° to 45°, and always tested on target domains with angles of 0° and 90°. As the number of domains seen during training decreases the domain gap between source and target increases, and the performance gaps between our method and others becomes more pronounced. Notably, when comparing our method with the recent test-time adaptation of Xiao et al. (2022), which

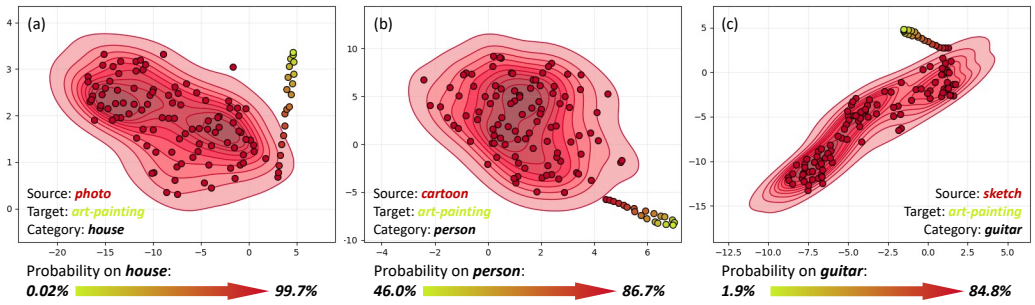

Figure 3: **Iterative adaptation of target samples.** We adapt the samples from target domain (*art-painting*) to different source domains (*photo*, *cartoon*, and *sketch* in (a), (b), (c)). Each subfigure shows the adaptation of one target sample. The adaptation procedure of the target samples is represented by the gradient color from green to red. In each figure, the target sample has the same label as the source data, but is mispredicted due to domain shifts. During adaptation, the target samples gradually approach the source distributions and eventually get correct predictions.

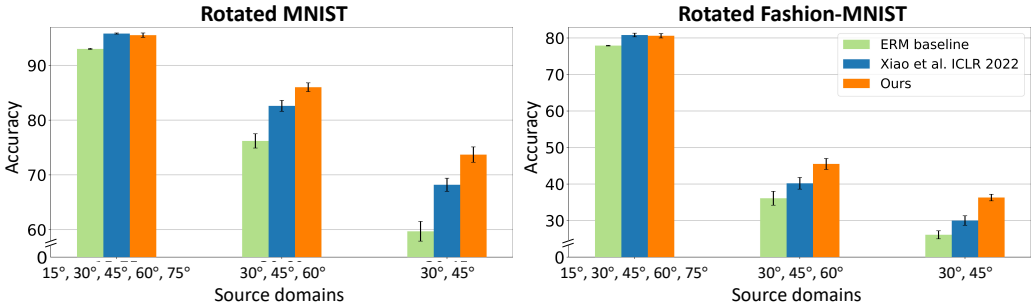

Figure 4: **Benefit for larger domain gaps.** We train on different source set distributions and evaluate on target sets with rotation angles of $0°$ and $90°$. As the domain gap between source and target sets increases, our method performs better than alternatives.

adapts a model to each target sample, shows adapting target samples better handles larger domain gaps than adapting the model.

Adaptation with different Langevin dynamics steps. We also investigate the effect of the Langevin dynamics step numbers during adaptation. Figure 5 shows the variety of the average energy and accuracy of the target samples adapted to the source distributions with different updating steps. The experiments are conducted on PACS with ResNet-18. The target domain is *art-painting*. With the step numbers less than 80, the average energy decreases consistently while the accuracy increases along with the increased number of updating steps, showing that the target samples are getting closer to the source distributions. When the step numbers are too large, the accuracy will decrease as the number of steps increases. We attribute this to $\mathbf{z}_t$ having imperfect categorical information, since it is approximated during inference from a single target sample $\mathbf{x}_t$ only. In this case, the label information would not be well preserved in $\mathbf{x}_t$ during the Langevin dynamics update, which causes an accuracy drop with a large number of updates. To demonstrate this, we conduct the experiment by replacing $p(\mathbf{z}_t)$ with $q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})$ during inference. $\mathbf{d}_\mathbf{x}$ is the class center of the same class as $\mathbf{x}_t$. Therefore, $q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})$ contains categorical information that is closer to the ground truth label. We regard this as the oracle model. As expected, the oracle

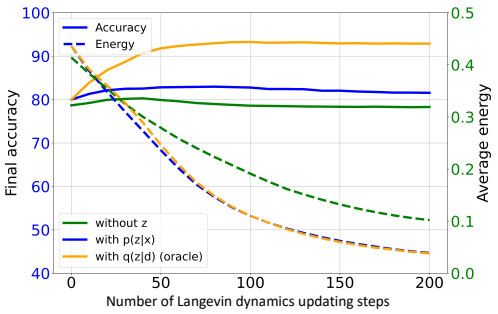

Figure 5: **Adaptation with different Langevin dynamics steps.** As the number of steps increases, energy decreases while accuracy increases. When the number of steps is too large, the accuracy without $\mathbf{z}$ or with $p(\mathbf{z}|\mathbf{x})$ drops slightly while the accuracy with $q(\mathbf{z}|\mathbf{d}_\mathbf{x})$ is more stable and better.

Table 2: **Comparisons on image and text datasets.** Our method achieves the best mean accuracy for all datasets, independent of the backbone.

	PACS		Office-Home		DomainNet	PHEME
	ResNet-18	ResNet-50	ResNet-18	ResNet-50	ResNet-50	DistilBERT
Iwasawa & Matsuo (2021)	81.40	85.10	57.00	68.30	-	-
Zhao et al. (2020)	81.46	85.34	-	-	-	-
Zhou et al. (2020a)	82.83	84.90	65.63	67.66	-	-
Gulrajani & Lopez-Paz (2020)	-	85.50	-	66.50	40.90	-
Wang et al. (2021)	83.09	86.23	64.13	67.99	-	75.8 ±0.23
Dubey et al. (2021)	-	84.50	-	68.90	43.90	-
Xiao et al. (2022)	84.15	**87.51**	66.02	71.07	-	76.1 ±0.21
This paper w/o adaptation	83.33 ±0.43	86.05 ±0.37	65.01 ±0.47	70.44 ±0.25	42.90 ±0.34	75.4 ±0.13
This paper w/ adaptation	**84.92** ±0.59	**87.70** ±0.28	**66.31** ±0.21	**72.07** ±0.38	**44.66** ±0.51	**76.5** ±0.18

model performs better as the number of steps increases and reaches stability after 100 steps. We also show the results without $\mathbf{z}$. We can see the performance and stability are both worse, which again demonstrates that $\mathbf{z}$ helps preserve label information in the target samples during adaptation. We provide visualizations and more analyses of $\mathbf{z}_t$ in Appendix D to further show that $\mathbf{z}_t$ captures the categorical information. In addition, the training and test time cost is also larger as the step number increases. Without adaptation, the test time cost for one test batch is about 0.05 second. The 20-step adaptation will take about 0.1 extra second. This number will increase to 0.25 second with 50 steps. To trade off the performance and time cost, we use 20 steps in the other experiments on PACS. More results and analysis is provided in Appendx E.

Comparisons on image datasets. PACS, Office-Home, and DomainNet are three widely used benchmarks in domain generalization. We conduct experiments on PACS and Office-Home based on both ResNet-18 and ResNet-50 and experiments on DomainNet based on ResNet-50. As shown in Table 2, our method achieves competitive and even the best overall performance in most cases. Moreover, our method performs better than most of the recent model adaptation methods (Iwasawa & Matsuo, 2021; Wang et al., 2021; Dubey et al., 2021). Compared with the most recent work (Xiao et al., 2022), our method is also competitive and even better. Table 2 also demonstrates the effectiveness of our sample adaptation. For each dataset and backbone, the proposed method achieves a good improvement after adaptation by the proposed discriminative energy-based model. We provide detailed comparisons on each target domain, as well as more experiments on corruption datasets and single source domain generalization, in Appendix E.

Generalization beyond image data. To show the generality of our method, we also conduct experiments on the natural language processing dataset PHEME. The dataset is proposed for rumour detection, which is a binary classification task. The results in Table 2 show similar conclusions as the image datasets. With adaptation, our method achieves a good improvement and performs better than the recent model adaptation methods. Detailed comparisons of each target domain are again provided in Appendix E.

4 Related Work

Domain generalization. One of the predominant methods is domain invariant learning (Muandet et al., 2013; Ghifary et al., 2016; Motiian et al., 2017; Seo et al., 2020; Zhao et al., 2020; Xiao et al., 2021a; Nguyen et al., 2021; Phung et al., 2021). Muandet et al. (2013) and Ghifary et al. (2016) learn domain invariant representations by matching the moments of features across source domains. Li et al. (Li et al., 2018b) further improved the model by learning conditional-invariant features. Recently, Mahajan et al. (2021) introduced causal matching to model within-class variations for generalization. Shi et al. (Shi et al., 2022) provided a gradient matching to encourage consistent gradient directions across domains. Different from these methods, Arjovsky et al. (2019) proposed invariant risk minimization to learn an invariant classifier, which is further improved by introducing an information bottleneck (Ahuja et al., 2021). Another widely used methodology is domain augmentation (Shankar et al., 2018; Volpi et al., 2018; Qiao et al., 2020; Zhou et al., 2020a;b; Yao et al., 2022), which generates more source domain data to simulate domain shifts during training. Meta-learning-based methods have also been studied for domain generalization (Li et al., 2018a; Balaji et al., 2018; Dou

et al., 2019; Bui et al., 2021). Li et al. (2018a) introduced the model agnostic meta-learning (Finn et al., 2017) into domain generalization. Du et al. (2020b) proposed the meta-variational information bottleneck for domain-invariant learning.

Domain generalization by test-time adaptation. Recently, adaptive methods have been proposed to better match the source-trained model and the target data at test time (Sun et al., 2020; Liang et al., 2020; Li et al., 2020; D'Innocente et al., 2019; Pandey et al., 2021; Iwasawa & Matsuo, 2021). Test-time adaptation (Sun et al., 2020; Wang et al., 2021; Liu et al., 2021; Zhou & Levine, 2021) fine-tunes (part of) a network trained on source domains by batches of target samples. Dubey et al. (2021) trained a domain embedding network and utilized a domain embedding of unlabeled data as auxiliary information for classification. Zhang et al. (2021) introduced adaptive risk minimization to optimize their model for effective adaptation to domain shifts. Xiao et al. (2022) proposed single-sample generalization that adapts a model to each target sample under a meta-learning framework. These methods adapt the model to the target samples. By contrast, in our work, we adapt the target data to source distributions by an energy-based model and predict the adapted samples with the source-trained classification model directly.

Energy-based model. The energy-based modelis a classical learning framework (Ackley et al., 1985; Hinton, 2002; Hinton et al., 2006; LeCun et al., 2006). Recently, (Xie et al., 2016; Nijkamp et al., 2019; 2020; Du & Mordatch, 2019; Du et al., 2021) further extend the energy-based model to high-dimensional data using contrastive divergence and Stochastic Gradient Langevin dynamics. Different from most of these works that only model the data distributions, some recent works model the joint distributions (Grathwohl et al., 2020; Xiao et al., 2021b). Grathwohl et al. (2020) modeled the joint distribution of data and labels to benefit classification. Xiao et al. (2021b) jointly model the distributions of data and latent variables of variational auto-encoder for image generation. In our work, we define the joint distribution of data and label to promote the classification of unseen target samples in domain generalization, and further incorporate a latent variable to incorporate the categorical information into the Langevin dynamics procedure. Energy-based models for various tasks have been proposed, e.g., image generation (Du & Mordatch, 2019; Du et al., 2020a; Nie et al., 2021), memory (Bartunov et al., 2020), out-of-distribution detection (Liu et al., 2020), and anomaly detection (Dehaene et al., 2020). Some methods also utilize energy-based models for domain adaptation (Zou et al., 2021; Xie et al., 2021; Kurmi et al., 2021). Different from these methods, we focus on domain generalization and utilize the energy-based model to express the source domain distributions without any target data during training. Instead, we adapt the target samples to the source distribution by Langevin dynamics at test time, without any fine-tuning operations.

5 Conclusion and Discussions

In this paper, we propose a discriminative energy-based model to adapt the target samples to the source data distributions for domain generalization. The energy-based model is designed on the joint space of input, output, and a latent variable, which is constructed by a domain specific classification model and an energy function. With the trained energy-based model, the target samples are adapted to the source distributions through Langevin dynamics and then predicted by the classification model. Since we aim to prompt the classification of the target samples, the model is trained to achieve label-preserving adaptation by incorporating the categorical latent variable. We evaluate the method on six image and text benchmarks. The results demonstrate its effectiveness and generality.

Compared with recent model adaptation methods, our method does not need to adjust the model parameters at test time, which requires batches of target samples to provide sufficient target information. One limitation of our proposed method is the iterative adaptation requirement for each target sample, which introduces an extra time cost in both training and test time. The problem can be mitigated by speeding up the energy minimization with optimization techniques during Langevin dynamics, e.g., Nesterov momentum (Nesterov, 1983), or by exploring one-step methods for target sample adaptation. We leave these explorations for future work. In addition, sample adaptation by Langevin dynamics is stochastic and might lead to the loss of the original information contained in the adapted samples. As a remedy that preserves the label information in the sample, we incorporate the categorical latent variable into the update in our discriminative energy model. Although the adapted samples remain stochastic, it does not hurt the classification tasks we consider. In fact our method achieves the best mean accuracy for all image and text datasets we consider.

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A DERIVATIONS

Derivation of energy-based sample adaptation. Recall our discriminative energy-based model

$$p_{\theta,\phi}(\mathbf{x},\mathbf{y}) = p_\phi(\mathbf{y}|\mathbf{x})\frac{\exp(-E_\theta(\mathbf{x}))}{Z_{\theta,\phi}}, \tag{12}$$

where $Z_{\theta,\phi} = \int p_\phi(\mathbf{y}|\mathbf{x})\exp(-E_\theta(\mathbf{x}))d\mathbf{x}d\mathbf{y}$ is the partition function. ϕ and θ denote the parameters of the classifier and energy function, respectively. To jointly train the parameters, we minimize the contrastive divergence proposed by Hinton (2002):

$$\mathcal{L} = \mathbb{D}_{\mathrm{KL}}[p_d(\mathbf{x},\mathbf{y})||p_{\theta,\phi}(\mathbf{x},\mathbf{y})] - \mathbb{D}_{\mathrm{KL}}[q_{\theta,\phi}(\mathbf{x},\mathbf{y})||p_{\theta,\phi}(\mathbf{x},\mathbf{y})], \tag{13}$$

where $p_d(\mathbf{x},\mathbf{y})$ denotes the the real data distribution and $q_{\theta,\phi}(\mathbf{x},\mathbf{y}) = \prod_\theta^t p(\mathbf{x},\mathbf{y})$ denotes t sequential MCMC samplings from the distribution expressed by the energy-based model (Du et al., 2021). The gradient of the first term with respect to θ and ϕ is

$$\begin{aligned}\nabla_{\theta,\phi}\mathbb{D}_{\mathrm{KL}}[p_d(\mathbf{x},\mathbf{y})||p_{\theta,\phi}(\mathbf{x},\mathbf{y})] &= \nabla_{\theta,\phi}\mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\big[\log\frac{p_d(\mathbf{x},\mathbf{y})}{p_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big] \\ &= \mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\big[\nabla_{\theta,\phi}\log p_d(\mathbf{x},\mathbf{y}) - \nabla_{\theta,\phi}\log p_{\theta,\phi}(\mathbf{x},\mathbf{y})\big] \\ &= \mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\big[-\nabla_{\theta,\phi}\log p_{\theta,\phi}(\mathbf{x},\mathbf{y})\big],\end{aligned} \tag{14}$$

while the gradient of the second term is

$$\begin{aligned}&\nabla_{\theta,\phi}\mathbb{D}_{\mathrm{KL}}[q_{\theta,\phi}(\mathbf{x},\mathbf{y})||p_{\theta,\phi}(\mathbf{x},\mathbf{y})] \\ =&\nabla_{\theta,\phi}\mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[\log\frac{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}{p_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big] \\ =&\nabla_{\theta,\phi}q_{\theta,\phi}(\mathbf{x},\mathbf{y})\nabla_{q_{\theta,\phi}}\mathbb{D}_{\mathrm{KL}}[q_{\theta,\phi}(\mathbf{x},\mathbf{y})||p_{\theta,\phi}(\mathbf{x},\mathbf{y})] + \mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[-\nabla_{\theta,\phi}\log p_{\theta,\phi}(\mathbf{x},\mathbf{y})\big].\end{aligned} \tag{15}$$

Combining eq. (14) and eq. (15), we have the overall gradient as:

$$\begin{aligned}\nabla_{\theta,\phi}\mathcal{L}_{all} = &-\big(\mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\big[\nabla_{\theta,\phi}\log p_{\theta,\phi}(\mathbf{x},\mathbf{y})\big] - \mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[\nabla_{\theta,\phi}\log p_{\theta,\phi}(\mathbf{x},\mathbf{y})\big] \\ &+ \nabla_{\theta,\phi}q_{\theta,\phi}(\mathbf{x},\mathbf{y})\nabla_{q_{\theta,\phi}}\mathbb{D}_{\mathrm{KL}}[q_{\theta,\phi}(\mathbf{x},\mathbf{y})||p_{\theta,\phi}(\mathbf{x},\mathbf{y})]\big).\end{aligned} \tag{16}$$

For the first two terms, the gradient can be further derived to

$$\begin{aligned}&\mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\big[\nabla_{\theta,\phi}\log p_{\theta,\phi}(\mathbf{x},\mathbf{y})\big] - \mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[\nabla_{\theta,\phi}\log p_{\theta,\phi}(\mathbf{x},\mathbf{y})\big] \\ =&\mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\big[\nabla_{\theta,\phi}(\log p_\phi(\mathbf{y}|\mathbf{x}) - E_\theta(\mathbf{x}) - \log Z_{\theta,\phi})\big] \\ -&\mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[\nabla_{\theta,\phi}(\log p_\phi(\mathbf{y}|\mathbf{x}) - E_\theta(\mathbf{x}) - \log Z_{\theta,\phi})\big].\end{aligned} \tag{17}$$

Moreover, $\nabla_{\theta,\phi}\log Z_{\theta,\phi}$ can be written as the expectation $\mathbb{E}_{p_{\theta,\phi}(\mathbf{x},\mathbf{y})}[\nabla_\phi\log p_\phi(\mathbf{y}|\mathbf{x}) - \nabla_\theta E_\theta(\mathbf{x})]$ (Song & Kingma, 2021; Xiao et al., 2021b), which is therefore canceled out in eq. (17) (Hinton, 2002). We then have the loss function for the first two terms as

$$\mathcal{L}_1 = \mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\big[E_\theta(\mathbf{x}) - \log p_\phi(\mathbf{y}|\mathbf{x})\big] - \mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[E_\theta(\mathbf{x}) - \log p_\phi(\mathbf{y}|\mathbf{x})\big]. \tag{18}$$

Furthermore, we have the loss function

$$\begin{aligned}\mathcal{L}_2 &= \mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[\log\frac{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}{p_{stop_grad(\theta,\phi)}(\mathbf{x},\mathbf{y})}\big] \\ &= -\mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[\log p_{stop_grad(\phi)}(\mathbf{y}|\mathbf{x}) - E_{stop_grad(\theta)}(\mathbf{x}) - \log Z_{stop_grad(\theta,\phi)}\big] \\ &\quad + \mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[\log q_{\theta,\phi}(\mathbf{x},\mathbf{y})\big],\end{aligned} \tag{19}$$

which has the same gradient as the last term in eq. (16) (Du et al., 2021). The $stop_grad$ here means that we do not backpropagate the gradients to update the parameters by the corresponding forward functions. Thus, these parameters can be treated as constants.

Since the gradient of θ and ϕ is stopped in $\log Z_{stop_grad(\theta,\phi)}$, we treat it as a constant independent of $q_{\theta,\phi}(\mathbf{x},\mathbf{y})$ and therefore remove it from the eq. (19). In addition, the term $\mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[\log p_\phi(\mathbf{y}|\mathbf{x})\big]$ in eq. (18) encourages wrong prediction of the updated samples from $q_{\theta,\phi}(\mathbf{x},\mathbf{y})$, which goes against

Table 3: Implementation details of our method per dataset and backbone.

Dataset	Backbone	Backbone learning rate	Step size	Number of steps
PACS	ResNet-18	0.00005	50	20
	ResNet-50	0.00001	50	20
Office-Home	ResNet-18	0.00001	100	20
	ResNet-50	0.00001	100	20
Rotated MNIST	ResNet-18	0.00005	50	20
Fashion-MNIST	ResNet-18	0.00005	50	20
PHEME	DistilBERT	0.00003	40	20

our goal of promoting classification by adapting target samples. The term $\mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[\log q_{\theta,\phi}(\mathbf{x},\mathbf{y})\big]$ in eq. (19) can be treated as a negative entropy of $q_{\theta,\phi}(\mathbf{x},\mathbf{y})$, which is always negative and hard to estimate. Therefore, we remove these two terms in the final loss function by applying an upper bound of the combination of eq. (18) and eq. (19) as:

$$\begin{aligned}\mathcal{L} = &-\mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\big[\log p_\phi(\mathbf{y}|\mathbf{x})\big] + \mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\big[E_\theta(\mathbf{x})\big] - \mathbb{E}_{\text{stop_grad}(\mathrm{q}_{\theta,\phi}(\mathbf{x},\mathbf{y}))}\big[E_\theta(\mathbf{x})\big] \\ &+ \mathbb{E}_{q_{\theta,\phi}(\mathbf{x},\mathbf{y})}\big[E_{\text{stop_grad}(\theta)}(\mathbf{x}) - \log p_{\text{stop_grad}(\phi)}(\mathbf{y}|\mathbf{x})\big].\end{aligned} \tag{20}$$

Energy-based sample adaptation with categorical latent variable. To keep the categorical information during sample adaptation, we introduce a categorical latent variable $\mathbf{z}$ into our discriminative energy-based model, which is defined as $p_{\theta,\phi}(\mathbf{x},\mathbf{y}) = \int p_{\theta,\phi}(\mathbf{x},\mathbf{y},\mathbf{z})d\mathbf{z} = \int p_\phi(\mathbf{y}|\mathbf{z},\mathbf{x})p_\phi(\mathbf{z}|\mathbf{x})\frac{\exp(-E_\theta(\mathbf{x}|\mathbf{z}))}{Z_{\theta,\phi}}d\mathbf{z}$. We optimize the parameters θ and ϕ also by the contrastive divergence $\mathbb{D}_{\mathrm{KL}}[p_d(\mathbf{x},\mathbf{y})||p_{\theta,\phi}(\mathbf{x},\mathbf{y})] - \mathbb{D}_{\mathrm{KL}}[q_{\theta,\phi}(\mathbf{x},\mathbf{y})||p_{\theta,\phi}(\mathbf{x},\mathbf{y})]$, which has similar gradient as eq. (14) and eq. (15). The latent variable $\mathbf{z}$ is estimated by variational inference, leading to a lower bound of $\log p_{\theta,\phi}(\mathbf{x},\mathbf{y}) \geq \mathbb{E}_{q_\phi(\mathbf{z})}[\log p_\phi(\mathbf{y}|\mathbf{z},\mathbf{x}) - E_\theta(\mathbf{x}|\mathbf{z}) - \log Z_{\theta,\phi}] + \mathbb{D}_{\mathrm{KL}}[q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})||p_\phi(\mathbf{z}|\mathbf{x})]$. We can then obtain the final loss function of the contrastive divergence in a similar way as eq. (20) by estimating the gradient and remove the terms that are hard to estimate or conflict to our final goal. The final objective function is:

$$\begin{aligned}\mathcal{L}_f = &\mathbb{E}_{p_d(\mathbf{x},\mathbf{y})}\Big[\mathbb{E}_{q_\phi(\mathbf{z})}[-\log p_\phi(\mathbf{y}|\mathbf{z},\mathbf{x})] + \mathbb{D}_{\mathrm{KL}}[q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})||p_\phi(\mathbf{z}|\mathbf{x})]\Big] + \mathbb{E}_{q_\phi(\mathbf{z})}\Big[\mathbb{E}_{p_d(\mathbf{x})}[E_\theta(\mathbf{x}|\mathbf{z})] \\ &- \mathbb{E}_{\text{stop_grad}(\mathrm{q}_\theta(\mathbf{x}))}[E_\theta(\mathbf{x},\mathbf{z})]\Big] + \mathbb{E}_{q_\theta(\mathbf{x})}\Big[\mathbb{E}_{q_{\text{stop_grad}(\phi)}(\mathbf{z})}\big[E_{\text{stop_grad}(\theta)}(\mathbf{x},\mathbf{z}) \\ &- \log p_{\text{stop_grad}(\phi)}(\mathbf{y}|\mathbf{z},\mathbf{x})\big] - \mathbb{D}_{\mathrm{KL}}[q_{\text{stop_grad}(\phi)}(\mathbf{z}|\mathbf{d}_\mathbf{x})||p_{\text{stop_grad}(\phi)}(\mathbf{z}|\mathbf{x})]\Big],\end{aligned} \tag{21}$$

B Algorithm

We describe the detailed training and test algorithm of our energy-based sample adaptation in Algorithm 1.

C Implementation details

Model. To be efficient, we train a shared backbone for all source domains while a domain-specific classifier and a neural-network-based energy function for each source domain. Both the prior distribution $p_\phi(\mathbf{z}|\mathbf{x})$ and posterior distribution $q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})$ of the latent variable $\mathbf{z}$ are generated by a neural network ϕ that consists of four fully connected layers with ReLU activation, which outputs the mean and variance of the distribution. Deployed on feature representations, the energy function consists of three fully connected layers with two dropout layers. The latent variable $\mathbf{z}$ is incorporated into the energy function by concatenating with the feature representation $\mathbf{x}$. We use the *swish* function as activation in the energy functions (Du et al., 2021). An illustration of our model is shown in Figure 6.

Training details and hyperparameters. We evaluate on PACS with both a ResNet-18 and ResNet-50 backbone, pretrained on ImageNet. We use Adam optimization and train for 10,000 iterations with a

Algorithm 1 Energy-based sample adaptation

TRAINING TIME

Require: Source domains $\mathcal{D}_s = \{D_s^i\}_{i=1}^S$ each with joint distribution $p_{d_s^i}(\mathbf{x}, \mathbf{y})$ of input data and label.
Require: Learning rate μ; the number of iterations N_{iter}; the number of steps K and step size λ of the energy function.
Initialize pretrained backbone ψ; $\phi^i, \theta^i, \mathcal{B}^i = \varnothing$ for each source domain D_s^i. ϕ: classification model; θ: neural-network-based energy function; $\mathcal{B}$: feature representations replay buffer.
for *iter* in N_{iter} **do**
  for D_s^i in $\mathcal{D}_s$ **do**
    Sample datapoints $\{(\mathbf{x}^i, \mathbf{y}^i)\} \sim p_{d_s^i}(\mathbf{x}, \mathbf{y})$.
    Sample datapoints $\{(\mathbf{x}^j, \mathbf{y}^j)\} \sim \{p_{d_s^j}(\mathbf{x}, \mathbf{y})\}_{j \neq i}$ with 50% probability and $\mathcal{B}$ otherwise.
    Feature representations $\mathbf{x}^i = f_\psi(\mathbf{x}^i), \mathbf{x}^j = f_\psi(\mathbf{x}^j)$
    for k in K **do**
      $\mathbf{x}_k^j \leftarrow \mathbf{x}_{k-1}^j - \nabla_{\mathbf{x}} E_{\theta^i}(\mathbf{x}_{k-1}^j | \mathbf{z}^j) + \omega, \quad \mathbf{z}^j \sim q_{\phi^i}(\mathbf{z}^j | \mathbf{d}_{\mathbf{x}^j}), \ \ \omega \sim \mathcal{N}(0, \sigma)$.
    end for
    $q_{\theta^i}(\mathbf{x}) \leftarrow \mathbf{x}_k^j, \qquad p_d(\mathbf{x}) \leftarrow p_{d_s^i}(\mathbf{x}^i)$.
    Update parameters: $(\psi, \phi^i) \leftarrow (\psi, \phi^i) - \lambda \nabla_{\psi, \phi^i} \mathcal{L}_{final}(p_d(\mathbf{x}))$
      //Gradient of the first term in $\mathcal{L}_{final}$ (eq. 21)
      $\theta^i \leftarrow \theta^i - \lambda \nabla_{\theta^i} \mathcal{L}_{final}(p_d(\mathbf{x}), q_{\theta^i}(\mathbf{x}))$.
      // Gradient of the last three terms in $\mathcal{L}_{final}$ (eq. 21)
    $\mathcal{B}^i \leftarrow \mathcal{B}^i \cup \mathbf{x}_k^j$
  end for
end for

TEST TIME

Require: Source domains $\mathcal{D}_s = \{D_s^i\}_{i=1}^S$; target samples $\mathbf{x}_t$ from the target domain; trained backbone ψ and domain specific model ϕ^i, θ^i for each source domain D_s^i.
Feature representation $\mathbf{x}_t = f_\psi(\mathbf{x}_t)$.
for D_s^i in $\mathcal{D}_s$ **do**
  for k in K **do**
    $\mathbf{x}_{t,k} \leftarrow \mathbf{x}_{t,k-1} - \nabla_{\mathbf{x}} E_{\theta^i}(\mathbf{x}_{t,k-1} | \mathbf{z}_t) + \omega, \quad \mathbf{z}_t \sim p_{\phi^i}(\mathbf{z}_t | \mathbf{x}_t), \ \ \omega \sim \mathcal{N}(0, \sigma)$.
  end for
  $\mathbf{y}_t^i = p_{\phi^i}(\mathbf{y}_t | \mathbf{x}_{t,k}, \mathbf{z}_t)$
end for
return $\mathbf{y}_t = \frac{1}{S} \sum_{i=1}^S \mathbf{y}_t^i$.

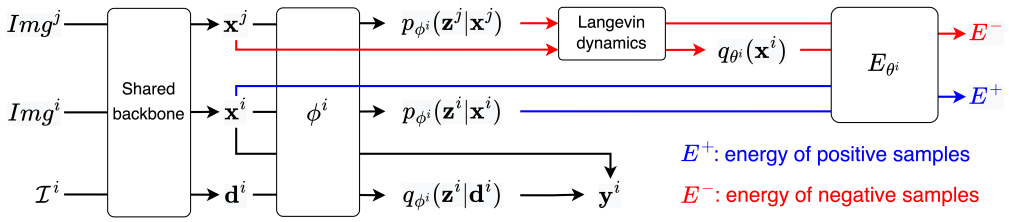

Figure 6: **Overall process of the proposed sample adaptation by discriminative energy-based model.** In each iteration, we train the classification model ϕ^i and energy function E_{θ^i} of one source domain D^i. The shared backbone and ϕ^i are trained by the images Img^i with the cross-entropy loss and KL divergence between $p_{\phi^i}(\mathbf{z}^i)$ and $q_{\phi^i}(\mathbf{z}^i)$. $\mathcal{I}^i$ denotes one batch of images from D^i, which generate the center features $\mathbf{d}^i$. The energy function E_{θ^i} is trained by using $\mathbf{x}^i$ as positive samples and adapted samples $q_{\theta^i}(\mathbf{x}^i)$ generated by $\mathbf{x}^j$ from other domains as negative samples. The adaptation is achieved by Langevin dynamics of E_{θ^i}. In inference, the target samples are adapted by Langevin dynamics of the energy function E_θ of each source domain and then predicted by eq. (11) in the main paper.

batch size of 128. We set the learning rate to 0.00005 for ResNet-18, 0.00001 for ResNet-50, and 0.0001 for the energy-based model and classification model. We use 20 steps of Langevin dynamics sampling to adapt the target samples to source distributions, with a step size of 50. Most of the

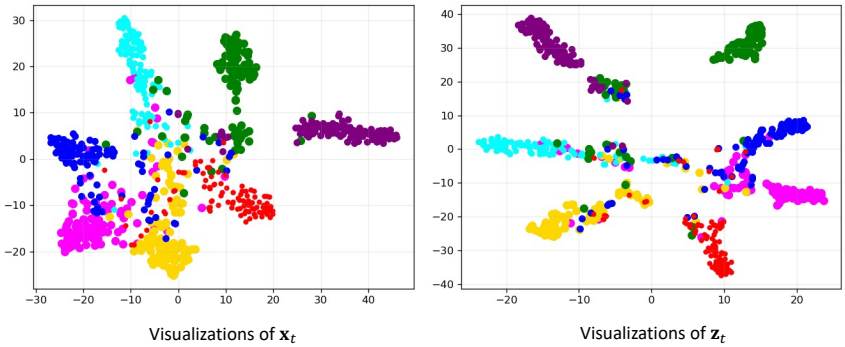

Figure 7: **Visualizations of the target features $\mathbf{x}_t$ and categorical latent variables $\mathbf{z}_t$.** We use *art-painting* on PACS as the target domain. Different colors denote different categories. $\mathbf{z}_t$ is obtained by $p_\phi(\mathbf{z}_t|\mathbf{x}_t)$. Most data points of z_t are clustered according to their labels, demonstrating that z_t can capture the categorical information.

experimental settings on Office-Home are the same as on PACS. The learning rate of the backbone is set to 0.00001 for both ResNet-18 and ResNet-50. For fair comparison, we evaluate the rotated MNIST and Fashion-MNIST with ResNet-18, following (Piratla et al., 2020). The other settings are also the same as PACS. On PHEME we conduct the experiments based on a pretrained DistilBERT. We set the learning rate as 0.00003 and use 20 steps of Langevin dynamics with a step size of 20.

We train all models on an NVIDIA Tesla V100 GPU for 10,000 iterations. The learning rates of the backbone are different for different datasets as shown in Table 3. The learning rates of the domain-specific classifiers and energy functions are both set to 0.0001 for all datasets. For each source domain, we randomly select 128 samples as a batch to train the backbone and classification model. We also select 128 samples from the other source domains together with the current domain samples to train the domain specific energy function. We use a replay buffer of size of 500 feature representations and apply spectral normalization on all weights of the energy function (Du & Mordatch, 2019). We use random noise with standard deviation $\lambda = 0.001$ and clip the gradients to have individual value magnitude of less than 0.01 similar to (Du & Mordatch, 2019). The step size and number of steps for Langevin dynamics are different for different datasets as shown in Table 3.

D VISUALIZATIONS

Visualizations of features and latent variables. To further show that $\mathbf{z}$ captures the categorical information in $\mathbf{x}$, we visualized the features $\mathbf{x}_t$ and latent variables $\mathbf{z}_t$ of the target samples in Figure 7, which shows that $\mathbf{z}_t$ actually captures the categorical information. Moreover, $\mathbf{z}_t$ is more discriminative than $\mathbf{x}_t$ as shown in the figure. Although $\mathbf{z}_t$ is approximated by only $\mathbf{x}_t$ during inference. It provides better categorical information because it is trained to do so. That is, during training, we minimize the KL divergence between $q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})$ and $p_\phi(\mathbf{z}|\mathbf{x})$ as in eq. (9) where $q_\phi(\mathbf{z}|\mathbf{d}_\mathbf{x})$ is essentially the class prototype containing the categorical information. As a result, the inference model of $p_\phi(\mathbf{z}|\mathbf{x})$ learns the ability to extract categorical information from a single sample.

More visualizations of the adaptation procedure. To further show the effectiveness of the iterative adaptation of target samples, we provide more visualizations on PACS in Figure 8. Subfigures in different rows show the adaptation of samples from different target domains to source domains. Similar with the visualizations in the main paper, the target samples gradually approach the source data distributions during the iterative adaptation. Therefore, the predictions of the target samples on the source domain classifier become more accurate after adaptation.

Failure cases. We also provide some failure cases on PACS in Figure 9 to gain more insights in our method. Our method is confused with samples that have objects of different categories (first row) and multiple objects or complex background (last three rows). A possible reason is that there is much noisy information contained in the latent variable of these samples, leading to adaptation without a clear direction, which behaves as wrong adaptation directions, e.g., visualization in row 1 column 4, or unstable updates with fluctuations in small regions, e.g., visualizations in row 2 column 3 and

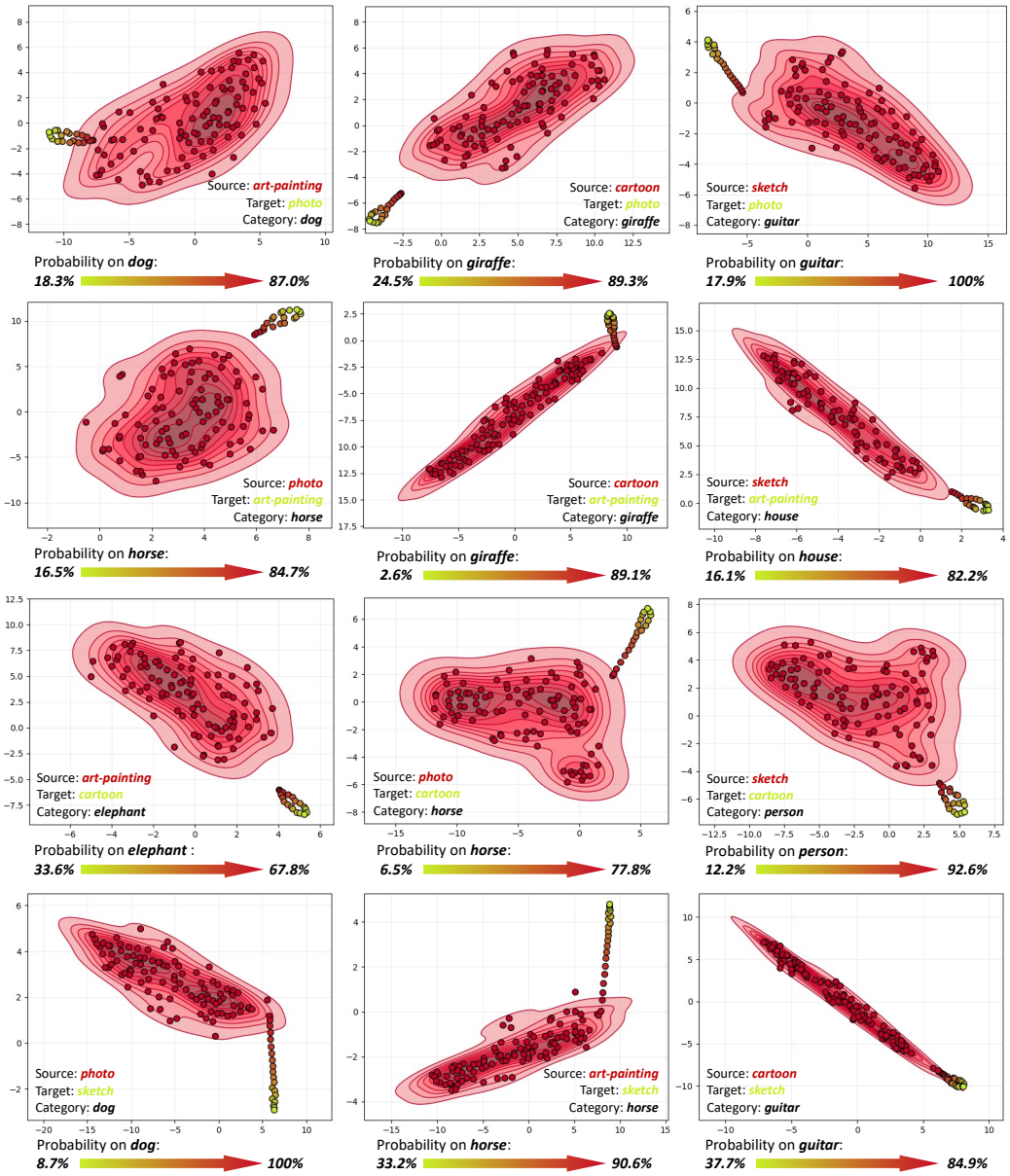

Figure 8: **More visualizations of the iterative adaptation on PACS.** We visualize the adaptation of samples from different target domains to source domains on PACS. Each subfigure shows the adaptation of one target sample to one source domain. The adaptation procedure of the target samples is represented by the gradient color from green to red. In each figure, the target sample has the same label as the source data, but is mispredicted due to domain shifts. During adaptation, the target samples gradually approach the source distributions and eventually get correct predictions.

row 3 column 4. Obtaining the latent variable with more accurate and clear categorical information can be one solution for these failure cases. We can also solve the problem by achieving more stable adaptations with some optimization techniques like Nesterov momentum (Nesterov, 1983). Moreover, although failing in these cases, the adaptation of the target sample to some source domains still improves the performance, e.g., the adaptation of the *photo* sample (row 1 column 2) and *cartoon* sample (row 3 column 3) to the *art-painting* domain and the adaptation of the *sketch* sample (row 4 column 4) to the *cartoon* domain, which further demonstrate the effectiveness of our iterative sample adaptation through the energy-based model. The results motivate another solution for these failure

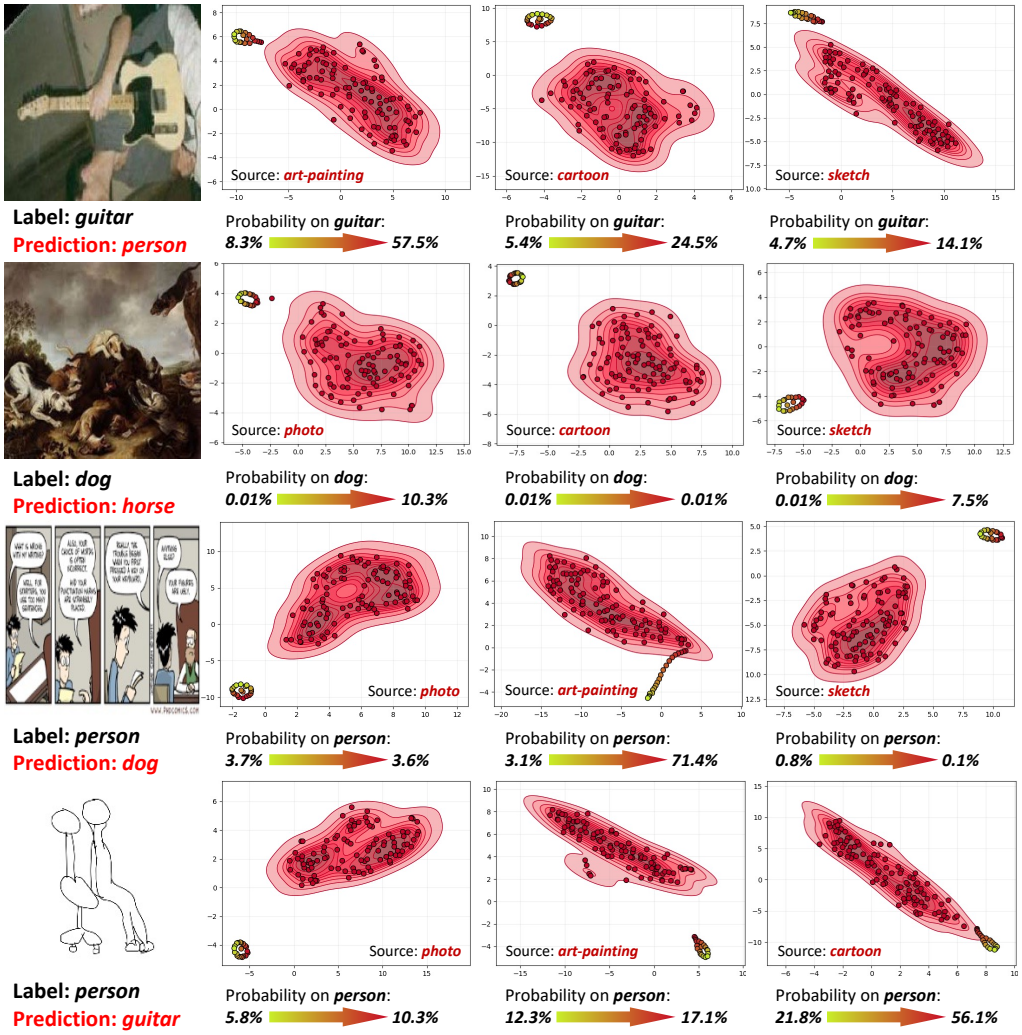

Figure 9: **Failure case visualizations of our method on PACS.** The visualization settings are the same as Figure 8. Our method makes wrong predictions on samples with complex background or multiple objects. However, our method still achieves good adaptation of these target samples to some source domains, which shows its effectiveness.

Table 4: **Training cost of the proposed method.** Compared with ERM, our method has about 20% more parameters, most of which come from the energy functions of source domains. Similar to test time, the time cost of training increases along with the number of steps of the energy-based model.

	Parameters	Adaptation steps	10000 iterations training time
ERM	11.18M	-	6.2 h
		20	7.9 h
		40	9.4 h
This paper	13.73M	60	10.6 h
		80	12.1 h
		100	14.0 h

cases, which is to learn to select the best source domain, or top-n source domains for adaptation and prediction of each target sample. We leave these explorations for future work.

Table 5: **Comparisons on PACS.** Our method achieves best mean accuracy with a ResNet-18 backbone and is competitive with ResNet-50.

Backbone	Method	**Photo**	**Art-painting**	**Cartoon**	**Sketch**	*Mean*
ResNet-18	Dou et al. (2019)	94.99	80.29	77.17	71.69	81.04
	Iwasawa & Matsuo (2021)	-	-	-	-	81.40
	Zhao et al. (2020)	**96.65**	80.70	76.40	71.77	81.46
	Wang et al. (2021)	95.49	81.55	77.67	77.64	83.09
	Zhou et al. (2020b)	96.10	**84.10**	78.80	75.90	83.70
	Xiao et al. (2022)	95.87	82.02	79.73	78.96	84.15
	This paper	96.05 ±0.37	82.28 ±0.31	**81.55** ±0.65	**79.81** ±0.41	**84.92** ±0.59
ResNet-50	Dou et al. (2019)	95.01	82.89	80.49	72.29	82.67
	Dubey et al. (2021)	-	-	-	-	84.50
	Iwasawa & Matsuo (2021)	-	-	-	-	85.10
	Zhao et al. (2020)	**98.25**	87.51	79.31	76.30	85.34
	Gulrajani & Lopez-Paz (2020)	97.20	84.70	80.80	79.30	85.50
	Wang et al. (2021)	97.96	86.30	82.53	78.11	86.23
	Seo et al. (2020)	95.99	87.04	80.62	**82.90**	86.64
	Xiao et al. (2022)	97.88	**88.09**	83.83	80.21	**87.51**
	This paper	97.67 ±0.14	**88.00** ±0.29	**84.75** ±0.39	80.40 ±0.38	**87.70** ±0.28

Table 6: **Comparisons on Office-Home.** Our method achieves the best mean accuracy using both a ResNet-18 and ResNet-50 backbone.

Backbone	Method	**Art**	**Clipart**	**Product**	**Real World**	*Mean*
ResNet-18	Iwasawa & Matsuo (2021)	47.00	46.80	68.00	66.10	57.00
	Wang et al. (2021)	56.45	52.06	73.19	74.82	64.13
	Xiao et al. (2022)]	59.39	**53.94**	**74.68**	76.07	66.02
	This paper	**60.08** ±0.33	**53.93** ±0.34	**74.50** ±0.39	**76.74** ±0.24	**66.31** ±0.21
ResNet-50	Gulrajani & Lopez-Paz (2020)	61.30	52.40	75.80	76.60	66.50
	Wang et al. (2021)	62.12	56.65	75.61	77.58	67.99
	Dubey et al. (2021)	-	-	-	-	68.90
	Xiao et al. (2022)	67.21	57.97	78.61	80.47	71.07
	This paper	**69.33** ±0.14	**58.37** ±0.30	**79.29** ±0.32	**81.26** ±0.26	**72.07** ±0.38

E DETAILED EXPERIMENTAL RESULTS

Time cost with different adaptation steps. As the number of steps increases, both the training and test time cost consistently increases for all target domains. The test time increases by more than 0.5 seconds for 100 iterations, which is ten times that without adaptation and might limit the application of the proposal. The training time cost is more than two times that for ERM for 100 iterations as shown in Table 4. Since the extra time cost is mainly caused by the iterative adaptation, potential solutions can be speeding up the Langevin dynamics with some optimization techniques like Nesterov momentum (Nesterov, 1983), or exploring some one-step methods for the target sample adaptation. In other experiments on PACS in the paper we use 20 steps for all target domains considering both the overall performance and the time cost.

Detailed comparisons. We provide the detailed performance of each target domain on PACS (Table 5), Office-Home (Table 6), and PHEME (Table 7). On PACS, our method achieves competitive results on each target domain and the best overall performance with both ResNet-18 and ResNet-50 as the backbone. Moreover, our method performs better than most of the recent model adaptation methods (Wang et al., 2021; Dubey et al., 2021; Iwasawa & Matsuo, 2021; Xiao et al., 2022). The conclusion on Office-Home and PHEME is similar to that on PACS. We achieve competitive and even better performance on each target domain.

Comparison with Tent. We also conducted experiments on rotated-MNIST to compare our method with Tent (Wang et al., 2021), which is a recent test-time adaptation method that fine-tunes the model with batches of target samples. We use images rotated from 15° to 75° as the source domains while 0° and 90° as the target ones. We implement Tent by fine-tuning the model for 10 steps with different

Table 7: **Generalization beyond image data.** Rumour detection on the PHEME microblog dataset. Our method achieves the best overall performance and is competitive in each domain.

	Charlie Hebdo	**Ferguson**	**German Wings**	**Ottawa Shooting**	**Sydney Siege**	*Mean*
ERM Baseline	79.4 $\pm$0.25	77.1 $\pm$0.36	**75.7** $\pm$0.12	68.2 $\pm$0.48	75.0 $\pm$0.28	75.1 $\pm$0.29
Wang et al. (2021)	80.1 $\pm$0.18	76.9 $\pm$0.56	74.7 $\pm$0.52	**72.0** $\pm$0.48	75.4 $\pm$0.34	75.8 $\pm$0.23
Xiao et al. (2022)	81.0 $\pm$0.52	77.2 $\pm$0.25	**75.7** $\pm$0.31	70.0 $\pm$0.46	**76.5** $\pm$0.22	76.1 $\pm$0.21
This paper	**81.8** $\pm$0.43	**77.8** $\pm$0.37	75.3 $\pm$0.14	**71.9** $\pm$0.28	75.6 $\pm$0.15	**76.5** $\pm$0.18

Table 8: **Comparison with Tent.** With limited test samples, Tent performs similar or even worse compared with the baseline while our method overcomes the lack of target samples.

Method	Number of samples for adaptation	Test accuracy
Baseline	-	94.22
Wang et al. (2021)	1	94.11
	32	94.46
	128	95.25
This paper	1	96.11

Table 9: **Experiments on CIFAR-10-C.** The model is trained on original data and evaluated on 15 different types of corruption. Our method achieves competitive results with Sun et al. (2020). Mimicking good domain shifts during training is important for our method.

Method	Error
Sun et al. (2020)	17.5
Wang et al. (2021)	**14.3**
This paper (noisy data as negative samples)	21.5
This paper (corrupted data as negative samples)	17.0

Table 10: **Domain similarity for ensemble prediction.** The experiments are conducted on PACS using ResNet-18. The results with cosine similarity and averaging are similar.

Settings	Photo	Art-painting	Cartoon	Sketch	*Mean*
Cosine similarity	95.93 $\pm$0.33	82.18 $\pm$0.37	81.24 $\pm$0.52	79.54 $\pm$0.77	84.76 $\pm$0.55
Average	96.05 $\pm$0.37	82.28 $\pm$0.31	81.55 $\pm$0.65	79.81 $\pm$0.41	84.92 $\pm$0.59

numbers of samples. These results are shown in Table 8. Since most of the model adaptation methods like Tent rely on batches of target samples for their test-time adaptation, our model will perform better in situations with very limited or even only one test sample. This is also demonstrated by the results in Table 8. Tent achieves slight improvements when adapted with small numbers of samples, e.g., 32, and even worse performance than baseline with one sample. By contrast, since our method achieves adaptation by adapting target samples to the source distributions without changing the source models, it overcomes the lack of target samples. The experiments are conducted on rotated-MNIST.

Results on CIFAR-10-C. To show the ability of our method of handling corruption distribution shifts and single source domain generalization, we conduct some experiments on CIFAR-10-C. We train the model on original data and evaluate it on the data with 15 types of corruption.

Since our method needs to mimic distribution shifts to train the discriminative energy-based model during training, for the single source domain setting, we generate the negative samples by adding random noise to the image and features of the clean data. We also use the other 4 corruption types (not contained in the evaluation corruption types) in CIFAR-10-C as the negative samples during training, which we regard as "corrupted data as negative samples". Note that these corrupted data are only used as negative samples to train the energy-based model. The number of source domains in test time is still one. As shown in Table 9, by mimicking better domain shifts during training, our method achieves competitive results with Sun et al. (Sun et al., 2020). The method performs worse with single source domain, although we generate extra negative samples to mimic the domain shifts. The reason can be that the randomly generated domain shifts do not well simulate the domain shift in test time.

Considering domain similarity for ensemble prediction. Since the final prediction in eq. (11) does not consider the domain similarity between target and source domains, we investigate the impact of such similarity for the final prediction. We compute the cosine similarity of the test sample to the center feature of each source domain as the importance for weighted prediction. Table 10 shows that the results considering domain similarity are close to the averaging method and even slightly worse. The reason can be that in our sample adaptation, we assume to be given only one test sample from an unknown target domain at a time. This makes it difficult to measure the closeness of the target domain to source domains.