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Bijective-Contrastive Estimation

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Abstract

In this paper, we propose a new classification-based learning criterion for energy-based models, called *Bijective-Contrastive Estimation* (BCE). We generate a collection of contrasting distributions using bijections, and solve all the classification problems between the original data distribution and the distributions induced by the bijections using a classifier parameterized by an energy model. We show that if the classification objective is minimized, the energy function will recover the data density up to a normalizing constant. This has the benefit of not having to explicitly specify a contrasting distribution, like noise contrastive estimation. Experimentally, we demonstrate that the proposed method works well on 2D synthetic datasets. We discuss the difficulty in high dimensional cases, and propose potential directions to explore for future work.

1. Introduction

Training energy-based models (EBM) via maximum likelihood estimation (MLE) is difficult. This is because likelihood evaluation under the density of the EBM requires computing the log-partition function, which involves an intractable integration. For numerical optimization, one only needs to estimate the gradient wrt the model parameters, but this still requires sampling from the energy model (Hinton, 2002), which itself is another hard problem and is often resolved by following some *Markov chain Monte Carlo* (MCMC) procedure. However, MCMC methods are notoriously computationally expensive and hard to tune, which prevents EBMs from being widely adopted among the practitioners. This computational bottleneck has therefore motivated the design of alternative training objectives of EBMs, such as score matching (SM, Hyvärinen (2005)), denoising score matching (DSM, Vincent (2011)), noise-contrastive estimation (NCE, Gutmann and Hyvärinen (2010)), and Stein discrepancy minimization (Liu et al., 2016; Grathwohl et al., 2020).

In our attempt to devise a new training criterion for EBMs, we draw inspiration from the recent development of flow-based methods. Notably, Dinh et al. (2019); Nielsen et al. (2020) demonstrate that the inverse model of a surjection map recovers the internal structure of the data distribution to a certain degree. In order to reconstruct the data distribution with a higher precision, a chain of bijection and surjection maps needs to be composed, resulting in solving multiple classification problems in sequel.

Motivated by this, we propose to use bijections to generate a collection of classification problems, which, when solved by parameterizing the classifier in a clever way, will recover the data density in the non-parametric limit. We refer to the corresponding principle of finite-sample parameter estimation as *Bijective-Contrastive Estimation* (BCE). As the EBM is trained to contrast the distributions induced by these bijections, it will learn to recover the

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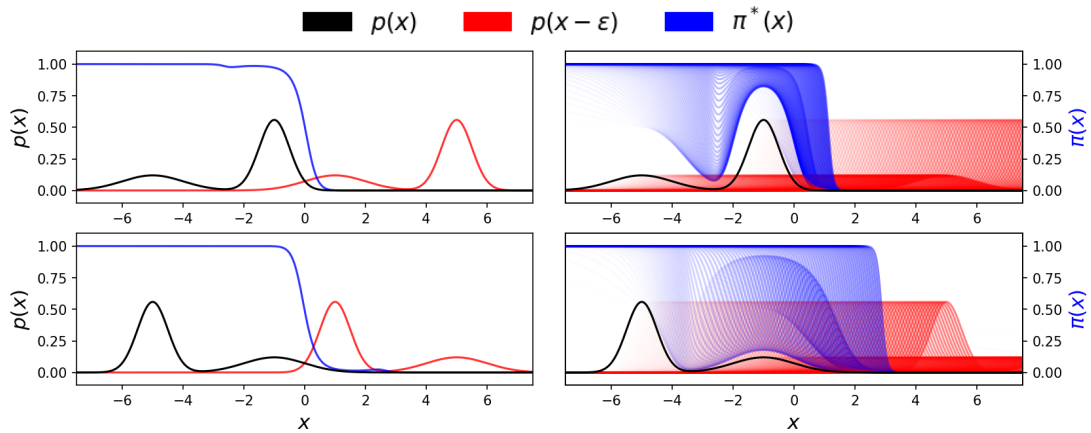

Figure 1: Examples of binary classification problems generated by bijections. Left: while two data densities are different (black solid lines in top and bottom-left), we have very similar Bayes optimal classifiers to differentiate $p(x)$ and $p(x-\epsilon)$. Right: a collection of optimal classifiers is fully governed by corresponding pdfs.

ratio of the corresponding density functions. By jointly solving a sufficiently large collection of classification problems with shared parameters, the EBM is guaranteed to recover the data distribution's density up to a normalizing constant.

2. Bijective-Contrastive Estimation (BCE)

2.1. How to contrast with bijections

In this section, we first show how to generate a binary classification problem using a bijection and demonstrate how to solve the classification problem with an energy model. We then conjecture that while using the energy model to solve a single classification problem will not be enough to recover the data density, we can do so by jointly solving sufficiently many classification problems.

Let ϵ be a constant. Suppose we have data associated with a probability density function $p(x)$ and another set of samples modified from the data; $x' = x + \epsilon$, whose density is then $p(x' - \epsilon)$. The two densities in the top-left of Figure 1 represent the data's density function (in black) and the perturbed one (in red). We consider a binary classification problem between these two distributions, which admits an optimal solution $\pi^*(x) = \frac{p(x)}{p(x)+p(x-\epsilon)}$ (i.e. the blue curve). This implies we can plug in a parametric density, or an unnormalized density using an energy model in place of $p(x)$, and hope to recover $p(x)$ by training the classifier. Nevertheless, we can't recover $p(x)$ solely from π^*. For example, the data density in the bottom-left of Figure 1 is another data density function which, with the same ϵ, produces a binary classification problem whose optimal classifier is almost indistinguishable from the one in the top-left.

While the optimal classifier generated by a single bijection may not be distinguishable for different data densities, we argue that the set of optimal classifiers generated by a sufficiently large collection of bijections will be uniquely dependent on the data density. Consider the same classification task above, but now with multiple ϵs. In Figure 1 (right), we plot a

hundred of $p(x-\epsilon)$ (as well as the optimal classifiers π^* corresponding to different values of ϵ) and color them by decreasing the transparency of solid lines inversely proportional to the ϵ values. Unlike the single classification case, the behaviors of the two sets of π^*s are distinguishable.

This reveals that with an increasing number of ϵ's, there will be less available densities that match all of the optimal classifiers of the generated problems. With a sufficiently large number of classification problems, we hope to rule out all but one density function – the true data density. This would imply that we can learn the data density by parameterizing the classifiers as a function of the energy and the bijections and jointly solving the classification problems. In the next section, by formalizing and generalizing the examples in this section, we propose a new classification-based learning principle for EBMs.

2.2. Bijective-Contrastive Estimation

Let $x \in \mathbb{R}^d \sim p_{\texttt{data}}(x)$ be the data, and $t : \mathbb{R}^d \to \mathbb{R}^d$ be a bijection. The probability density of $x_t := t(x)$ can be conveniently expressed as $p(x_t) = p_{\texttt{data}}(t^{-1}(x_t))|J_{t^{-1}}(x_t)|$ by the change-of-variable formula, where $J_f(x)$ denotes Jacobian matrix of f wrt x. Similar to the previous example, let us first consider a classification problem to differentiate between x and x_t for the fixed t when the observation is a sample drawn from either $p_{\texttt{data}}(x)$ or $p(x_t)$ with equal probability. Let $\pi(x)$ be a classifier $\pi : \mathbb{R}^d \to [0,1]$, solving the following classification objective:

$$\mathcal{L}(\pi; t) := -\mathop{\mathbb{E}}_{x}\left[\log \pi(x)\right] - \mathop{\mathbb{E}}_{x_t}\left[\log(1-\pi(x_t))\right] = -\mathop{\mathbb{E}}_{x}\left[\log \pi(x) + \log(1-\pi(t(x)))\right], \tag{1}$$

which admits a minimizer

$$\pi^*(x) = \frac{p_{\texttt{data}}(x)}{p_{\texttt{data}}(x) + p_{\texttt{data}}(t^{-1}(x))|J_{t^{-1}}(x)|}.$$

That is, $\mathcal{L}(\pi^*; t) \leq \mathcal{L}(\pi; t)$ for any π. Let $p(x; f) = e^{-f(x)}/Z(f)$, where f is the energy model and $Z(f)$ is the normalizing constant. We can parameterize the classifier as

$$\pi(x; f) := \frac{p(x; f)}{p(x; f) + p(t^{-1}(x); f)|J_{t^{-1}}(x)|} = \frac{e^{-f(x)}}{e^{-f(x)} + e^{-f(t^{-1}(x))}|J_{t^{-1}}(x)|}. \tag{2}$$

Plugging $\pi(x; f)$ into Equation (1), we can redefine it as a loss functional of f

$$\mathcal{L}(f; t) = -\mathop{\mathbb{E}}_{x}\left[\log \frac{e^{-f(x)}}{e^{-f(x)} + e^{-f(t^{-1}(x))}|J_{t^{-1}}(x)|} + \log \frac{e^{-f(x)}}{e^{-f(t(x))}|J_t(x)| + e^{-f(x)}}\right]. \tag{3}$$

As discussed in the previous section, f^* that satisfies $p_{\texttt{data}}(x) \propto e^{-f^*(x)}$ will be the only minimizer of $\mathcal{L}(f; t)$ for any t. Motivated from this, we propose to minimize an expected loss over a distribution of bijections:

$$\mathcal{L}_{\texttt{BCE-b}}(f) = -\mathop{\mathbb{E}}_{x,t}\left[\log \frac{e^{-f(x)}}{e^{-f(x)} + e^{-f(t^{-1}(x))}|J_{t^{-1}}(x)|} + \log \frac{e^{-f(x)}}{e^{-f(t(x))}|J_t(x)| + e^{-f(x)}}\right]. \tag{4}$$

We refer to learning energy functions by minimizing Equation (4) (expectation taken over $p_{\texttt{data}}$ or an empirical distribution) as ***Bijective-Contrastive Estimation* (BCE)**. We call the binary classification form of Equation (4) *binary BCE objective*. We let $p(t)$[1] denote the density of the bijection t. We show that under some assumption on $p(t)$, the minimizer f^* of the BCE loss is unique up to a normalizing constant and $e^{-f^*(x)}$ is proportional to the data density.

Theorem 1 (Uniqueness of BCE-based estimator) *Let $\mathcal{F}$ be all measurable functions. If $\operatorname{supp}(p_{\texttt{data}}) \subseteq \{t^{-1}(x) \in \mathbb{R}^d : p(t) > 0\}$ for any x such that $p_{\texttt{data}}(x) > 0$, then*

$$p_{\texttt{data}}(x) \propto e^{-f^*(x)} \quad \forall x \in \mathbb{R}^d \iff \mathcal{L}_{\texttt{BCE-b}}(f^*) \leq \mathcal{L}_{\texttt{BCE-b}}(f) \quad \forall f \in \mathcal{F}. \tag{5}$$

Corollary 2 (Addition is sufficient) *If $t(x) \coloneqq x + \epsilon$ where $\epsilon \in \mathbb{R}^d$ is a random variable with a density function $p(\epsilon)$ that is non-zero everywhere, then the minimizer f^* of the BCE objective in Equation (4) satisfies $p_{\texttt{data}}(x) \propto e^{-f^*(x)}$ $\forall x \in \mathbb{R}^d$.*

The proofs are deferred to Appendix A. Theorem 1 shows that BCE is powerful enough to recover $p_{\texttt{data}}$ up to a normalizing constant. Moreover, according to Corollary 2 very simple classes of bijections suffice, for example the standard normal distribution.

2.3. Variants of objective functions

For additive bijections, we observe that t and t^{-1} have the same density if $p(\epsilon)$ is standard normal. In this paper, if the distribution of bijections in BCE satisfies $p(t) = p(t^{-1})$, we informally refer to this property as *inverse-symmetry*. Inverse-symmetry allows us to simplify Equation (4) to (neglecting a multiplier of 2)

$$\mathcal{L}_{\texttt{BCE-b}}(f) = -\mathop{\mathbb{E}}_{x,t}\left[\log \frac{e^{-f(x)}}{e^{-f(x)} + e^{-f(t(x))}|J_t(x)|}\right]. \tag{6}$$

In addition to the additions, random permutations and matrix-vector product of data with orthogonal matrices are also simple bijections that are inverse-symmetric.

Inverse-symmetry also largely simplifies the computation of the multiclass classification loss, which would normally have quadratically many terms, to be

$$\mathcal{L}_{\texttt{BCE-m}}(f) = -\mathop{\mathbb{E}}_{x,t_1,\ldots,t_n}\left[\log \frac{e^{-f(x)}}{e^{-f(x)} + \sum_{i=1}^{n} e^{-f(t_i(x))}|J_{t_i}(x)|}\right], \tag{7}$$

where $t_1, \ldots, t_n \sim p(t)$. Here, we neglect a multiplier of n. We find that training with multiclass BCE tends to be more stable as it has smaller gradient variance.

1. In this article, we assume that the bijections have real-valued representations. For convenience, we abuse notations and refer to $p(t)$ as a density function on the real-valued representations of t's. When we write $y = t(x)$, we refer to the functional form of t that maps x to y.

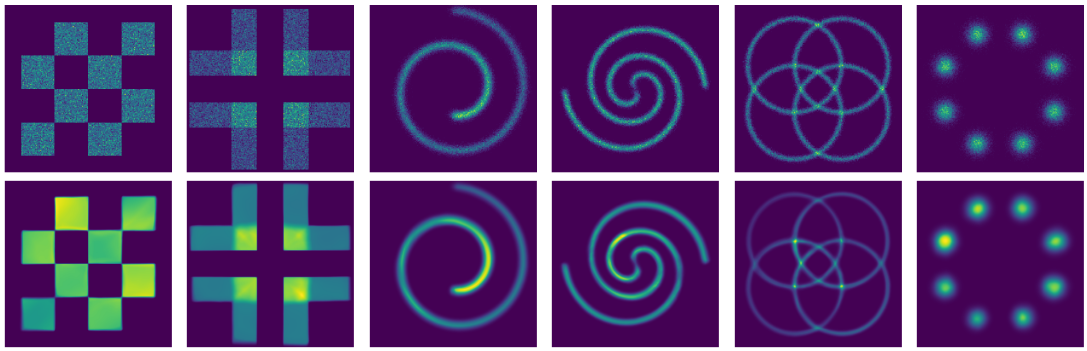

Figure 2: Density estimation on 2D synthetic datasets. First row: 2D histogram of synthetic datasets. Second row: unnormalized density functions learned by BCE.

2.4. Relation to noise contrastive estimation

The most closely related work to ours is noise-contrastive estimation (NCE, Gutmann and Hyvärinen (2010)), which uses a tractable noise distribution $q(x)$ and learns the energy function via the following objective,

$$\mathcal{L}_{\texttt{NCE}}(f) = -\mathop{\mathbb{E}}_{x\sim p_{\texttt{data}}}\left[\log \frac{e^{-f(x)}}{e^{-f(x)}+q(x)}\right] - \mathop{\mathbb{E}}_{x\sim q}\left[\log \frac{q(x)}{e^{-f(x)}+q(x)}\right].$$

If $q(x)$ is defined to be nonzero wherever $p_{\texttt{data}}(x)$ is nonzero, then $e^{-f^*(x)} = p_{\texttt{data}}(x)$ if f^* minimizes the NCE objective[2]. While NCE uses a pre-defined noise distribution q to contrast against, BCE uses bijections to generate many contrasting distributions non-parametrically.

3. Experiment on 2D synthetic datasets

In order to demonstrate that by minimizing the BCE loss, we can learn the correct data density, we run density estimation experiments on six 2D synthetic datasets. We use binary BCE loss as in Equation (6), additive bijections for the perturbation, and standard normal distribution for the additive bijections. We use a ReLU network with three 1,000-unit hidden layers, and train it using the Adam optimizer (Kingma and Ba, 2015) with $\beta_1 = 0.9, \beta_2 = 0.999$. We run 50K iterations. Mini-batch size and learning rate are set to 256 and 0.0001, respectively. The results are presented in Figure 2. We see that the energy-based model trained by BCE successfully learns the densities of a variety of 2D synthetic datasets.

4. Difficulties in modeling high-dimensional data

In preliminary experiments, we observe that the proposed method did not work well on high dimensional data. On the MNIST dataset, we train the EBM via BCE and evaluate the quality of samples generated by running Langevin dynamics (Grenander and Miller, 1994), but the generated samples all fail to resemble the true data samples. We conjecture that this

2. In NCE, the normalizing constant is commonly absorbed in $f(x)$ as a parameter.

is a result from using the cross entropy loss, which causes two types of vanishing gradients problems: the loss does not provide meaningful learning signals when $t(x)$ is either too far from or too close to the data manifold. The first case occurs when we use a simple family of bijections for BCE. For instance, simple addition of unstructured noise to highly structured data generates samples that are easily off the data manifolds. Hence the classifiers can achieve near-perfect accuracy while the energy fails to learn the density. The gradients wrt the energy can also vanish when $p(t(x))$ is too close to the data density, *e.g.* when t is almost identity.

Similarly to BCE, the first type of vanishing gradient problem also prevents NCE from scaling up, occurring when $q(x)$ is too far from $p_{\texttt{data}}(x)$. Recently, Rhodes et al. (2020) tackle this by generating a sequence of NCE problems, each of which contrasts two consecutive intermediate distributions interpolated between the data and a noise distribution. When the two distributions are close enough, one can potentially mitigate the vanishing gradient problem. On the other hand, in generative adversarial nets (GANs, Goodfellow et al. (2014)), the vanishing gradient problem has been addressed by regularizing the discriminator (Arjovsky et al., 2017). We leave the ideas of generating intermediate distributions and regularizing the classifiers for future work.

5. Conclusion

In this paper, we propose a new classification-based EBM training method, called *Bijective-Contrastive Estimation* (BCE). We prove that the data density (up to a normalizing constant) is the only minimizer of the BCE loss. In the experiment, we show that the energy trained with BCE accurately models the 2D synthetic data distributions. We discuss the difficulty of BCE in modeling high-dimensional data due to the vanishing gradient problems, and suggest future direction for addressing this issue.

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Appendix A. Proofs

Proof of Theorem 1

Step 1 In order to prove Theorem 1, we first introduce another optimization problem equivalent to minimizing $\mathcal{L}_{\texttt{BCE-b}}(f)$ in Equation (4). Consider a following data generation process.

$$x = \begin{cases} \tilde{x}, & \text{if } y = 1, \\ t(\tilde{x}), & \text{otherwise.} \end{cases},$$

where $\tilde{x} \sim p_{\texttt{data}}(\tilde{x})$, $t \sim p(t)$, and $y \sim \text{Bernoulli}\left(\frac{1}{2}\right)$. We define the likelihoods of x given y, t as $p(x|y=1,t) = p_{\texttt{data}}(x)$ and $p(x|y=0,t) = p_{\texttt{data}}(t^{-1}(x))|J_{t^{-1}}(x)|$. Let $q(y|x,t;f)$ be a variational posterior parameterized by an energy f, whose likelihoods are defined as

$$q(x|y=1,t;f) \coloneqq \frac{e^{-f(x)}}{Z(f)} \text{ and } q(x|y=0,t;f) \coloneqq \frac{e^{-f(t^{-1}(x))}|J_{t^{-1}}(x)|}{Z(f)}. \tag{8}$$

Then, the minimization of the BCE objective in Equation (4) is equivalent to minimizing the expected KL-divergence between the true posterior $p(y|x,t)$ and the variational posterior $q(y|x,t)$:

$$\arg\min_f \mathcal{L}_{\texttt{BCE-b}}(f) = \arg\min_f \mathop{\mathbb{E}}_t \left[D_{KL}\left(p(y|x,t) \| q(y|x,t;f)\right)\right], \tag{9}$$

where

$$p(y|x,t) = \frac{p(x|y,t)}{p_{\texttt{data}}(x) + p_{\texttt{data}}(t^{-1}(x))|J_{t^{-1}}(x)|}$$

$$\text{and } \; q(y|x,t;f) = \frac{q(x|y,t;f)}{\underbrace{\frac{e^{-f(x)}}{Z(f)}}_{=\, q(x|y=1,t;f)} + \underbrace{\frac{e^{-f(t^{-1}(x))}|J_{t^{-1}}(x)|}{Z(f)}}_{=\, q(x|y=0,t;f)}}.$$

The equality holds since $\mathcal{L}_{\texttt{BCE-b}}(f)$ is the cross entropy term in the expected KL and the entropy term of $p(y|x,t)$ does not depends on f.

Step 2 Due to Equation (9), proving Theorem 1 is equivalent to show that if $\text{supp}(p_{\texttt{data}}) \subseteq \{t^{-1}(x) \in \mathbb{R}^d : p(t) > 0\}$ for any x such that $p_{\texttt{data}}(x) > 0$, then

$$p_{\texttt{data}}(x) \propto e^{-f^*(x)} \quad \forall x \in \mathbb{R}^d \iff \mathop{\mathbb{E}}_t \left[D_{KL}\left(p(y|x,t) \| q(y|x,t;f^*)\right)\right] = 0. \tag{10}$$

Proving from LHS to RHS is straightforward. Here, we focus on the direction from RHS to LHS. From the RHS in Equation (10), we have

$$\begin{aligned} &\mathop{\mathbb{E}}_t \left[D_{KL}\left(p(y|x,t) \| q(y|x,t;f)\right)\right] = 0 \\ &\overset{*}{\iff} D_{KL}\left(p(y|x,t) \| q(y|x,t;f)\right) = 0 \quad \forall t \in \text{supp}(p(t)) \\ &\iff p(y|x,t) = q(y|x,t;f) \\ &\qquad \forall x \in \text{supp}(p_{\texttt{data}}) \cup \{x \in \mathbb{R}^d : p_{\texttt{data}}(t^{-1}(x)) > 0\}, \\ &\qquad \forall y \in \{0,1\}, \forall t \in \text{supp}(p(t)), \end{aligned} \tag{11}$$

where $(*)$ is due to $D_{KL}(\cdot\|\cdot) \geq 0$. We can rewrite Equation (11) as following: for any $t \in \text{supp}(p(t))$ and $x \in \text{supp}(p_{\texttt{data}}) \cup \{x \in \mathbb{R}^d : p_{\texttt{data}}(t^{-1}(x)) > 0\}$,

$$\frac{p_{\texttt{data}}(x)}{p_{\texttt{data}}(x) + p_{\texttt{data}}(t^{-1}(x))|J_{t^{-1}}(x)|} = \frac{e^{-f(x)}}{e^{-f(x)} + e^{-f(t^{-1}(x))}|J_{t^{-1}}(x)|}. \tag{12}$$

Recall that for any $x_0 \in \text{supp}(p_{\texttt{data}})$, $p_{\texttt{data}}(x_0) > 0$, and thus we have

$$\begin{aligned}
&\frac{p_{\texttt{data}}(x_0)}{p_{\texttt{data}}(x_0) + p_{\texttt{data}}(t^{-1}(x_0))|J_{t^{-1}}(x_0)|} = \frac{e^{-f(x_0)}}{e^{-f(x_0)} + e^{-f(t^{-1}(x_0))}|J_{t^{-1}}(x_0)|} \\
&\Rightarrow\ 1 \Bigg/ \left(1 + \frac{p_{\texttt{data}}(t^{-1}(x_0))|J_{t^{-1}}(x_0)|}{p_{\texttt{data}}(x_0)}\right) = 1 \Bigg/ \left(1 + \frac{e^{-f(t^{-1}(x_0))}|J_{t^{-1}}(x_0)|}{e^{-f(x_0)}}\right) \\
&\Rightarrow\ \frac{p_{\texttt{data}}(t^{-1}(x_0))}{p_{\texttt{data}}(x_0)} = \frac{e^{-f(t^{-1}(x_0))}}{e^{-f(x_0)}} \\
&\Rightarrow\ p_{\texttt{data}}(t^{-1}(x_0)) \propto e^{-f(t^{-1}(x_0))} \quad \forall t \in \text{supp}(p(t)) \\
&\overset{\dagger}{\Rightarrow}\ p_{\texttt{data}}(x') \propto e^{-f(x')} \quad \forall x' \in \mathbb{R}^d,
\end{aligned} \tag{13}$$

where $(\dagger)$ holds due to $\text{supp}(p_{\texttt{data}}) \subseteq \{t^{-1}(x) \in \mathbb{R}^d : p(t) > 0\}$ for any $x \in \text{supp}(p_{\texttt{data}})$ and $p_{\texttt{data}}$ is a probability density function.

■

Proof of Corollary 2 For $t(x) = x + \epsilon$ where $\epsilon \in \mathbb{R}^d$ is a random variable with a density function $p(\epsilon)$ that is non-zero everywhere, we can rewrite Equation (13) in Theorem 1 as follows; for any $x_0 \in \text{supp}(p_{\texttt{data}})$ we have

$$p_{\texttt{data}}(x_0 - \epsilon) \propto e^{-f(x_0 - \epsilon)} \quad \forall \epsilon \in \mathbb{R}^d. \tag{14}$$

Without loss of generality, we can take $x_0 = 0$ and $p_{\texttt{data}}(x_0) > 0$. Plugging it in Equation (14) and flipping the sign of ϵ, we have

$$p_{\texttt{data}}(\epsilon) \propto e^{-f(\epsilon)} \quad \forall \epsilon \in \mathbb{R}^d.$$

■