Variational (Gradient) Estimate of the Score Function in Energy-based Latent Variable Models

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Abstract

This paper presents new estimates of the score function and its gradient with respect to the model parameters in a general energy-based latent variable model (EBLVM). The score function and its gradient can be expressed as combinations of expectation and covariance terms over the (generally intractable) posterior of the latent variables. New estimates are obtained by introducing a variational posterior to approximate the true posterior in these terms. The variational posterior is trained to minimize a certain divergence (e.g., the KL divergence) between itself and the true posterior. Theoretically, the divergence characterizes upper bounds of the bias of the estimates. In principle, our estimates can be applied to a wide range of objectives, including kernelized Stein discrepancy (KSD), score matching (SM)-based methods and exact Fisher divergence with a minimal model assumption. In particular, these estimates applied to SM-based methods outperform existing methods in learning EBLVMs on several image datasets.

1. Introduction

Energy-based models (EBMs) (LeCun et al., 2006) associate an energy to each configuration of visible variables, which naturally induces a probability distribution by normalizing the exponential negative energy. Such models have found applications in a wide range of areas, such as image synthesis (Du & Mordatch, 2019; Nijkamp et al., 2020), out-of-distribution detection (Grathwohl et al., 2020a; Liu et al., 2020) and controllable generation (Nijkamp et al., 2019). Based on EBMs, energy-based latent variable models (EBLVMs) (Swersky et al., 2011; Vértes et al., 2016) incorporate latent variables to further improve the expressive power (Salakhutdinov & Hinton, 2009; Bao et al., 2020) and to enable representation learning (Welling et al., 2004; Salakhutdinov & Hinton, 2009; Srivastava & Salakhutdinov, 2012) and conditional sampling (see results in Sec. 4.2).

Notably, the score function (SF) of an EBM is defined as the gradient of its log-density with respect to the visible variables, which is independent of the partition function and thereby tractable. Due to its tractability, the SF-based methods are appealing in both learning (Hyvärinen, 2005; Liu et al., 2016) and evaluating (Grathwohl et al., 2020b) EBMs, compared to many other approaches (Hinton, 2002; Tieleman, 2008; Gutmann & Hyvärinen, 2010; Salakhutdinov, 2008) (see a comprehensive discussion in Sec. 6). In particular, score matching (SM) (Hyvärinen, 2005), which minimizes the expected squared distance between the score function of the data distribution and that of the model distribution, and its variants (Kingma & LeCun, 2010; Vincent, 2011; Saremi et al., 2018; Song et al., 2019; Li et al., 2019; Pang et al., 2020) have shown promise in learning EBMs.

Unfortunately, the score function and its gradient with respect to the model parameters in EBLVMs are generally intractable without a strong structural assumption (e.g., the joint distribution of visible and latent variables is in the exponential family (Vértes et al., 2016)) and thereby SF-based methods are not directly applicable to general EBLVMs. Recently, bi-level score matching (BiSM) (Bao et al., 2020) applies SM to general EBLVMs by reformulating a SM-based objective as a bilevel optimization problem, which learns a deep EBLVM on natural images and outperforms an EBM of the same size. However, BiSM is not problemless — practically BiSM is optimized by gradient unrolling (Metz et al., 2017) of the lower level optimization, which is time and memory consuming (see a comparison in Sec. 4.1).

In this paper, we present variational estimates of the score function and its gradient with respect to the model parameters in general EBLVMs, referred to as VaES and VaGES respectively. The score function and its gradient can be expressed as combinations of expectation and covariance terms over the posterior of the latent variables. VaES and VaGES are obtained by introducing a variational posterior, which approximates the true posterior in these terms by minimizing a certain divergence between itself and the true

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2. Method

As mentioned in Sec. 1, the score function has been used in a wide range of methods (Hyvärinen, 2005; Liu et al., 2016; Grathwohl et al., 2020b), while it is generally intractable in EBLVMs without a strong structural assumption. In this paper, we present estimates of the score function and its gradient w.r.t. the model parameters in a general EBLVM. Formally, an EBLVM defines a joint probability distribution over the visible variables $v$ and latent variables $h$ as follows

$$p_\theta(v, h) = \tilde{p}_\theta(v, h) \frac{Z(\theta)}{e^{-\mathcal{E}_\theta(v, h)} / Z(\theta)},$$

where $\mathcal{E}_\theta(v, h)$ is the energy function parameterized by $\theta$, $\tilde{p}_\theta(v, h) = e^{-\mathcal{E}_\theta(v, h)}$ is the unnormalized distribution and $Z(\theta) = \int e^{-\mathcal{E}_\theta(v, h)}dv$ is the partition function. As shown by Vértes et al. (2016), the score function of an EBLVM can be written as an expectation over the posterior:

$$\nabla_v \log p_\theta(v, h) = \mathbb{E}_{p_\theta(h|v)}[\nabla_v \log \tilde{p}_\theta(v, h)],$$

where $p_\theta(h|v) = \int p_\theta(v, h)dh$ is the marginal distribution and $p_\theta(h|v)$ is the posterior. We then show that the gradient of the score function w.r.t. the model parameters can be decomposed into an expectation term and a covariance term over the posterior (proof in Appendix A):

$$\frac{\partial \nabla_v \log p_\theta(v)}{\partial \theta} = \mathbb{E}_{p_\theta(h|v)}\left[\frac{\partial \nabla_v \log \tilde{p}_\theta(v, h)}{\partial \theta}\right]$$

$$+ \text{Cov}_{p_\theta(h|v)}(\nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h)),$$

where the first term is the expectation of a random matrix $\frac{\partial \nabla_v \log \tilde{p}_\theta(v, h)}{\partial \theta}$ with $h \sim p_\theta(h|v)$ and the second term is the covariance between two random vectors $\nabla_v \log \tilde{p}_\theta(v, h)$ and $\nabla_\theta \log \tilde{p}_\theta(v, h)$ with $h \sim p_\theta(h|v)$.

2.1. Variational (Gradient) Estimate of the Score Function in EBLVMs

Eq. (2) and (3) naturally suggest Monte Carlo estimates, while both of them need samples from the posterior $p_\theta(h|v)$, which is generally intractable. As for approximate inference, we present an amortized variational approach (Kingma & Welling, 2014) that considers

$$\mathbb{E}_{q_\phi(h|v)}[\nabla_v \log \tilde{p}_\theta(v, h)],$$

and

$$\mathbb{E}_{q_\phi(h|v)}\left[\frac{\partial \nabla_v \log \tilde{p}_\theta(v, h)}{\partial \theta}\right]$$

$$+ \text{Cov}_{q_\phi(h|v)}(\nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h)),$$

respectively, where $q_\phi(h|v)$ is a variational posterior parameterized by $\phi$. Note that the covariance term in Eq. (5) is a variational estimate of that in Eq. (3), not derived from taking gradient to Eq. (4). We optimize some divergence between $q_\phi(h|v)$ and $p_\theta(h|v)$

$$\min_{\phi} \mathbb{E}_{p_D(v)}[D(q_\phi(h|v)||p_\theta(h|v))],$$

where $p_D(v)$ denotes the data distribution. Specifically, if we set $D$ in Eq. (6) as the KL divergence or the Fisher divergence, then Eq. (6) is tractable. For clarity, we refer the readers to Appendix B for a derivation and a general analysis of the tractability of other divergences.

Below, we consider Monte Carlo estimates based on the variational approximation. According to Eq. (4), the variational estimate of the score function (VaES) is

$$\text{VaES}(v; \theta, \phi) = \frac{1}{L} \sum_{i=1}^{L} \nabla_v \log \tilde{p}_\theta(v, h_i),$$

where $h_i \sim q_\phi(h|v)$ and $L$ is the number of samples from $q_\phi(h|v)$. Similarly, according to Eq. (5), the variational estimate of the expectation term $e(v; \theta)$ is

$$\hat{e}(v; \theta, \phi) = \frac{1}{L} \sum_{i=1}^{L} \frac{\partial \nabla_v \log \tilde{p}_\theta(v, h_i)}{\partial \theta},$$

where $h_i \sim q_\phi(h|v)$. As for the covariance term $c(v; \theta, \phi)$, we estimate it with the sample covariance matrix (Fan et al.,
According to Eq. (5), the variational estimate is
\[
\hat{c}(v; \theta, \phi) = \frac{1}{L-1} \sum_{i=1}^{L} \nabla_v \log \tilde{p}_\theta(v, h_i) \frac{\partial \log \tilde{p}_\theta(v, h_i)}{\partial \theta} \\
- \frac{1}{(L-1)L} \sum_{i=1}^{L} \nabla_v \log \tilde{p}_\theta(v, h_i) \sum_{i=1}^{L} \frac{\partial \log \tilde{p}_\theta(v, h_i)}{\partial \theta},
\]
(9)
where \( h_i \uparrow \equiv q_\phi(h|v) \), \( \nabla_v \) outputs column vectors and \( \frac{\partial}{\partial \theta} \) outputs row vectors. With Eq. (8) and (9), the variational gradient estimate of the score function (VaGES) is
\[
\text{VaGES}(v; \theta, \phi) = \hat{c}(v; \theta, \phi) + \hat{c}(v; \theta, \phi).
\]
(10)

Remark: Although Eq. (8) includes second derivatives, in practice we only need to calculate the product of them and vectors. Similar to the Hessian-vector products (Song et al., 2019), only two backpropagations are required in the calculation (since \( z^T \frac{\partial \nabla_v \log \tilde{p}_\theta(v, h_i)}{\partial \theta} = 2z^T \nabla_v \log \tilde{p}_\theta(v, h_i) \)).

2.2. Bounding the Bias

Notice that VaES\((v; \theta, \phi)\) and VaGES\((v; \theta, \phi)\) are actually biased estimates due to the difference between \( q_\phi(h|v) \) and \( p_\m(h|v) \). Firstly, we show that the bias of VaES\((v; \theta, \phi)\) and VaGES\((v; \theta, \phi)\) can be bounded by the square root of the KL divergence between \( q_\phi(h|v) \) and \( p_\m(h|v) \) under some assumptions on boundedness, as characterized in Theorem 1 and Theorem 2.

Theorem 1. (VaES, KL, proof in Appendix C) Suppose \( \nabla_v \log \tilde{p}_\theta(v, h) \) is bounded w.r.t. \( v, h \) and \( \theta \), then the bias of VaES\((v; \theta, \phi)\) can be bounded by the square root of the KL divergence between \( q_\phi(h|v) \) and \( p_\m(h|v) \) up to multiplying a constant.

Theorem 2. (VaGES, KL, proof in Appendix C) Suppose \( \nabla_v \log \tilde{p}_\theta(v, h) \), \( \nabla_\theta \log \tilde{p}_\theta(v, h) \) and \( \frac{\partial}{\partial \theta} \nabla_v \log \tilde{p}_\theta(v, h) \) are bounded w.r.t. \( v, h \) and \( \theta \), then the bias of VaGES\((v; \theta, \phi)\) can be bounded by the square root of the KL divergence between \( q_\phi(h|v) \) and \( p_\m(h|v) \) up to multiplying a constant.

Remark: The boundedness assumptions in Theorem 1,2 are not difficult to satisfy when \( h \) is discrete. For example, if \( v \) comes from a compact set (which is naturally satisfied on image data), \( \theta \) comes from a compact set (which can be satisfied by adding weight decay to \( \theta \)), \( \log \tilde{p}_\theta(v, h) \) is second continuously differentiable w.r.t. \( v \) and \( \theta \) (which is satisfied in neural networks composed of smooth functions) and \( h \) comes from a finite set (which is satisfied in most commonly used discrete distributions, e.g., the Bernoulli distribution), then \( \nabla_v \log \tilde{p}_\theta(v, h) \), \( \nabla_\theta \log \tilde{p}_\theta(v, h) \) and \( \frac{\partial}{\partial \theta} \nabla_v \log \tilde{p}_\theta(v, h) \) are bounded w.r.t. \( v, h \) and \( \theta \) by the extreme value theorem of continuous functions on compact sets.

In Fig. 1 (a), we numerically validate Theorem 1,2 in Gaussian restricted Boltzmann machines (GRBMs) (Hinton & Salakhutdinov, 2006). The biases of VaES and VaGES in such models are linearly proportional to the square root of the KL divergence. Theorem 1,2 strongly motivate us to set \( D \) as the KL divergence in Eq. (6) when \( h \) is discrete.

Then, we show that under extra assumptions on the Stein regularity (see Def. 2) and boundedness of the Stein factors (see Def. 3), the bias of VaES\((v; \theta, \phi)\) and VaGES\((v; \theta, \phi)\) can be bounded by the square root of the Fisher divergence (Johnson, 2004) between \( q_\phi(h|v) \) and \( p_\m(h|v) \), as characterized in Theorem 3 and Theorem 4. We first introduce some definitions, which will be used in the theorems.

Definition 1. (Ley et al., 2013) Suppose \( p \) is a probability density defined on \( \mathbb{R}^n \) and \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) is a function, we define \( g_p^r \) as a solution of the Stein equation \( S_p g = f - E_p f \), where \( g : \mathbb{R}^n \rightarrow \mathbb{R} \) and \( S_p g(x) \equiv \nabla_v \log p(x)^T g(x) + \text{Tr}(\nabla_v g(x)) \). (See Appendix D for the existence of the solution.)

Definition 2. Suppose \( p,q \) are probability densities defined on \( \mathbb{R}^n \) and \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \) is a function, we say \( f \) satisfies the Stein regular condition w.r.t. \( p,q \) if \( \forall i \in \mathbb{Z} \cap [1, m], \lim_{|x| \to \infty} \frac{q(x)g^r_{p,q}(x)}{q(x)g^r_{p,q}(x)} = 0 \).

Definition 3. (Ley et al., 2013) Suppose \( p,q \) are probability densities defined on \( \mathbb{R}^n \) and \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \) is a function satisfying the Stein regular condition w.r.t. \( p,q \), we define \( n^r_{f,p,q} \equiv \sqrt{E_{q(x)}(\sum_{i=1}^{m} \|g^r_{p,q}(x)\|^2)} \), referred to as the Stein factor of \( f \) w.r.t. \( p,q \).

Theorem 3. (VaES, Fisher, proof in Appendix D) Suppose (1) \( \forall (v, \theta, \phi), \nabla_v \log \tilde{p}_\theta(v, h) \) as a function of \( h \) satisfies the Stein regular condition w.r.t. \( p_\m(h|v) \) and \( q_\phi(h|v) \) and (2) the Stein factor of \( \nabla_v \log \tilde{p}_\theta(v, h) \) as a function of \( h \) w.r.t. \( p_\m(h|v) \), \( q_\phi(h|v) \) is bounded w.r.t. \( v, \theta \) and \( \phi \), then the bias of VaES\((v; \theta, \phi)\) can be bounded by the square root of the Fisher divergence between \( q_\phi(h|v) \) and \( p_\m(h|v) \) up to multiplying a constant.

![Figure 1](image_url)
Theorem 4. (VaGES, Fisher, proof in Appendix D)
Suppose (1) $\forall (v, \theta, \phi)$, $\nabla_v \log p_\theta(v, h)$, $\nabla_\theta \log p_\theta(v, h)$, $\nabla_v \log \hat{p}_\theta(v, h)$, $\nabla_\theta \log \hat{p}_\theta(v, h)$, $\frac{\partial \log \hat{p}_\theta(v, h)}{\partial \theta}$ and $\frac{\partial \log \hat{p}_\theta(v, h)}{\partial \theta}$ as functions of $h$ satisfy the Stein regular condition w.r.t. $p_\theta(h|v)$ and $q_\phi(h|v)$ and (2) the Stein factors of $\nabla_v \log p_\theta(v, h)$, $\nabla_v \log \hat{p}_\theta(v, h)$, $\nabla_v \log p_\theta(v, h)$, $\nabla_\theta \log p_\theta(v, h)$, $\nabla_\theta \log \hat{p}_\theta(v, h)$ and $\frac{\partial \log \hat{p}_\theta(v, h)}{\partial \theta}$ as functions of $h$ w.r.t. $p_\theta(h|v)$, $q_\phi(h|v)$ are bounded w.r.t. $v, \theta$ and $\phi$. (3) $\nabla_v \log p_\theta(v, h)$ and $\nabla_v \log \hat{p}_\theta(v, h)$ are bounded w.r.t. $v, h$ and $\theta$, then the bias of VaGES$(v, \theta, \phi)$ can be bounded by the square root of the Fisher divergence between $q_\phi(h|v)$ and $p_\theta(h|v)$ up to multiplying a constant.

Although the boundedness of the Stein factors has only been verified under some simple cases (Ley et al., 2013), and hasn‘t been extended to more complex cases, e.g., when $\hat{p}_\theta(v, h)$ is parameterized by a neural network, we find it work in practice when choosing $D$ in Eq. (6) as the Fisher divergence (see Sec. 4.2) to learn $q_\phi(h|v)$. In Fig. 1 (b), we numerically validate Theorem 3.4 in a Gaussian model (GM), whose energy is $E_\theta(v, h) = \frac{1}{2\sigma^2}||v - b||^2 + \frac{1}{2}||h - c||^2 - v^\top W h$ with $\theta = (\sigma, W, b, c)$. The biases of VaES and VaGES in such models are linearly proportional to the square root of the Fisher divergence.

2.3. Langevin Dynamics Corrector
Sometimes $p_\theta(h|v)$ can be complex for $q_\phi(h|v)$ to approximate, especially in deep models. To improve the inference performance, we can run a few Langevin dynamics steps (Welling & Teh, 2011) to correct samples from $q_\phi(h|v)$, which has been successfully applied to correct the solution of a numerical SDE solver (Song et al., 2020). Specifically, a Langevin dynamics step updates $h$ by

$$h \leftarrow h + \frac{\alpha}{2} \nabla_h \log p_\theta(h|v) + \epsilon, \epsilon \sim \mathcal{N}(0, \alpha). \tag{11}$$

In practice, the standard deviation of $\epsilon$ is often smaller than $\sqrt{\alpha}$ to allow a faster convergence (Du & Mordatch, 2019; Nijkamp et al., 2020; 2019; Grathwohl et al., 2020a). Since Langevin dynamics requires $p_\theta(h|v)$ to be differentiable w.r.t. $h$, we only apply the corrector when $h$ is continuous.

3. Learning EBLVMs with KSD
In this section, we show that VaES and VaGES can extend kernelized Stein discrepancy (KSD) (Liu et al., 2016) to learn general EBLVMs. The KSD between the data distribution $p_D(v)$ and the model distribution $p_\theta(v)$ with the kernel

$$k(v_1, v_2) \text{ is defined as }$$

$$\text{KSD}(p_D, p_\theta) \triangleq \mathbb{E}_{v_1, v_2 \sim p_D} [k(v_1, v_2) \nabla_{v_1} \log p_\theta(v_1) \nabla_{v_2} \log p_\theta(v_2) + \nabla_{v_1} \log p_\theta(v_1) \nabla_{v_2} k(v_1, v_2) + \nabla_{v_2} k(v_1, v_2) \nabla_{v_1} \log p_\theta(v_1) + \text{Tr}(\nabla_{v_1} \nabla_{v_2} k(v_1, v_2))], \tag{12}$$

which properly measures the difference between $p_D(v)$ and $p_\theta(v)$ under some mild assumptions (Liu et al., 2016). To learn an EBLVM, we use the gradient-based optimization to minimize KSD$(p_D, p_\theta)$, where the gradient w.r.t. $\theta$ is

$$\frac{\partial \text{KSD}(p_D, p_\theta)}{\partial \theta} = 2\mathbb{E}_{v_1, v_2 \sim p_D} [(k(v_1, v_2) \nabla_{v_1} \log p_\theta(v_1) + \nabla_{v_1} \log p_\theta(v_1) \nabla_{v_2} k(v_1, v_2) + \nabla_{v_2} k(v_1, v_2) \nabla_{v_1} \log p_\theta(v_1) + \text{Tr}(\nabla_{v_1} \nabla_{v_2} k(v_1, v_2))]. \tag{13}$$

Estimating $\nabla_{v_1} \log p_\theta(v_1)$ and $\frac{\partial \nabla_{v_1} \log p_\theta(v_1)}{\partial \theta}$ with VaES and VaGES respectively, the variational stochastic gradient estimate of KSD (VaGES-KSD) is

$$\frac{2}{M} \sum_{i=1}^{M} [k(v_i, v'_i) \text{VaES}(v_i; \theta, \phi) + \nabla_{v_i} k(v_i, v'_i)^\top \text{VaGES}(v'_i; \theta, \phi)], \tag{14}$$

where the union of $v_i, v'_i$ and $v_i, v'_i$ is a mini-batch from the data distribution, and $\text{VaES}(v_i; \theta, \phi)$ and $\text{VaGES}(v'_i; \theta, \phi)$ are independent.

3.1. Experiments
Setting. Since KSD itself suffers from the curse of dimensionality issue (Gong et al., 2020), we illustrate the validity of VaGES-KSD by learning Gaussian restricted Boltzmann machines (GRBMs) (Welling et al., 2004; Hinton & Salakhutdinov, 2006) on the 2-D checkerboard dataset.
whose distribution is shown in Appendix G.1. The energy function of a GRBM is

$$E_\theta(v, h) = \frac{1}{2}\sigma^2 \|v - b\|^2 - c^\top h - v^\top W h,$$

(15)

with learnable parameters \(\theta = (\sigma, W, b, c)\). Since GRBM has a tractable posterior, we can directly learn it using KSD (see Eq. (12)). We also compare another baseline where \(p_\theta(v)\) is estimated by importance sampling (Owen, 2013) (i.e., \(p_\theta(v) \approx \frac{1}{L} \sum_{i=1}^L \tilde{p}_\theta(v|h_i), h_i \sim \text{unif}(h)\), where \(\text{unif}\) means the uniform distribution) and we call it IS-KSD. We use the RBF kernel \(k(v, v') = \exp(-\|v-v\|^2_{2\sigma^2})\) with \(\sigma = 0.1\). \(q_\phi(h|v)\) is a Bernoulli distribution parameterized by a fully connected layer with the sigmoid activation and we use the Gumbel-Softmax trick (Jang et al., 2017) for reparameterization of \(q_\phi(h|v)\) with 0.1 as the temperature. \(D\) in Eq. (6) is the KL divergence. See Appendix F.1 for more experimental details.

**Result.** As shown in Fig. 2, VaGES-KSD outperforms IS-KSD on all \(L\) (the number of samples from \(q_\phi(h|v)\)) and is comparable to the KSD (the test log-likelihood curves of VaGES-KSD are very close to KSD when \(L = 5, 10\)).

### 4. Learning EBLVMs with Score Matching

In this section, we show that VaES and VaGES can extend two score matching (SM)-based methods (Vincent, 2011; Li et al., 2019) to learn general EBLVMs. The first one is the denoising score matching (DSM) (Vincent, 2011), which minimizes the Fisher divergence \(D_F\) between a perturbed data distribution \(p_{\sigma_0}(v)\) and the model distribution \(p_\theta(v)\):

$$J_{DSM}(\theta) \triangleq D_F(p_{\sigma_0}||p_\theta)$$

$$= \frac{1}{2} \mathbb{E}_{p_D(w)p_{\sigma_0}(v|w)} \left\| \nabla_v \log p_\theta(v) - \nabla_v \log p_{\sigma_0}(v|w) \right\|^2_2,$$

where \(p_D(w)\) is the data distribution, \(p_{\sigma_0}(v|w) = \mathcal{N}(v|w, \sigma_0^2 I)\) is the Gaussian perturbation with a fixed noise level \(\sigma_0, p_{\sigma_0}(v) = \int p_D(w)p_{\sigma_0}(v|w)dw\) is the perturbed data distribution and \(\sigma_0\) means equivalence in parameter optimization.

The second one is the multiscale denoising score matching (MDSM) (Li et al., 2019), which uses different noise levels to scale up DSM to high-dimensional data:

$$J_{MDSM}(\theta)$$

$$= \frac{1}{2} \mathbb{E}_{p_D(w)p(\sigma)p_{\sigma_0}(v|w)} \left\| \nabla_v \log p_\theta(v) - \nabla_v \log p_{\sigma_0}(v|w) \right\|^2_2,$$

where \(p(\sigma)\) is a prior distribution over the flexible noise level \(\sigma\) and \(\sigma_0\) is a fixed noise level. We extend DSM and MDSM to learn EBLVMs. Firstly we write Eq. (16) and (17) in a general form for the convenience of discussion

$$J(\theta) = \frac{1}{2} \mathbb{E}_{p_D(w,v)} \left\| \nabla_v \log p_\theta(v) - \nabla_v \log p_{\sigma_0}(v|w) \right\|^2_2,$$

where \(p_D(w, v)\) is the joint distribution of \(w\) and \(v\) (specifically, \(p_D(w, v) = p_D(w)p_{\sigma_0}(v|w)\) for Eq. (16) and \(p_D(w, v) = \sum_{\sigma} p_D(w)p(\sigma)p_{\sigma_0}(v|w)\) for Eq. (17)). We use gradient-based optimization to minimize \(J(\theta)\) and its gradient w.r.t. \(\theta\)

$$\frac{\partial J(\theta)}{\partial \theta} = \mathbb{E}_{p_D(w,v)} \left\{ \nabla_v \log p_\theta(v) - \nabla_v \log p_{\sigma_0}(v|w) \right\} \frac{\partial \nabla_v \log p_\theta(v)}{\partial \theta}.$$

Estimating \(\nabla_v \log p_\theta(v)\) and \(\frac{\partial \nabla_v \log p_\theta(v)}{\partial \theta}\) with VaES and VaGES respectively, the variational stochastic gradient estimate of the SM-based methods (VaGES-SM) is

$$\frac{1}{M} \sum_{i=1}^M \left[ \nabla_v \log p_\theta(v_i|w_i) \right] \text{VaGES}(v_i; \theta, \phi)$$

where \(\{w_{1:M}, v_{1:M}\}\) is a mini-batch from \(p_D(w, v)\), and VaES(\(v_i; \theta, \phi\)) and VaGES(\(v_i; \theta, \phi\)) are independent. We explicitly denote our methods as VaGES-DSM or VaGES-MDSM according to which objective is used.

### 4.1. Comparison in GRBMs

**Setting.** We firstly consider the GRBM (see Eq. (15)), which is a good benchmark to compare existing methods. We consider the Frey face dataset, which consists of grayscale images of size \(20 \times 28\), and the checkerboard dataset (mentioned in Sec. 3.1). \(q_\phi(h|v)\) is a Bernoulli distribution parameterized by a fully connected layer with the sigmoid activation and we use the Gumbel-Softmax trick (Jang et al., 2017) for reparameterization of \(q_\phi(h|v)\) with 0.1 as the temperature. \(D\) in Eq. (6) is the KL divergence. See Appendix F.2.1 for more experimental details.

**Comparison with BiSM.** As mentioned in Sec. 1, bi-level score matching (BiSM) (Bao et al., 2020) learns general EBLVMs by reformulating Eq. (16) and (17) as bi-level optimization problems, referred to as BiDSM and BiMDSM respectively, which serves as the most direct baseline (see Appendix I for an introduction to BiSM). We make a comprehensive comparison between VaGES-SM and BiSM on the Frey face dataset, which explores all hyperparameters involved in these two methods. Specifically, both methods sample from a variational posterior and optimize the variational posterior, so they share two hyperparameters \(L\) (the number of \(h\) sampled from the variational posterior) and \(K\) (the number of times updating the variational posterior on each mini-batch). Besides, BiSM has an extra hyperparameter \(N\), which specifies the number of gradient unrolling steps. In Fig. 3, we plot the test log-likelihood, the test score matching (SM) loss (Hyvärinen, 2005), which is the Fisher divergence up to an additive constant, the time
and memory consumption by grid search across \( L, K \) and \( N \). VaGES-DSM takes about 40\% time and 90\% memory on average to achieve a similar performance with BiDSM \((N=5)\). VaGES-DSM outperforms BiDSM \((N=0,2)\), and meanwhile it takes less time than BiDSM \((N=2)\) and the least memory.

**Comparison with other methods.** For completeness, we also compare with DSM \((\text{Vincent}, 2011)\), CD-based methods \((\text{Hinton}, 2002; \text{Tieleman}, 2008)\) and noise contrastive estimation (NCE)-based methods \((\text{Gutmann} & \text{Hyv"arinen}, 2010; \text{Rhodes} & \text{Gutmann}, 2019)\) on the checkerboard dataset. VaGES-DSM is competitive to the baselines (e.g., CD and DSM) that leverage the tractability of the posterior in GRBM and outperforms the variational NCE \((\text{Rhodes} & \text{Gutmann}, 2019)\). See results in Appendix G.2.1.

### 4.2. Learning Deep EBLVMs

**Setting.** Then we show that VaGES-SM can scale up to learn general deep EBLVMs and generate natural images. Following BiSM \((\text{Bao et al., 2020})\), we consider the deep EBLVM with the following energy function

\[
E_\theta(v, h) = g_3(g_2(g_1(v; \theta_1), h), \theta_2),
\]

where \( h \) is continuous, \( \theta = (\theta_1, \theta_2) \), \( g_1 \) a vector-valued neural network that outputs a feature sharing the same dimension with \( h \), \( g_2 \) is an additive coupling layer \((\text{Dinh et al., 2015})\) and \( g_3 \) is a scalar-valued neural network. We consider the MNIST dataset \((\text{LeCun et al., 2010})\), which consists of gray-scaled handwritten digits of size \( 28 \times 28 \), the CIFAR10 dataset \((\text{Krizhevsky et al., 2009})\), which consists of color natural images of size \( 32 \times 32 \) and the CelebA dataset \((\text{Liu et al., 2015})\), which consists of color face images. We resize CelebA to \( 64 \times 64 \). \( q_\phi(h|v) \) is a Gaussian distribution parameterized by a 3-layer convolutional neural network. \( D \) in Eq. \((6)\) is the Fisher divergence. We use the Langevin dynamics corrector (see Sec. 2.3) to correct samples from \( q_\phi(h|v) \). As for the step size \( \alpha \) in Langevin dynamics, we empirically find that the optimal one is approximately proportional to the dimension of \( h \) (see Appendix F.2.2), perhaps because Langevin dynamics converges to its stationary distribution slower when \( h \) has a higher dimension and thereby requires a larger step size, so we fix the ratio of the step size \( \alpha \) in Langevin dynamics to the dimension of \( h \) on one dataset and the ratio is \( 2 \times 10^{-4} \) on MNIST and CIFAR10 and \( 10^{-5} \) on CelebA. The standard deviation of the noise \( \epsilon \) in Langevin dynamics is \( 10^{-4} \). See Appendix F.2.2 for more experimental details, e.g., how hyperparameters are selected and time consumption.

**Sample quality.** Since the EBLVM defined by Eq. \((21)\) has an intractable posterior, BiSM is the only applicable baseline mentioned in Section 4.1. We quantitatively evaluate the sample quality with the FID score \((\text{Heusel et al., 2017})\) in Tab. 1 and VaGES-MDSM achieves comparable performance to BiMDSM. Since there are relatively few baselines of learning deep EBLVMs, we also compare with other baselines involving learning EBMs in Tab. 1. We mention that VAE-EBLVM \((\text{Han et al., 2020})\) and CoopNets \((\text{Xie et al., 2018})\) report FID results on a subset of CelebA and on a different resolution of CelebA respectively. For fairness, we don’t include these results on CelebA. We provide image samples and Inception Score results in Appendix G.2.2.

**Interpolation in the latent space.** As argued in prior work \((\text{Bao et al., 2020})\), the conditional distribution \( p_\theta(v|h) \)
of a deep EBLVM can be multimodal, so we want to explore how a local modal of \( p_\theta(v|h) \) evolves as \( h \) changes. Since \( v \) is of high dimension, we are not able to plot the landscape of \( p_\theta(v|h) \). Alternatively, we study how a fixed particle moves in different landscapes according to the annealed Langevin dynamics (Li et al., 2019) by interpolating \( h \). Specifically, we select two points in the latent space and interpolate linearly between them to get a class of conditional distributions \( \{p_\theta(v|h_i)\}_{i=1}^5 \). Then we fix an initial point \( v_0 \) and run annealed Langevin dynamics on these conditional distributions with a shared noise. These annealed Langevin dynamics trajectories are shown in Fig. 4. Starting from the same initial noise, the trajectory evolves smoothly as \( h \) changes smoothly. More interpolation results can be found in Appendix G.2.2.

**Sensitivity analysis.** We also study how hyperparameters influence the performances of VaGES-SM in deep EBLVMs, including the dimension of \( h \), the number of convolutional layers, the number of \( h \) sampled from \( q_\phi(h|v) \), the number of times of updating \( \phi \), the number of Langevin dynamics steps, the noise level in Langevin dynamics and which divergence to use in Eq. (6). These results can be found in Appendix G.2.2. In brief, increasing the number of convolutional layers will improve the performance, while the dimension of \( h \), the number of \( h \) sampled from \( q_\phi(h|v) \), the noise level in Langevin dynamics and using the KL divergence instead of the Fisher divergence in Eq. (6) don’t affect the result very much. Besides, setting both the number of times updating \( \phi \) and the number of Langevin dynamics steps to 5 is enough for a stable training process.

5. Evaluating EBLVMs with Exact Fisher Divergence

In this setting we are given an EBLVM and a set of samples \( \{v_i\}_{i=1}^N \) from the data distribution \( p_D(v) \). We want to measure how well the model distribution \( p_\theta(v) \) approximates \( p_D(v) \), which needs an absolute value representing the difference between them. This task is more difficult than model comparison, which only needs relative values (e.g., log-likelihood) to compare between different models. Specifically, we consider the Fisher divergence of the maximum form (Hu et al., 2018; Grathwohl et al., 2020b) to measure how well \( p_\theta(v) \) approximates \( p_D(v) \):

\[
D^\theta_F (p_D||p_\theta) \triangleq \max_{f \in \mathcal{F}} \mathbb{E}_{p_D(v)} \mathbb{E}_{p(\epsilon)} \left[ \nabla_v \log p_\theta(v)^\top f(v) + \epsilon^\top \nabla_v f(v) \epsilon - \frac{1}{2} \|f(v)\|_2^2 \right],
\]

where \( \mathcal{F} \) is the set of functions \( f : \mathbb{R}^d \rightarrow \mathbb{R}^d \) satisfying \( \lim_{|v| \rightarrow \infty} p_D(v) f(v) = 0 \) and \( p(\epsilon) \) is a noise distribution (e.g., Gaussian distribution) introduced for computation efficiency (Grathwohl et al., 2020b). Such a form can also be understood as the Stein discrepancy (Gorham & Mackey, 2017) with \( L_2 \) constraint on the function space \( \mathcal{F} \) and has been applied to evaluate GRBMs (Grathwohl et al., 2020b). Under some mild assumptions (see Appendix E), Eq. (22) is equal to the exact Fisher divergence. In practice, \( \mathcal{F} \) is approximated by a neural network \( \{f_\eta : \eta \in \mathcal{H}\} \), where \( \eta \) is the parameter and \( \mathcal{H} \) is the parameter space. We optimize the right hand side of Eq. (22) and the gradient w.r.t. \( \eta \) is

\[
\mathbb{E}_{p_D(v)} \mathbb{E}_{p(\epsilon)} \left[ \nabla_v \log p_\theta(v)^\top \frac{\partial f_\eta(v)}{\partial \eta} \right] + \frac{\partial \epsilon^\top \nabla_v f_\eta(v) \epsilon}{\partial \eta} - \frac{1}{2} \frac{\partial \|f_\eta(v)\|_2^2}{\partial \eta}. \tag{23}
\]
We initialize a GRBM as $p$. We validate the effectiveness of VaGES-Fisher in GRBMs.

The dimensions of $v$ and $h$ are the same and we experiment on dimensions of 200 and 500. See Appendix F.3 for more experimental details. The result is shown in Fig. 5. We compare the Fisher divergence estimated by VaGES-Fisher with the accurate Fisher divergence. Under both dimensions, our estimated Fisher divergence is close to the accurate one.

5.1. Experiments

We validate the effectiveness of VaGES-Fisher in GRBMs. We initialize a GRBM as $p_D(v)$, perturb its weight with increasing noise and estimate the Fisher divergence between the initial GRBM and the perturbed one by VaGES-Fisher. The dimensions of $v$ and $h$ are the same and we experiment on dimensions of 200 and 500. See Appendix F.3 for more experimental details. The result is shown in Fig. 5. We compare the Fisher divergence estimated by VaGES-Fisher with the accurate Fisher divergence. Under both dimensions, our estimated Fisher divergence is close to the accurate one.

6. Related Work

Learning EBLVMs with MLE. A popular class of learning methods is the maximum likelihood estimate (MLE). Such methods have to deal with both the model posterior and the partition function. Some methods impose structural assumptions on the model. Among them, contrastive divergence (CD) (Hinton, 2002) and its variants (Tieleman, 2008; Qiu et al., 2020) estimate the gradient of the partition function with respect to the model parameters using Gibbs sampling (Geman & Geman, 1984) when the posterior can be sampled efficiently. Furthermore, when the model is fully visible, scalable methods (Du et al., 2018; Du & Mordatch, 2019; Nijkamp et al., 2020; 2019; Grathwohl et al., 2020a) are applicable by estimating such gradient with Langevin dynamics. In deep models with multiple layers of latent variables such as DBNs (Hinton et al., 2006; Lee et al., 2009) and DBMs (Salakhutdinov & Hinton, 2009), the greedy layer-wise learning algorithm (Hinton et al., 2006; Bengio et al., 2006) is applicable by exploring their hierarchical structures. Some recent methods (Kuleshov & Ermon, 2017; Li et al., 2020) attempt to learn general EBLVMs by variational inference. However, such methods suffer from high variance (Kuleshov & Ermon, 2017) or high bias (Li et al., 2020) of the variational bounds for the partition function in high-dimensional space.

Learning EBLVMs without partition functions. As mentioned in Sec. 1, the score matching (SM) is a popular class of learning methods, which eliminate the partition function by considering the score function, and the recent bi-level score matching (BiSM) is a scalable extension of SM to learn general EBLVMs. Prior to BiSM, extensions of SM (Swersky et al., 2011; Vértes et al., 2016) impose structural assumptions on the model, e.g., a tractable posterior (Swersky et al., 2011) or a jointly exponential family model (Vértes et al., 2016). Recently, Song & Ermon (2019; 2020) use a score network to directly model the score function of the data distribution. Incorporating latent variables to such a model is currently an open problem and we leave it as future work. The noise contrastive estimation (NCE) (Gutmann & Hyvärinen, 2010) is also a learning method which eliminates the partition function and variational noise contrastive estimation (VNCE) (Rhodes & Gutmann, 2019) is an extension of NCE to general EBLVMs based on variational methods. However, such methods have to manually design a noise distribution, which in principle should be close to the data distribution and is challenging in high-dimensional space. There are alternative approaches to handling the partition function, e.g., Doubly Dual Embedding (Dai et al., 2019a), Adversarial Dynamics Embedding (Dai et al., 2019b) and Fenchel Mini-Max Learning (Tao et al., 2019), and extending theses methods for learning EBLVMs would be interesting future work.

Evaluating EBLVMs. The log-likelihood is commonly used to compare fully visible models on the same dataset and the annealed importance sampling (Neal, 2001; Salakhutdinov, 2008) is often used to estimate the partition function in the log-likelihood. For a general EBLVM, a lower bound of the log-likelihood (Kingma & Welling, 2014; Burda et al., 2016) can be estimated by introducing a variational posterior together with estimating the partition function. The log-likelihood is a relative value and the corresponding absolute value (i.e., the KL divergence) is generally intractable since the entropy of the data distribution is unknown.

7. Conclusion

We propose new variational estimates of the score function and its gradient with respect to the model parameters in general energy-based latent variable models (EBLVMs). We
rewrite the score function and its gradient as combinations of expectation and covariance terms over the model posterior. We approximate the model posterior with a variational posterior and analyze its bias. With samples drawn from the variational posterior, the expectation terms are estimated by Monte Carlo and the covariance terms are estimated by sample covariance matrix. We apply our estimates to kernelized Stein discrepancy (KSD), score matching (SM)-based methods and exact Fisher divergence. In particular, these estimates applied to SM-based methods are more time and memory efficient compared with the complex gradient unrolling in the strongest baseline bi-level score matching (BiSM) and meanwhile can scale up to natural images in deep EBLVMs. Besides, we also present interpolation results of annealed Langevin dynamics trajectories in the latent space in deep EBLVMs.

Software and Data
Codes in https://github.com/baofff/VaGES.

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A. Proof of the Decomposition of the Gradient of the Score Function

Proof. Firstly we have

\[ \mathbb{E}_{\theta|v} \left[ \nabla_v \log p_\theta(h|v) \right] = \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(h|v) \right] = \int \frac{\nabla_v \log \tilde{p}_\theta(h|v) \mid p_\theta(h|v)}{p_\theta(h|v)} \, dh \]

\[ = \int \nabla_v \log \tilde{p}_\theta(h|v) \, dh = \nabla_v \int p_\theta(h|v) \, dh = \nabla_v 1 = 0, \tag{25} \]

and similarly we have \( \mathbb{E}_{\theta|v} \left[ \nabla_\theta \log \tilde{p}_\theta(v|h) \right] = 0 \). Thereby, we have

\[ \nabla_v \log \tilde{p}_\theta(v) = \nabla_v \log \tilde{p}_\theta(v) + \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v|h) \right] = \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v, h) \right], \]

and similarly we have \( \nabla_\theta \log \tilde{p}_\theta(v) = \mathbb{E}_{\theta|v} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \).

Taking derivatives to Eqn. (25) w.r.t. \( \theta \), we have

\[ \mathbb{E}_{\theta|v} \left[ \frac{\partial \nabla_v \log \tilde{p}_\theta(h|v)}{\partial \theta} \right] + \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v, h) \frac{\partial \log \tilde{p}_\theta(h|v)}{\partial \theta} \right] = 0. \tag{26} \]

The second term in the left side of Eqn. (26) can be written as

\[ \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v, h) \frac{\partial \log \tilde{p}_\theta(v|h)}{\partial \theta} \right] = \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v, h) \frac{\partial \log \tilde{p}_\theta(v|h)}{\partial \theta} \right] - \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v, h) \frac{\partial \log \tilde{p}_\theta(v)}{\partial \theta} \right] \]

\[ = \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v, h) \frac{\partial \log \tilde{p}_\theta(v|h)}{\partial \theta} \right] - \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v, h) \frac{\partial \log \tilde{p}_\theta(v)}{\partial \theta} \right] \]

\[ = \text{Cov}_{\theta|v} \left( \nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v|h) \right) = \text{Cov}_{\theta|v} \left( \nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v|h) \right). \]

Thereby, we have

\[ \frac{\partial \nabla_v \log \tilde{p}_\theta(v)}{\partial \theta} = \frac{\partial \nabla_v \log \tilde{p}_\theta(v)}{\partial \theta} \]

\[ = \frac{\partial \nabla_v \log \tilde{p}_\theta(v)}{\partial \theta} + \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v|h) \right] + \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v|h) \frac{\partial \log \tilde{p}_\theta(h|v)}{\partial \theta} \right] \]

\[ = \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v, h) \right] + \mathbb{E}_{\theta|v} \left[ \nabla_v \log \tilde{p}_\theta(v|h) \frac{\partial \log \tilde{p}_\theta(h|v)}{\partial \theta} \right] + \text{Cov}_{\theta|v} \left( \nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h) \right). \]

B. The Tractability of the Commonly Used Divergences between Posteriors

The tractability of the KL divergence or the Fisher divergence between the variational posterior and the true posterior in EBLVMs has been shown by Bao et al. (2020) and we restate the results for completeness. Besides, we also analyze the tractability of the reverse KL divergence, the total variation distance (Pollard, 2005), the maximum mean discrepancy (Li et al., 2017) and the Wasserstein distance (Arjovsky et al., 2017) between the two posteriors in EBLVMs.
The KL divergence is tractable. The gradient of the KL divergence between \( q_\phi(h|v) \) and \( p_\theta(h|v) \) w.r.t. \( \phi \) is
\[
\nabla_\phi D_{KL}(q_\phi(h|v)||p_\theta(h|v)) = \nabla_\phi \mathbb{E}_{q_\phi(h|v)} \log \frac{q_\phi(h|v)}{p_\theta(h|v)} = \nabla_\phi \mathbb{E}_{q_\phi(h|v)} \log \frac{q_\phi(h|v)p_\theta(v)}{\tilde{p}_\theta(v,h)} = \nabla_\phi \mathbb{E}_{q_\phi(h|v)} \log \frac{q_\phi(h|v)}{\tilde{p}_\theta(v,h)}.
\]
The last term doesn’t depend on the partition function or the marginal distribution of an EBLVM and thereby is tractable.

The Fisher divergence is tractable. The Fisher divergence between \( q_\phi(h|v) \) and \( p_\theta(h|v) \) is
\[
D_F(q_\phi(h|v)||p_\theta(h|v)) = \frac{1}{2} \mathbb{E}_{q_\phi(h|v)} \| \nabla_h \log q_\phi(h|v) - \nabla_h \log p_\theta(h|v) \|_2^2
\]
Again, the last term doesn’t depend on the partition function or the marginal distribution of an EBLVM and thereby is tractable. Furthermore, its gradient w.r.t. \( \phi \) is tractable.

The reverse KL divergence is generally intractable. The gradient of the reverse KL divergence between \( q_\phi(h|v) \) and \( p_\theta(h|v) \) w.r.t. \( \phi \) is
\[
\nabla_\phi D_{KL}(p_\theta(h|v)||q_\phi(h|v)) = \nabla_\phi \mathbb{E}_{p_\theta(h|v)} \log \frac{p_\theta(h|v)}{q_\phi(h|v)} = -\mathbb{E}_{p_\theta(h|v)} \nabla_\phi \log q_\phi(h|v). \]
Since \( p_\theta(h|v) \) is generally intractable, the reverse KL divergence is generally intractable.

The total variation distance is generally intractable. The gradient of total variation distance (Pollard, 2005) between \( q_\phi(h|v) \) and \( p_\theta(h|v) \) w.r.t. \( \phi \) is
\[
\nabla_\phi V(q_\phi(h|v), p_\theta(h|v)) = \nabla_\phi \frac{1}{2} \mathbb{E}_{q_\phi(h|v)} \| 1 - \frac{p_\theta(h|v)}{q_\phi(h|v)} \|_1 = \nabla_\phi \frac{1}{2} \mathbb{E}_{q_\phi(h|v)} \| 1 - \frac{p_\theta(h|v)}{q_\phi(h|v)} \|_1.
\]
Since \( p_\theta(h|v) \) is generally intractable, the total variation distance is generally intractable.

Maximum mean discrepancy is generally intractable. Given a kernel \( k \), the gradient of the square of maximum mean discrepancy (Li et al., 2017) between \( q_\phi(h|v) \) and \( p_\theta(h|v) \) w.r.t. \( \phi \) is
\[
\nabla_\phi M_k(q_\phi(h|v), p_\theta(h|v)) = \nabla_\phi \mathbb{E}_{h,h'} q_\phi(h|v)k(h,h') + \mathbb{E}_{h,h'} p_\theta(h|v)k(h,h') - 2 \mathbb{E}_{h,h'} q_\phi(h|v) k(h,h') - 2 \mathbb{E}_{h,h'} p_\theta(h|v) k(h,h') \nabla_\phi \mathbb{E}_{h,h'} q_\phi(h|v) k(h,h').
\]
Since \( p_\theta(h|v) \) is generally intractable, the maximum mean discrepancy is generally intractable.

The Wasserstein distance is generally intractable. The Wasserstein distance (Arjovsky et al., 2017) between \( q_\phi(h|v) \) and \( p_\theta(h|v) \) is
\[
\mathbb{W}(q_\phi(h|v), p_\theta(h|v)) = \frac{1}{K} \sup_{f \in \mathcal{F} \setminus \{0\}} \mathbb{E}_{q_\phi(h|v)} f(h) - \mathbb{E}_{p_\theta(h|v)} f(h).
\]
Generally \( \{ f : \| f \|_{Lip} \leq K \} \) is approximated by a neural network \( f_w \) with weight clipping and the Wasserstein distance is optimized by a bi-level optimization (Arjovsky et al., 2017). The lower level problem requires samples from the generally intractable posterior \( p_\theta(h|v) \). Thereby, the Wasserstein distance is generally intractable.

C. Proof of Theorem 1 and Theorem 2

Lemma 1. Suppose \( P, Q \) are two probability measures on \( \Omega \), and \( f : \Omega \rightarrow \mathbb{R}^m \), then we have \( \| \mathbb{E}_P f - \mathbb{E}_Q f \|_2 \leq \| f \|_{\infty} \sqrt{2D_{KL}(Q||P)} \), where \( \| f \|_{\infty} = \sup_{\omega \in \Omega} \| f(\omega) \|_2 \).

Proof. Let \( S = (P + Q)/2 \), then \( P, Q \) are absolutely continuous w.r.t. \( S \), and we have
\[
\| \mathbb{E}_P f - \mathbb{E}_Q f \|_2 = \| \int f \, dP - \int f \, dQ \|_2 = \| \int \frac{dP}{dS} \frac{dP}{dS} dS - \int f \frac{dQ}{dS} dS \|_2 = \| \int \left( \frac{dP}{dS} - \frac{dQ}{dS} \right) dS \|_2 \leq \| f \|_2 \| \frac{dP}{dS} - \frac{dQ}{dS} \|_{Lip} \leq \| f \|_{\infty} \sqrt{2D_{KL}(Q||P)}.
\]
According to Pinsker’s inequality (Tsybakov, 2008), we have \( \int \frac{dP}{dS} - \frac{dQ}{dS} \| dS \leq \sqrt{2D_{KL}(Q||P)} \). Thereby, \( \| \mathbb{E}_P f - \mathbb{E}_Q f \|_2 \leq \| f \|_{\infty} \sqrt{2D_{KL}(Q||P)} \).
Variational (Gradient) Estimate of the Score Function in Energy-based Latent Variable Models

**Theorem 1.** (VaES, KL divergence) Suppose $\nabla_v \log \tilde{p}_\theta(v, h)$ is bounded w.r.t. $v$, $h$ and $\theta$, then the bias of VaES($v; \theta, \phi$) can be bounded by the square root of the KL divergence between $q_\phi(h|v)$ and $p_\theta(h|v)$ up to multiplying a constant.

**Proof.** According to Lemma 1, we have

$$||E_{q_\phi(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)] - E_{p_\theta(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)]||_2 \leq \sup_h ||\nabla_v \log \tilde{p}_\theta(v, h)||_2 \sqrt{2D_{KL}(q_\phi(h|v)||p_\theta(h|v))}.$$  

By the boundedness of $\nabla_v \log \tilde{p}_\theta(v, h)$, $\exists A < \infty, \forall v, h, \forall \theta, ||\nabla_v \log \tilde{p}_\theta(v, h)||_2 \leq A$. Let $C = \sqrt{2}A$, then

$$||E_{q_\phi(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)] - \nabla_v \log p_\theta(v)||_2 = ||E_{q_\phi(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)] - E_{p_\theta(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)]||_2$$

$$\leq A \sqrt{2D_{KL}(q_\phi(h|v)||p_\theta(h|v))} = C \sqrt{D_{KL}(q_\phi(h|v)||p_\theta(h|v))}.$$  

\[\square\]

**Definition 1.** Suppose $A$ is a matrix, we define $||A||_2 \triangleq \sqrt{\sum_{i,j} A_{i,j}^2}.$

**Lemma 2.** Suppose $a, b$ are two vectors, then $||ab^T||_2 = ||a||_2||b||_2.$

**Proof.** $||ab^T||_2 = \sqrt{\sum_{i,j} a_i^2 b_j^2} = ||a||_2||b||_2.$  

\[\square\]

**Theorem 2.** (VaGES, KL divergence) Suppose $\nabla_v \log \tilde{p}_\theta(v, h)$, $\nabla_\theta \log \tilde{p}_\theta(v, h)$ and $\frac{\partial \nabla_v \log \tilde{p}_\theta(v, h)}{\partial \theta}$ are bounded w.r.t. $v$, $h$ and $\theta$, then the bias of VaGES($v; \theta, \phi$) can be bounded by the square root of the KL divergence between $q_\phi(h|v)$ and $p_\theta(h|v)$ up to multiplying a constant.

**Proof.** According to Thm. 1, $\exists C_1 < \infty$, s.t.

$$||E_{q_\phi(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)] - \nabla_v \log p_\theta(v)||_2 \leq C_1 \sqrt{D_{KL}(q_\phi(h|v)||p_\theta(h|v))}.$$  

Similarly, $\exists C_2 < \infty$, s.t.

$$||E_{q_\phi(h|v)} [\nabla_\theta \log \tilde{p}_\theta(v, h)] - \nabla_\theta \log p_\theta(v)||_2 \leq C_2 \sqrt{D_{KL}(q_\phi(h|v)||p_\theta(h|v))},$$

and $\exists C_3 < \infty$, s.t.

$$||E_{q_\phi(h|v)} \left[ \frac{\partial \nabla_v \log \tilde{p}_\theta(v, h)}{\partial \theta} \right] - E_{p_\theta(h|v)} \left[ \frac{\partial \nabla_v \log \tilde{p}_\theta(v, h)}{\partial \theta} \right]||_2 \leq C_3 \sqrt{D_{KL}(q_\phi(h|v)||p_\theta(h|v))}.$$  

By the boundedness of $\nabla_v \log \tilde{p}_\theta(v, h)$ and $\nabla_\theta \log \tilde{p}_\theta(v, h)$, $\nabla_v \log \tilde{p}_\theta(v, h) \frac{\partial \log \tilde{p}_\theta(v, h)}{\partial \theta}$ is also bounded. Thereby, $\exists C_4 < \infty$, s.t.

$$||E_{q_\phi(h|v)} \left[ \nabla_v \log \tilde{p}_\theta(v, h) \frac{\partial \log \tilde{p}_\theta(v, h)}{\partial \theta} \right] - E_{p_\theta(h|v)} \left[ \nabla_v \log \tilde{p}_\theta(v, h) \frac{\partial \log \tilde{p}_\theta(v, h)}{\partial \theta} \right]||_2$$

$$\leq C_4 \sqrt{D_{KL}(q_\phi(h|v)||p_\theta(h|v))}.$$  

By the boundedness of $\nabla_v \log \tilde{p}_\theta(v, h)$ and $\nabla_\theta \log \tilde{p}_\theta(v, h)$, we can assume $C < \infty$ is a constant that bounds
As a result, thereby, proof.

D. Proof of Theorem 3 and Theorem 4

\[ \| \nabla_v \log \tilde{p}_\theta(v, h) \|_2 \text{ and } \| \nabla_\theta \log \tilde{p}_\theta(v, h) \|_2 \text{. Then, by the triangle inequality and Lemma 2, we have} \]

\[ \| E_{q_\phi(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)] E_{q_\phi(h|v)} \left[ \frac{\partial \log \tilde{p}_\theta(v, h)}{\partial \theta} \right] - E_{p_\theta(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)] E_{p_\theta(h|v)} \left[ \frac{\partial \log \tilde{p}_\theta(v, h)}{\partial \theta} \right] \|_2 \]

\[ \leq \| E_{q_\phi(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)] E_{q_\phi(h|v)} \left[ \frac{\partial \log \tilde{p}_\theta(v, h)}{\partial \theta} \right] - E_{p_\theta(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)] E_{p_\theta(h|v)} \left[ \frac{\partial \log \tilde{p}_\theta(v, h)}{\partial \theta} \right] \|_2 \]

\[ + \| E_{q_\phi(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)] E_{q_\phi(h|v)} \left[ \frac{\partial \log \tilde{p}_\theta(v, h)}{\partial \theta} \right] - E_{p_\theta(h|v)} [\nabla_v \log \tilde{p}_\theta(v, h)] E_{p_\theta(h|v)} \left[ \frac{\partial \log \tilde{p}_\theta(v, h)}{\partial \theta} \right] \|_2 \]

\[ \leq (C_2 + C_1) \sqrt{D_{KL}(q_\phi(h|v)||p_\theta(h|v))} \]

Therefore,

\[ \| \text{Cov}_{q_\phi(h|v)} (\nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h)) - \text{Cov}_{p_\theta(h|v)} (\nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h)) \|_2 \]

\[ \leq \| \text{Cov}_{q_\phi(h|v)} (\nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h)) - \text{Cov}_{p_\theta(h|v)} (\nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h)) \|_2 \]

\[ \leq (C_4 + C_2 + C_1) \sqrt{D_{KL}(q_\phi(h|v)||p_\theta(h|v))} \]

As a result,

\[ \| \text{Cov}_{q_\phi(h|v)} (\nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h)) + \text{Cov}_{q_\phi(h|v)} (\nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h)) \|_2 \]

\[ \leq (C_4 + C_2 + C_1 + C_3) \sqrt{D_{KL}(q_\phi(h|v)||p_\theta(h|v))}. \]

D. Proof of Theorem 3 and Theorem 4

Definition 2. Suppose \( p \) is a probability density on \( \mathbb{R}^n \) and \( g : \mathbb{R}^n \to \mathbb{R}^n \), we define \( S_p g(x) \triangleq \nabla_x p(x) \nabla_g(x) + \text{Tr}(\nabla_x g(x)) \).

Lemma 3. (Liu & Wang, 2016) Suppose \( p \) is a probability density on \( \mathbb{R}^n \) and \( g : \mathbb{R}^n \to \mathbb{R}^n \) is a function satisfying

\[ \lim_{||x|| \to \infty} p(x)g(x) = 0, \text{ then } E_{p(x)} [S_p g(x)] = 0. \]

Proof.

\[ 0 = \int \nabla_x (p(x)g(x)) \, dx = \int p(x) \nabla_x g(x) + p(x)g(x) \nabla_x \log p(x) \nabla_x g(x) \, dx = E_{p(x)} [\nabla_x g(x) + g(x) \nabla_x \log p(x) \nabla_x g(x)]. \]

Thereby,

\[ 0 = \text{Tr}(E_{p(x)} [\nabla_x g(x) + g(x) \nabla_x \log p(x) \nabla_x g(x)]) = E_{p(x)} [\text{Tr}(\nabla_x g(x)) + \nabla_x \log p(x) \nabla_x g(x)] = E_{p(x)} [S_p g(x)]. \]
Lemma 4. Suppose \( p, q \) are probability densities on \( \mathbb{R}^n \) and \( g : \mathbb{R}^n \to \mathbb{R}^n \) satisfies \( \lim_{\|x\| \to \infty} q(x)g(x) = 0 \), we have

\[
|E_q S_p g| \leq \sqrt{E_q(||g(x)||^2 \sqrt{D_F(q||p)}}
\]

Proof. By Lemma 3, we have \( \mathbb{E}_q S_q g = 0 \). Thereby,

\[
|E_q S_p g| = |E_q S_p g - E_q S_q g| = \mathbb{E}_q g(x)^T (\nabla_x \log p(x) - \nabla_x \log q(x)) \\
\leq \mathbb{E}_q ||g(x)|| \cdot ||\nabla_x \log p(x) - \nabla_x \log q(x)|| \leq \sqrt{\mathbb{E}_q ||g(x)||^2 \mathbb{E}_q ||\nabla_x \log p(x) - \nabla_x \log q(x)||^2} \\
= \sqrt{\mathbb{E}_q ||g(x)||^2 \sqrt{D_F(q||p)}}. 
\]

Definition 3. (Ley et al., 2013) Suppose \( p \) is a probability density defined on \( \mathbb{R}^n \) and \( f : \mathbb{R}^n \to \mathbb{R} \) is a function, we define \( g_f^p \) as a solution of the Stein equation \( S_p g = f - E_p f \).

Remark. The solution of the Stein equation exists. For example, let \( h = f - E_p f \), then

\[
g_1(x) = \frac{1}{p(x)} \int_{-\infty}^{x_1} p(t, x_2, \ldots, x_n)h(t, x_2, \ldots, x_n)dt, \quad g_2(x) = \ldots = g_n(x) = 0
\]
is a solution.

Definition 4. Suppose \( p, q \) are probability densities defined on \( \mathbb{R}^n \) and \( f : \mathbb{R}^n \to \mathbb{R}^m \) is a function, we say \( f \) satisfies the Stein regular condition w.r.t. \( p, q \) iff \( \forall i \in \mathbb{Z} \cap [1, m], \lim_{||x|| \to \infty} q(x)g^p f_i(x) = 0 \).

Definition 5. (Ley et al., 2013) Suppose \( p, q \) are probability densities defined on \( \mathbb{R}^n \) and \( f : \mathbb{R}^n \to \mathbb{R}^m \) is a function satisfying the Stein regular condition w.r.t. \( p, q \), we define \( \kappa^{p,q}_f \triangleq \sqrt{\mathbb{E}_q(x) \sum_{i=1}^{m} ||g_f^p(x)||^2} \) referred to as the Stein factor of \( f \) w.r.t. \( p, q \).

Lemma 5. Suppose \( p, q \) are probability densities defined on \( \mathbb{R}^n \) and \( f : \mathbb{R}^n \to \mathbb{R}^m \) is a function satisfying the Stein regular condition w.r.t. \( p, q \), then we have \( ||E_q f - E_p f||_2 \leq \kappa^{p,q}_f \sqrt{D_F(q||p)} \).

Proof. By Lemma 4, we have \( ||E_q f - E_p f|| = ||E_q(f - E_p f)|| = ||E_q S_p g_f^p|| \leq \sqrt{\mathbb{E}_q(||g_f^p(x)||^2 \sqrt{D_F(q||p)}}. \]

Thereby, \( ||E_q f - E_p f|| = \sqrt{\sum_{i=1}^{n} ||E_q(f_i - E_p f_i)||^2 \leq \sqrt{\sum_{i=1}^{n} \mathbb{E}_q(||g_f^p(x)||^2 D_F(q||p)} = \kappa^{p,q}_f \sqrt{D_F(q||p)}}. \]

Theorem 3. (continuous \( h \), VaES) Suppose (1) \( \forall (v, \theta, \phi), \nabla_v \log \tilde{p}_\theta(v, h) \) as a function of \( h \) satisfies the Stein regular condition w.r.t. \( p_\theta(h|v) \) and \( q_\phi(h|v) \) and (2) the Stein factor of \( \nabla_v \log \tilde{p}_\theta(v, h) \) as a function of \( h \) w.r.t. \( p_\theta(h|v), q_\phi(h|v) \) is bounded w.r.t. \( v, \theta \) and \( \phi \), then the bias of VaES \((v, \theta, \phi)\) can be bounded by the square root of the Fisher divergence between \( q_\phi(h|v) \) and \( p_\theta(h|v) \) up to multiplying a constant.

Proof. It can be directly derived from Lemma 5.

Theorem 4. (continuous \( h \), VaGES) Suppose (1) \( \forall (v, \theta, \phi), \nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\phi(v, h), \nabla_v \log \tilde{p}_\phi(v, h) \) as functions of \( h \) satisfy the Stein regular condition w.r.t. \( p_\theta(h|v) \) and \( q_\phi(h|v) \) and (2) the Stein factors of \( \nabla_v \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\phi(v, h), \nabla_v \log \tilde{p}_\phi(v, h) \) as functions of \( h \) w.r.t. \( p_\theta(h|v), q_\phi(h|v) \) are bounded w.r.t. \( v, \theta \) and \( \phi \), (3) \( \nabla_v \log \tilde{p}_\theta(v, h) \) and \( \nabla_\theta \log \tilde{p}_\phi(v, h) \) are bounded w.r.t. \( v, h \) and \( \theta \), then the bias of VaGES \((v, \theta, \phi)\) can be bounded by the square root of the Fisher divergence between \( q_\phi(h|v) \) and \( p_\theta(h|v) \) up to multiplying a constant.

Proof. According to Lemma 5, \( \exists C_1 < \infty \), s.t.

\[
||E_{q_\phi(h|v)}[\nabla_v \log \tilde{p}_\theta(v, h)] - \nabla_v \log \tilde{p}_\theta(v)||_2 \leq C_1 \sqrt{D_F(q_\phi(h|v)||p_\theta(h|v))},
\]
Thereby,

\[ \exists C_2 < \infty, \text{ s.t.} \]

\[ \|\mathbb{E}_{q_\phi(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] - \nabla_\theta \log \tilde{p}_\theta(v) \|_2 \leq C_2 \sqrt{D_F(q_\phi(h|v)||p_\theta(h|v))}, \]

\[ \exists C_3 < \infty, \text{ s.t.} \]

\[ \|\mathbb{E}_{q_\phi(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] - \mathbb{E}_{p_\theta(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v) \right] \|_2 \leq C_3 \sqrt{D_F(q_\phi(h|v)||p_\theta(h|v))}, \]

and \( \exists C_4 < \infty, \text{ s.t.} \)

\[ \|\mathbb{E}_{q_\phi(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] - \mathbb{E}_{p_\theta(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \|_2 \leq C_4 \sqrt{D_F(q_\phi(h|v)||p_\theta(h|v))}. \]

By the boundedness of \( \nabla_\theta \log \tilde{p}_\theta(v, h) \) and \( \nabla_\theta \log \tilde{p}_\theta(v, h) \), we can assume \( C < \infty \) is a constant that bounds \( \|\nabla_\theta \log \tilde{p}_\theta(v, h)\|_2 \) and \( \|\nabla_\theta \log \tilde{p}_\theta(v, h)\|_2 \). After establishing the above bounds w.r.t. the Fisher divergence, the rest proof is exactly the same as Theorem 2. For completeness, we restate the proof as follows. By the triangle inequality and Lemma 2, we have

\[ \|\mathbb{E}_{q_\phi(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] - \mathbb{E}_{p_\theta(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \mathbb{E}_{p_\theta(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \|_2 \]

\[ \leq \|\mathbb{E}_{q_\phi(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \|_2 \|\mathbb{E}_{q_\phi(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \mathbb{E}_{p_\theta(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \|_2 \]

and

\[ \|\mathbb{E}_{q_\phi(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] - \mathbb{E}_{p_\theta(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \|_2 \leq (C_2 + C_1) \sqrt{D_F(q_\phi(h|v)||p_\theta(h|v))}. \]

Thereby,

\[ \|\text{Cov}_{q_\phi(h|v)}(\nabla_\theta \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h)) - \text{Cov}_{p_\theta(h|v)}(\nabla_\theta \log \tilde{p}_\theta(v, h), \nabla_\theta \log \tilde{p}_\theta(v, h))\|_2 \]

\[ \leq \|\mathbb{E}_{q_\phi(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] - \mathbb{E}_{p_\theta(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \|_2 \]

\[ + \|\mathbb{E}_{q_\phi(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \mathbb{E}_{q_\phi(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] - \mathbb{E}_{p_\theta(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \mathbb{E}_{p_\theta(h|v)} \left[ \nabla_\theta \log \tilde{p}_\theta(v, h) \right] \|_2 \]

\[ \leq (C_4 + C_2 + C_1) \sqrt{D_F(q_\phi(h|v)||p_\theta(h|v))}. \]
As a result,

\[
\|\text{Cov}_{q_{θ}(h|v)}(\nabla_v \log \tilde{p}_θ(v, h), \nabla_θ \log \tilde{p}_θ(v, h)) + \mathbb{E}_{q_{θ}(h|v)} \left[ \frac{∂\nabla_v \log \tilde{p}_θ(v, h)}{∂θ} \right] - \frac{∂\nabla_v \log p_θ(v)}{∂θ} \|_2 \\
= \|\text{Cov}_{q_{θ}(h|v)}(\nabla_v \log \tilde{p}_θ(v, h), \nabla_θ \log \tilde{p}_θ(v, h)) + \mathbb{E}_{q_{θ}(h|v)} \left[ \frac{∂\nabla_v \log \tilde{p}_θ(v, h)}{∂θ} \right] - \mathbb{E}_{p_θ(h|v)} \left[ \frac{∂\nabla_v \log \tilde{p}_θ(v, h)}{∂θ} \right] \|_2 \\
- \text{Cov}_{p_θ(h|v)}(\nabla_v \log \tilde{p}_θ(v, h), \nabla_θ \log \tilde{p}_θ(v, h)) - \mathbb{E}_{p_θ(h|v)}(\nabla_v \log \tilde{p}_θ(v, h), \nabla_θ \log \tilde{p}_θ(v, h)) \|_2 \\
\leq \|\text{Cov}_{q_{θ}(h|v)}(\nabla_v \log \tilde{p}_θ(v, h), \nabla_θ \log \tilde{p}_θ(v, h)) - \text{Cov}_{p_θ(h|v)}(\nabla_v \log \tilde{p}_θ(v, h), \nabla_θ \log \tilde{p}_θ(v, h)) \|_2 \\
+ \|\mathbb{E}_{q_{θ}(h|v)} \left[ \frac{∂\nabla_v \log \tilde{p}_θ(v, h)}{∂θ} \right] - \mathbb{E}_{p_θ(h|v)} \left[ \frac{∂\nabla_v \log \tilde{p}_θ(v, h)}{∂θ} \right] \|_2 \]
\]
\[
\leq (C_4 + CC_2 + CC_3 + C_3)\sqrt{D_F(q_θ(h|v)||p_θ(h|v))}. 
\]

\[\Box\]

E. Consistency between \(D^m_F\) and \(D_F\)

**Theorem 5.** Suppose \(\lim_{||v||→∞} p_D(v)(\nabla_v \log p_θ(v) - \nabla_v \log p_D(v)) = 0\) and \(\mathbb{E}_{p(ε)}[εε^T] = I\), then \(D^m_F(p_D||p_θ) = D_F(p_D||p_θ)\), where \(D_F(p_D||p_θ) = \frac{1}{2} \mathbb{E}_{p_D(v)} ||\nabla_v \log p_θ(v) - \nabla_v \log p_D(v)||_2^2\) is the Fisher divergence between \(p_D\) and \(p_θ\).

**Proof.** By the assumption \(\mathbb{E}_{p(ε)}[εε^T] = I\), we have \(\mathbb{E}_{p(ε)}[ε^T \nabla_v f(v) ε] = \text{Tr}(\nabla_v f(v))\). Thereby, \(D^m_F(p_D||p_θ) = \max_{f ∈ F} \mathbb{E}_{p_D(v)} [\nabla_v \log p_θ(v)^T f(v) + \text{Tr}(\nabla_v f(v)) - \frac{1}{2}||f(v)||_2^2]\).

Suppose \(f ∈ F\), i.e., \(f\) is a function from \(\mathbb{R}^d\) to \(\mathbb{R}^d\) and \(\lim_{||v||→∞} p_D(v) f(v) = 0\), by the Stein’s identity, we have \(\mathbb{E}_{p_D(v)} [\nabla_v \log p_D(v)^T f(v) + \text{Tr}(\nabla_v f(v))] = 0\). Thereby, we have

\[
\mathbb{E}_{p_D(v)} \left[ \nabla_v \log p_D(v)^T f(v) + \text{Tr}(\nabla_v f(v)) - \frac{1}{2}||f(v)||_2^2 \right] = 0 \\
= \mathbb{E}_{p_D(v)} \left[ \nabla_v \log p_θ(v)^T f(v) + \text{Tr}(\nabla_v f(v)) - \frac{1}{2}||f(v)||_2^2 \right] - \mathbb{E}_{p_D(v)} \left[ \nabla_v \log p_D(v)^T f(v) + \text{Tr}(\nabla_v f(v)) \right] \\
= \mathbb{E}_{p_D(v)} \left[ (\nabla_v \log p_θ(v) - \nabla_v \log p_D(v))^T f(v) - \frac{1}{2}||f(v)||_2^2 \right] \\
\leq \frac{1}{2} \mathbb{E}_{p_D(v)} ||(\nabla_v \log p_θ(v) - \nabla_v \log p_D(v))||_2^2 = D_F(p_D||p_θ).
\]

The equality is achieved when \(f(v) = \nabla_v \log p_θ(v) - \nabla_v \log p_D(v)\), which is a function in \(F\) by assumption. As a result, \(D^m_F(p_D||p_θ) = D_F(p_D||p_θ)\).

\[\Box\]
F. Additional Experimental Details

F.1. Learning EBLVMs with KSD

Additional setting. We generate 60,000 samples for training and 10,000 samples for testing on checkerboard. The dimension of $h$ is 4. We use the Adam optimizer and the learning rate is $10^{-3}$. We train 100,000 iterations and the batch size is 100. The log-likelihood is estimated by annealed importance sampling (Salakhutdinov & Murray, 2008), where we use 2,000 samples and 2,000 middle states to estimate the log-partition function. We run 1,000 steps Gibbs sampling to sample from GRBMs. The variational parameter $\phi$ is updated for $K = 5$ times on each minibatch.

F.2. Learning EBLVMs with Score Matching

F.2.1. Comparison in GRBMs

Following BiSM (Bao et al., 2020), we split 1,400 images for training, 300 images for validation and 265 images for testing on Frey face\(^1\); we generate 60,000 samples for training and 10,000 samples for testing on checkerboard; the dimension of $h$ is 400 on Frey face and 4 on checkerboard; we use the Adam optimizers with learning rates $2 \times 10^{-4}$ for training on Frey face and $10^{-3}$ for training on checkerboard; we train 20,000 iterations on Frey face and 100,000 iterations on checkerboard; the batch size is 100 for both datasets; we select the best model trained on Frey face according to the validation log-likelihood. The log-likelihood is estimated by annealed importance sampling (Salakhutdinov & Murray, 2008), where we use 2,000 samples and 2,000 middle states to estimate the log-partition function. We run 1,000 steps Gibbs sampling to sample from GRBMs. The time comparison on Frey face is conducted on 1 GeForce GTX 1080 Ti GPU with 2,000 training iterations. The number of samples from $q_{\phi}(h|v)$ is $L = 2$ and the variational parameter $\phi$ is updated for $K = 5$ times on each minibatch by default.

F.2.2. Learning Deep EBLVMs

Additional setting. Following BiSM (Bao et al., 2020), we split 60,000 samples for training on MNIST, 50,000 samples for training on CIFAR10 and 182,637 samples for training on CelebA; the dimension of $h$ is 50; we use the Adam optimizers with learning rates $10^{-3}$ for training on MNIST and $5 \times 10^{-5}$ for training on CIFAR10 and CelebA; we train 100,000 iterations on MNIST and 300,000 iterations on CIFAR10 and CelebA; the batch size is 100 for all datasets. $g_1$ consists of a $6k$-layer ResNet, where $k = 2, 3, 3$ for MNIST, CIFAR10 and CelebA respectively and $g_3$ is an MLP containing one fully connected layer. The structure of the deep EBLVM is shown in Fig. 6. The number of samples from $q_{\phi}(h|v)$ is $L = 2$ and the variational parameter $\phi$ is updated for $K = 5$ times on each minibatch. Following a similar protocol with Song & Ermon (2019); Li et al. (2019); Bao et al. (2020), we save one checkpoint every 5000 iterations and select the best CIFAR10 and CelebA models according to the FID score on 1000 samples. The FID score reported in Section 4.2 is estimated on 50,000 samples using the official code\(^2\).

Hyperparameter selection. Since we compare with BiSM (Bao et al., 2020), we use the same hyperparameters as BiSM when they can be shared (e.g., the model types and structures, the divergence to learn $q_{\phi}(h|v)$, the dimensions of $h$, the batch size, the optimizers and corresponding learning rates). As for $L$ (the number of samples from $q_{\phi}(h|v)$, we find it enough to set it to 2 (the minimal number of samples required in a sample covariance matrix) in our considered models. As for $K$, we set it to 5, so that it will ensure the convergence of training $q_{\phi}(h|v)$ and meanwhile have an acceptable computational cost. As for the step size and the standard deviation of the noise in Langevin dynamics, we grid search the optimal one, as shown in Tab. 2. We find that the optimal step size is approximately proportional to the dimension of $h$, perhaps because Langevin dynamics converges to its stationary distribution slower when $h$ has a higher dimension. The standard deviation can work in range $[10^{-4}, 10^{-2}]$.

\(^1\)http://www.cs.nyu.edu/~roweis/data.html
\(^2\)https://github.com/bioinf-jku/TTUR
We train 20,000 iterations and the batch size is 100. The number of samples from the GRBM is initialized as a standard Gaussian distribution by letting $q = 0$.

Additional setting.

The temperature range is $[0.2, 10]$ and the step size is $10^{-3}$.

2 hidden layers and each layer has the same width.

$\phi$ is a Bernoulli distribution parameterized by a fully connected layer with the sigmoid activation and we use the Gumbel-Softmax trick (Jang et al., 2017) for reparameterization.

$2,000$ samples for validation and $2,000$ samples for testing. We use the Adam optimizer and the learning rate is $10^{-4}$.

We get $20,000$ samples from the initial GRBM, and split $16,000$ samples for training, $1,000$ samples for validation and $2,000$ samples for testing. We use the Adam optimizer and the learning rate is $10^{-4}$.

We get $20,000$ samples from the initial GRBM, and split $16,000$ samples for training, $1,000$ samples for validation and $2,000$ samples for testing. We use the Adam optimizer and the learning rate is $10^{-4}$.

We get $20,000$ samples from the initial GRBM, and split $16,000$ samples for training, $1,000$ samples for validation and $2,000$ samples for testing. We use the Adam optimizer and the learning rate is $10^{-4}$.

**Sampling.** Since we compare with BiSM (Bao et al., 2020), we use the same sampling algorithm as BiSM. For deep EBLVMs, we first randomly select a training data point and inference its approximate posterior mean; we then sample from $p(v|h)$ with $h$ equal to the approximate posterior mean using the annealed Langevin dynamics technique (Li et al., 2019). The temperature range is $[1, 100]$ and the step size is $0.02$ in annealed Langevin dynamics.

**Devices and training time.** The time and memory consumption of VaGES with different batch sizes (BS) is displayed in Tab. 3. We also include that of BiSM. The time and memory consumption in deep EBLVMs of VaGES and BiSM is consistent with GRBMs (see Fig. 3 in the full paper). Besides, training an EBLVM takes about 2.8 times as long as training an EBM (the one trained by MDSM in Tab. 1 (a) in the full paper). The additional cost is reasonable, since (i) the EBLVM improves the expressive power (see Tab. 1 (a) in the full paper) based on a similar model structure and a comparable amount of parameters (244MB for the EBLVM and 238MB for the EBM), and (ii) the EBLVM enables manipulation in the latent space (see Fig. 4 in the full paper).

**F.3. Evaluating EBLVMs with Exact Fisher Divergence**

**Dataset Setting VaGES BiSM (N=0) BiSM (N=2) BiSM (N=5)**

| Dataset | Setting | VaGES | BiSM (N=0) | BiSM (N=2) | BiSM (N=5) |
|---------|---------|-------|------------|------------|------------|
| CIFAR10 | 1GPU BS=64 | 24m/5.8GB | 19m/6.8GB | 25m/7.8GB | 34m/9.5GB |
|         | 2GPUs BS=100 | 35m/8.2GB | 28m/11.1GB | 43m/13.2GB | 66m/16.4GB |
| CelebA  | 1GPU BS=16 | 26m/8.0GB | 21m/7.9GB | 26m/9.2GB | 35m/10.2GB |
|         | 6GPUs BS=100 | 90m/52.4GB | 67m/51.9GB | 100m/58.7GB | 124m/60.1GB |

**F.4. Numerical Validation of Theorems**

In the two posteriors $p_{\phi}(h|v)$ and $q_{\phi}(h|v)$, we fix $v$, $\theta$ and only vary $\phi$ to plot the relationship between the biases and the divergences. As for $v$, we randomly select a sample from the Frey face training dataset and fix $v$ as the sample. As for
we randomly initialize it with the uniform noise and don’t change it anymore. As for \( \phi \), we initialize it such that the variational posterior \( q_\phi(h|v) \) is equal to the true posterior \( p_\theta(h|v) \). After initialization, we perturb \( \phi \) with an increasing Gaussian noise level and record the corresponding biases and divergences.

The dimension of \( h \) is 400. As for the GRBM, \( q_\phi(h|v) \) is a Bernoulli distribution parameterized by a fully connected layer with the sigmoid activation. As for the Gaussian model, \( q_\phi(h|v) \) is a Gaussian distribution parameterized by a fully connected layer.

G. Additional Results

G.1. Learning EBLVMs with KSD

The density of the checkerboard dataset is shown in Fig. 7 (a). The densities of GRBMs learned by KSD, VaGES-KSD and IS-KSD are shown in Fig. 7 (b-h). Our VaGES-KSD is comparable to the KSD baseline and is better than the IS-KSD baseline. The result is consistent with the test log-likelihood results in Fig. 2 in the full paper.

Figure 7. Density plots of GRBMs trained by KSD, VaGES-KSD and IS-KSD. \( L \) is the number of samples from \( q_\phi(h|v) \).
G.2. Learning EBLVMs with Score Matching

G.2.1. COMPARISON IN GRBM

We compare with DSM (Vincent, 2011), BiSM (Bao et al., 2020), CD-based methods (Hinton, 2002; Tieleman, 2008) and noise contrastive estimation (NCE)-based methods (Gutmann & Hyvärinen, 2010; Rhodes & Gutmann, 2019) on the checkerboard dataset. In Fig. 8, we plot the test log-likelihood of different methods under the same setting. The result of VaGES-DSM is similar to CD, DSM and BiDSM and slightly better than PCD and NCE-based methods after convergence. The convergence speed of VaGES-DSM is faster than BiDSM. Besides, we show the densities of GRBMs learned by these methods in Fig. 9. The performance of VaGES-DSM is similar to CD, DSM and BiDSM and better than PCD, NCE and VNCE, which agrees with the test log-likelihood results after convergence in Fig. 8.

Figure 8. Comparison of different methods on checkerboard. The test log-likelihood is averaged over 10 runs.

Figure 9. Density plots of GRBMs trained by different methods on checkerboard.
G.2.2. Learning Deep EBLVMs

Sample quality. We show samples from EBLVMs learned on MNIST, CIFAR10 and CelebA in Fig. 10. We also evaluate the Inception Score on CIFAR10 and VaGES gets 7.53, which is better than baselines such as VAE-EBLVM (Han et al., 2020) (7.17) and EBM (Du & Mordatch, 2019) (6.78).

Figure 10. Samples from EBLVMs.
Interpolation in the latent space. We show more interpolation results in Fig. 11.

Figure 11. Interpolation of annealed Langevin dynamics trajectories in the latent space in EBLVMs.
Sensitivity analysis. We study how hyperparameters influence the performances of VaGES-SM in deep EBLVMs. The result is shown in Tab. 4. Increasing the number of convolutional layers will improve the performance, while the dimension of $h$, the number of $h$ sampled from $q_\phi(h|v)$ and the noise level in Langevin dynamics don’t affect the result very much. Setting both the number of times updating $\phi$ and the number of Langevin dynamics steps to 5 is enough for a stable training. Besides, we also try using the KL divergence to learn the variational posterior and get a FID of 29.13, which doesn’t affect the result very much.

| (a) Dimensions of $h$ | (b) # convolutional layers | (c) $h$ sampled from $q_\phi(h|v)$ | (d) Noise level in Langevin dynamics | (e) # times updating $\phi$ ($K$) | # Langevin dynamics steps ($C$) |
|-----------------------|---------------------------|----------------------------------|-----------------------------------|----------------------------------|---------------------------|
| 20 50 100             | 12 18 24                  | 2 5 10                           | $10^{-4}$ $10^{-3}$ $10^{-2}$     | FID 26.55 28.09 27.78            | FID 36.17 28.09 25.98     |
| FID 26.55 28.09 27.78 | FID 28.09 31.21 29.26     | FID 28.09 25.83 30.47            |                                   | Div Div Div Div Div Div Div Div |

H. Additional Attempts on Improving Estimates

We can directly apply the control variate technique (Owen, 2013) to VaES. By noticing that

$$\mathbb{E}_{q_\phi(h|v)} \nabla_v \log q_\phi(h|v) = \int q_\phi(h|v) \nabla_v q_\phi(h|v) \, q_\phi(h|v) \, dh = \nabla_v \int q_\phi(h|v) \, dh = 0,$$  

(27)

we can subtract $\nabla_v \log q_\phi(h|v)$ from VaES without changing the value of the expectation, and the resulting variational estimate is

$$\text{VaES-CV}(v; \theta, \phi) = \frac{1}{L} \sum_{i=1}^{L} \nabla_v \log \tilde{p}_\theta(v, h_i), \quad h_i \overset{i.i.d.}{\sim} q_\phi(h|v).$$  

(28)

When the variational posterior $q_\phi(h|v)$ is equal to the true posterior $p_\theta(h|v)$, $\text{VaES-CV}(v; \theta, \phi) = \nabla_v \log \tilde{p}_\theta(v, h) = \nabla_v \log \hat{p}_\theta(v)$ is exactly equal to the score function and has zero bias and variance. Empirically, we study how the control variate influences the performance over different objectives on the checkerboard dataset in GRBMs. As shown in Fig. 12, the control variate only marginally improves the performance of VaGES-KSD and makes no difference to VaGES-DSM. As a result, we don’t make the control variate a default technique in VaES, since it will introduce some extra computation, while the improvement is marginal.

Figure 12. How the control variate (CV) influences the performance over different objectives on the checkerboard dataset in GRBMs. The test log-likelihood is averaged over 10 runs.
I. An Introduction to BiSM

BiSM (Bao et al., 2020) approximates the score function via variational inference first:

\[ \nabla_v \log p(v; \theta) = \nabla_v \log \frac{\tilde{p}(v, h; \theta)}{p(h|v; \theta)} - \nabla_v \log Z(\theta) = \nabla_v \log \frac{\tilde{p}(v, h; \theta)}{p(h|v; \theta)}, \]

and then gets the gradient of a certain objective via solving a complicated bi-level optimization problem:

\[ \min_{\theta \in \Theta} J_{Bi}(\theta, \phi^*(\theta)), \quad J_{Bi}(\theta, \phi) = \mathbb{E}_{q(v, \epsilon)} \mathbb{E}_{q(h|v; \phi)} F \left( \nabla_v \log \frac{\tilde{p}(v, h; \theta)}{q(h|v; \phi)}, \epsilon, v \right), \]

where \( \Theta \) is the hypothesis space of the model, \( F \) depends on the certain objective, \( q(v, \epsilon) \) is the joint distribution of the data and additional noise and \( \phi^*(\theta) \) is defined as follows:

\[ \phi^*(\theta) = \arg \min_{\phi \in \Phi} G(\theta, \phi), \quad \text{with } G(\theta, \phi) = \mathbb{E}_{q(v, \epsilon)} D \left( q(h|v; \phi) || p(h|v; \theta) \right). \]

BiSM uses gradient unrolling to solve the problem, where the lower level problem \( \phi^*(\theta) \) is approximated by the output of \( N \) steps gradient descent on \( G(\theta, \phi) \) w.r.t. \( \phi \), which is denoted by \( \phi^N(\theta) \). Finally, the model is updated with the approximate gradient \( \nabla_\theta J_{Bi}(\theta, \phi^N(\theta)) \), whose bias converges to zero in a linear rate in terms of \( N \) when \( G \) is strongly convex. The gradient unrolling requires an \( O(N) \) time and memory.

Gradient unrolling of small steps is of large bias and that of large steps is time and memory consuming. Thus, BiSM with 0 gradient unrolling suffers from an additional bias besides the variational approximation. Instead, VaGES directly approximates the gradient of score function and its bias is controllable as presented in Sec. 2.2.