Learning Deep Generative Models with Short Run Inference Dynamics

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Abstract

This paper studies the fundamental problem of learning deep generative models that consist of one or more layers of latent variables organized in top-down architectures. Learning such a generative model requires inferring the latent variables for each training example based on the posterior distribution of these latent variables. The inference typically requires Markov chain Monte Carlo (MCMC) such as Langevin dynamics [27] or Hamiltonian Monte Carlo (HMC) [30]. Such MCMC posterior sampling can be time consuming and can be difficult to scale up to big training data. The convergence of MCMC sampling is also questionable even after a long running time.

An alternative to MCMC posterior sampling is variational inference, which employs a simple factorized distribution to approximate the posterior distribution. Classical variational inference methods assume an approximate posterior distribution for each observed example, where the approximate posterior distribution is parametrized by some variational parameters that are specific to each example and that can be optimized by minimizing the Kullback-Leibler divergence between the approximate distribution and the true posterior.

More recently, in the context of the generator network which consists of a single layer of latent vector at the top, the variational auto-encoder (VAE) [25, 35] learns an extra inference network that maps each input example to the approximate posterior distribution, in particular, the mean vector and the diagonal variance-covariance matrix of the approximate multivariate Gaussian posterior. Unlike classical variational methods, the parameters of the inference network are shared by all the training and testing examples, and they are learned together with the parameters of the generator network by jointly maximizing a lower bound of the log-likelihood.

Despite the success of VAE, it has the following shortcomings. (1) It requires a separate inference model with a separate set of parameters. These parameters are to be learned together with the parameters of the generative model. (2) The design of the inference model is not automatic, especially for generative models with multiple layers of latent vectors, which may have complex relationships un-

1. Introduction

Deep generative models have seen many applications such as image and video synthesis, and unsupervised or semi-supervised learning. Such models usually consist of one or more layers of latent variables organized in top-down architectures. Learning such latent variable models from training examples is a fundamental problem, and this is the problem that this paper is concerned with.

Learning latent variable models usually requires inferring the latent variables based on their joint posterior distribution, i.e., the conditional distribution of the latent variables given each observed example. The inference typically requires Markov chain Monte Carlo (MCMC) such as Langevin dynamics [27] or Hamiltonian Monte Carlo (HMC) [30]. Such MCMC posterior sampling can be time consuming and can be difficult to scale up to big training data. The convergence of MCMC sampling is also questionable even after a long running time.

An alternative to MCMC posterior sampling is variational inference, which employs a simple factorized distribution to approximate the posterior distribution. Classical variational inference methods assume an approximate posterior distribution for each observed example, where the approximate posterior distribution is parametrized by some variational parameters that are specific to each example and that can be optimized by minimizing the Kullback-Leibler divergence between the approximate distribution and the true posterior.

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Despite the success of VAE, it has the following shortcomings. (1) It requires a separate inference model with a separate set of parameters. These parameters are to be learned together with the parameters of the generative model. (2) The design of the inference model is not automatic, especially for generative models with multiple layers of latent vectors, which may have complex relationships un-

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nder their joint posterior distribution. It is a highly non-trivial task to design an inference model to adequately capture the explaining-away competitions and bottom-up and top-down interactions between multiple layers of latent variables.

In this article, we propose a simple method that lies in between MCMC posterior sampling and variational inference. Specifically, we propose to use a short run inference dynamics guided by the posterior distribution of the latent variables as an approximate inference engine. To make it more concrete, we employ a finite-step gradient descent on the negative log-posterior distribution of the latent variables. For each training example, we initialize such a short run gradient flow from the prior distribution such as Gaussian or uniform noise distribution, and run a finite number (e.g., 20) of steps of gradient descent updates. This amounts to a residual network or a recurrent neural network (RNN) that transforms the initial noise distribution to an approximate posterior distribution. We optimize the step size of the gradient flow by minimizing the Kullback-Leibler divergence between the approximate distribution produced by this short run inference dynamics and the true posterior distribution. Thanks to the computing capacities of the modern deep learning platforms, it is possible to compute the approximate distribution and its entropy, and optimize the aforementioned Kullback-Leibler divergence. This is similar to variational inference, except that the variational parameter is the step size of the gradient descent, or in general, the tuning parameters of the short run inference dynamics. Our experiments show that the proposed method outperforms the VAE in terms of reconstruction error and synthesis quality.

The proposed method is similar to MCMC posterior sampling except that we focus on the optimization of a short run version of MCMC sampling. Such short run inference dynamics is easily affordable on current deep learning platforms and there is no much difficulty to scale it up to big datasets. The proposed method is also similar to variational inference except that the inference model is simply a noise initialized finite-step gradient flow, where the only extra parameter is the step sizes of the gradient flow or in general some tuning parameters of the short run inference dynamics.

One major advantage of the proposed method is that it is natural and automatic. For models with multiple layers of latent variables that may be organized in complex top-down architectures, the gradient descent update of the log-posterior of the latent variables can be automatically obtained on modern deep learning platforms. Such gradient descent update naturally integrates explaining-away competitions and bottom-up and top-down interactions between multiple layers of latent variables. By optimizing the step size of the gradient descent update using the variational criterion, it is possible to have a good approximate posterior distribution and an efficient inference engine. It thus enables researchers to explore sophisticated generative models without worrying about constructing the presumably more sophisticated inference models.

2. Contributions and related work

The following are contributions of our paper.

- We propose short run inference dynamics for inferring latent variables in deep generative models.
- We provide a method to determine the optimal step size or in general tuning parameters of the short run inference dynamics.
- We demonstrate learning of multi-layer latent variable models with high quality samples and reconstructions.

The following are themes related to our work.

(1) Variational inference. As mentioned above, VAE [25, 35, 39, 11] is the prominent method for learning generator network. The original inference model has been generalized to flow-based inference models such as normalizing flows. Our short run gradient flow can also be viewed as a flow model. The difference is that the gradient flow is obtained automatically from the log-posterior of latent variables. There is no need to design an extra inference model or flow-based model for inference, and there is no need to learn an extra set of parameters except some tuning parameters of the gradient descent algorithm such as step size. More importantly, the gradient descent update is readily available for models with multiple layers of latent variables, whereas designing inference models for such generative models can be a highly non-trivial task.

(2) Alternating back-propagation. [12, 42] propose to learn the generator network by maximum likelihood, and the learning algorithm iterates the following two steps: (a) inferring the latent variables by Langevin dynamics that samples from the posterior distribution of the latent variables. (b) updating the model parameters based on the inferred latent variables. Both steps involve gradient computations based on back-propagation, thus the name “alternating back-propagation”. In the training stage, in step (a), the Langevin dynamics is initialized from the values of the latent variables produced in the previous epoch. This is usually called persistent chain in the literature. In our work, in step (a), we always initialize the finite-step (e.g., 20-step) gradient descent updates from the prior noise distribution. This can be called non-persistent chain. It is also a non-convergent chain because we do not expect the chain to converge to the target distribution. But we do optimize the step size (or in general, the tuning parameters) of the gradient descent update based on a variational criterion. This
allows us to use very affordable short run inference dynamics for learning, and moreover, the same short run inference dynamics can be used for testing examples as well.

(3) Short run MCMC for energy-based model. Recently [32] proposes to learn short run MCMC for energy-based model. An energy-based model is in the form of an unnormalized probability density function, where the log-density or the energy function is parametrized by a bottom-up neural network. [32] shows that it is possible to learn short run MCMC such as 100-step Langevin dynamics that can generate images of high synthesis quality, and they justify the learn short run MCMC as a valid flow-like model. However, the energy-based model itself is not well learned. Our method follows a similar strategy, but it is intended for approximately sampling from the posterior distribution of latent variables. Our optimization method can help reduce the gap between the short run MCMC and the corresponding energy-based model, so that the energy-based model may also be properly learned.

(4) Attractor dynamics. In computational neuroscience, the dynamics of the neuron activities is often modeled by attractor dynamics [19, 2, 33]. However, the objective function of the attractor dynamics is often implicit, thus it is unclear what is the computational problem that the attractor dynamics is solving. For the attractor dynamics to be implemented in real time, the dynamics is necessarily a short run dynamics. Our short run inference dynamics is guided by a top-down model with a well-defined objective function in terms of the log-posterior of the latent variables. It may be connected to the attractor dynamics and help us understand the latter. We shall explore this direction in future work.

3. Deep generative models

3.1. Joint, marginal, and posterior distributions

Let $x$ be the observed example, such as an image. Let $z$ be the latent variables, which may consist of latent variables at multiple layers organized in a top-down architecture. We may consider $z$ as forming an interpretation or explanation of $x$.

The joint distribution of $(x, z)$ is $p_\theta(x, z)$, where $\theta$ consists of model parameters. The marginal distribution of $x$ is $p_\theta(x) = \int p_\theta(x, z)dz$. Given $x$, the inference of $z$ can be based on the posterior distribution $p_\theta(z|x) = p_\theta(x, z)/p_\theta(x)$.

3.2. Five families of models

To put our work in context, we review the following classes of models, which correspond to different ways of specifying $p_\theta(x, z)$ or $p_\theta(x)$.

(1) Generator network. This model assumes a $d$-dimensional noise vector $z$ at the top-layer. The prior distribution $p(z)$ is known, such as $z \sim \mathcal{N}(0, I_d)$, where $I_d$ is the $d$-dimensional identity matrix. Given $z$, $x = g_\theta(z) + \epsilon$, where $g_\theta(z)$ is a top-down convolutional neural network (sometimes called deconvolutional network due to the top-down nature), where $\theta$ consists of all the weight and bias terms of this top-down network. $\epsilon$ is usually assumed to be Gaussian white noise with mean 0 and variance $\sigma^2$. Thus $p_\theta(x|z)$ is such that $[x|z] \sim \mathcal{N}(g_\theta(z), \sigma^2 I_D)$, where $D$ is the dimensionality of $x$. For this model

$$\log p_\theta(x, z) = \log[p_\theta(z)p_\theta(x|z)]$$

$$= -\frac{1}{2} \left[ \|z\|^2 + \|x - g_\theta(z)\|^2/\sigma^2 \right] + c,$$

where $c$ is a constant independent of $\theta$.

In the generator network, units in the latent vector $z$ may carry semantic meanings in that if we varying the units of $z$, we can observe semantically meaningful variations in $x$.

(2) Multi-layer generator network. While it is computationally convenient to have a latent noise vector at the top layer, it does not account for the fact that patterns can appear at multiple layers of compositions or abstractions (e.g., face $\rightarrow$ (eyes, nose, mouth) $\rightarrow$ (edges, corners) $\rightarrow$ pixels), where variations and randomness occur at multiple layers. To capture such a hierarchical structure, it is desirable to introduce multiple layers of latent variables organized in a top-down architecture. Specifically, we have $z = (z_l, l = 1, ..., L)$, where layer $L$ is the top layer, and layer 1 is the bottom layer above $x$. For notational simplicity, we let $x = z_0$. We can then specify $p_\theta(z)$ as

$$p_\theta(z) = p_\theta(z_L) \prod_{l=0}^{L-1} p_\theta(z_l|z_{l+1}).$$

One concrete example is $z_L \sim \mathcal{N}(0, I)$, $[z_l|z_{l+1}] \sim \mathcal{N}(\mu_l(z_{l+1}), \sigma^2_l(z_{l+1}))$, $l = 0, ..., L - 1$. where $\mu_l()$ and $\sigma^2_l()$ are the mean vector and the diagonal variance-covariance matrix of $z_l$ respectively, and they are functions of $z_{l+1}$. $\theta$ collects all the parameters in these functions. $p_\theta(x, z)$ can be obtained similarly to Equation (2).

(3) Energy-based model (EBM). The EBM [29, 31, 21, 44, 43, 9, 26, 32, 8, 20, 28] specifies $p_\theta(x)$ directly, and it does not involve any latent variables $z$. Specifically, $p_\theta(x) = \frac{1}{Z(\theta)} \exp(f_\theta(x))$, where $f_\theta$ is parametrized by a bottom-up neural network. $-f_\theta(x)$ is called the energy function.

(4) Latent energy-based model. The latent EBM [18, 38] specifies $p_\theta(x, z)$ directly, instead of specifying $p_\theta(z)$ and $p_\theta(x|z)$ separately as in the generator network or multi-layer generator network. Specifically, $p_\theta(x, z) = \frac{1}{Z(\theta)} \exp(f_\theta(x, z))$, where $-f_\theta(x, z)$ is the joint energy function. In general, both the generator model and its multi-layer version can be written in this form with closed form $Z(\theta)$, thus they are special cases of latent EBM. However,
Unlike \( f_\theta(x) \) of the EBM in (3), \( f_\theta(x, z) \) in latent EBM typically only involves singleton (unitary) and pairwise (binary) terms for biological plausibility.

(5) Flow-based model. The flow-based model [6, 7, 23, 10, 3, 41] is similar to the generator network, except that \( z \) and \( x \) are of the same dimensionality, and \( x = g_\theta(z) \) with an invertible \( g_\theta \). As a result, \( p_\theta(x) \) can be obtained in closed form, similar to the EBM. Unlike EBM, the density for the flow-based model is normalized, or in other words, the normalizing constant is in closed form. Computational feasibility requires that \( g_\theta \) composes a sequence of transformations, thus a flow, whose inverse and Jacobian can be efficiently computed. Here we present the flow-based model as a generative model. It can also be used as an inference model to approximate the posterior \( p(z|x) \) [34, 24].

To connect the above models to our work, we focus on (1) and (2). However, our method is applicable to (3) and (4) as well. For (3), our optimization method can be used to optimize the short run MCMC that samples \( p_\theta(x) \). Our short run inference dynamics is also related to the flow-based inference model in (5).

3.3. Learning and inference

Let \( p_{\text{data}}(x) \) be the data distribution that generates the example \( x \). The learning of parameters \( \theta \) of \( p_\theta(x) \) can be based on \( \min_\theta \text{KL}(p_{\text{data}}(x) || p_\theta(x)) \), where \( \text{KL}(p || q) = E_p[\log(p(x) / q(x))] \) is the Kullback-Leibler divergence between \( p \) and \( q \) (or from \( p \) to \( q \) since \( \text{KL}(p || q) \) is asymmetric). If we observe training examples \( \{x_i, i = 1, ..., n \} \sim p_{\text{data}} \), the above minimization can be approximated by maximizing the log-likelihood

\[
L(\theta) = \frac{1}{n} \sum_{i=1}^{n} \log p_\theta(x_i),
\]

which leads to the maximum likelihood estimate (MLE).

The gradient of the log-likelihood, \( L'(\theta) \), can be computed according to the following identity:

\[
\frac{\partial}{\partial \theta} \log p_\theta(x) = \frac{1}{p_\theta(x)} \frac{\partial}{\partial \theta} p_\theta(x) = \int \frac{\partial}{\partial \theta} \log p_\theta(x, z) \frac{p_\theta(x, z)}{p_\theta(x)} dz = E_{p_\theta(z|x)} \left[ \frac{\partial}{\partial \theta} \log p_\theta(x, z) \right].
\]

The above expectation can be approximated by Monte Carlo samples from \( p_\theta(x, z) \).

For generator network or its multi-layer version, \( \frac{\partial}{\partial \theta} \log p_\theta(x, z) \) is in closed form. For latent EBM, \( \frac{\partial}{\partial \theta} \log p_\theta(x, z) = \frac{\partial}{\partial \theta} f_\theta(x, z) - E_{p_\theta(x, z)} \left[ \frac{\partial}{\partial \theta} f_\theta(x, z) \right] \), where the expectation can be approximated by Monte Carlo samples from \( p_\theta(x, z) \). In this work, we shall focus on generator network and its multi-layer version. We shall leave latent EBM to future work.

The MLE learning can be accomplished by gradient descent. Each learning iteration updates \( \theta \) by

\[
\theta_{t+1} = \theta_t + \eta_t \frac{1}{n} \sum_{i=1}^{n} E_{p_{\theta_t}(z_i|x_i)} \left[ \frac{\partial}{\partial \theta} \log p_\theta(x_i, z_i) \right],
\]

where \( \eta_t \) is the step size or learning rate, and \( E_{p_{\theta_t}(z_i|x_i)} \) can be approximated by Monte Carlo sampling from \( p_{\theta_t}(z_i|x_i) \).

4. Short run inference dynamics

4.1. Langevin dynamics

Sampling from \( p_\theta(z|x) \) usually requires MCMC. One convenient MCMC is Langevin dynamics [27], which iterates

\[
z_{k+1} = z_k + s \frac{\partial}{\partial z} \log p_\theta(z_k|x) + \sqrt{2s} \epsilon_k,
\]

where \( \epsilon_k \sim \mathcal{N}(0, I) \), \( k \) indexes the time step of the Langevin dynamics, and \( s \) is the step size. The Langevin dynamics consists of a gradient descent term on \(- \log p_\theta(z|x)\). In the case of generator network, it amounts to gradient descent on \( ||z||^2/2 + ||x - g_\theta(z)||^2/2\sigma^2 \), which is penalized reconstruction error. The Langevin dynamics also consists of a white noise diffusion term \( \sqrt{2s} \epsilon_k \) to create randomness for sampling from \( p_\theta(z|x) \). For small step size \( s \), the marginal distribution of \( z_k \) will converge to \( p_\theta(z|x) \) as \( k \to \infty \) regardless of the initial distribution of \( z_0 \). More specifically, let \( q_k(z) \) be the marginal distribution of \( z_k \) of the Langevin dynamics, then \( \text{KL}(q_k(z) || p_\theta(z|x)) \to 0 \) monotonically, that is, by increasing \( k \), we reduce \( \text{KL}(q_k(z) || p_\theta(z|x)) \).

Thus MCMC is consistent with variational approximation. Both seek to minimize \( \text{KL}(q(z) || p_\theta(z|x)) \) over \( q \) within a certain class.

4.2. Noise initialized short run dynamics

It is impractical to run long chains to sample from \( p_\theta(z|x) \). We thus propose the following short run inference dynamics.

\[
z_0 \sim p(z),
\]

\[
z_{k+1} = z_k + s \frac{\partial}{\partial z} \log p_\theta(z_k|x), \; k = 1, ..., K,
\]

where \( p(z) \) is the prior distribution of \( z \). In the case of generator network, \( p(z) = \mathcal{N}(0, L_q) \). Starting from \( p(z) \), we run \( K \) steps of gradient descent on \(- \log p_\theta(z|x)\) with step size \( s \), and we take \( z_K \) to be an approximate sample from \( p_\theta(z|x) \).
Compared to the Langevin dynamics, we remove the white noise term $\sqrt{2}\varepsilon_k$. In practice, the noise term $\sqrt{2}\varepsilon_k$ has minimal usefulness for the following two reasons. (1) In the beginning stage, when the reconstruction error is big relative to $\sigma^2$, the gradient of $-\log p_\theta(z|x) = (\|z\|^2 + \|x - g_\theta(z)\|^2/\sigma^2)/2 + c$ dominates the noise term, which is negligible. (2) When the Langevin dynamics get to a local mode, the noise term can hardly get the chain jump out of the local mode, if the mode is deep. That is, running long chain without noise term, starting from the noise prior can afford it, it still cannot guarantee mode traversing and convergence to the target distribution. Thus we opt to run short chain without noise term, starting from the noise prior distribution $p(z)$, so that the randomness or possible multimodality comes from the initial $p(z)$ instead of the almost useless noise term, and we optimize the step size $s$ to let the distribution of $z_K$ approximate the true posterior $p_\theta(z|x)$.

We can write the above dynamics as

$$z_0 \sim p(z), \quad z_{k+1} = z_k + sR(z_k), \quad k = 1, ..., K,$$

(12)

where $R(z) = \frac{\partial}{\partial z} \log p_\theta(z|x)$, where we omit $x$ and $\theta$ in $R(z)$ for the simplicity of notation. For finite $K$, this dynamics is a $K$-layer residual network, or $K$-step RNN. In a recent paper, [3] studies the residual network as a flow-based model.

### 4.3. Flow-like inference model

To further simplify the notation, we may write the dynamics as

$$z_0 \sim p(z), \quad z_K = F(z_0),$$

(13)

where $F$ composes the $K$ steps of gradient descent. The above model can be considered a flow-based model, where $F$ consists of $K$-step flow of gradient updates. Let the distribution of $z_K$ be $q_s(z)$, where we include the notation $s$ to make it explicit that the distribution of $z_K$ depends on the step size $s$. Recall that the distribution of $z_K$ also depends on $x$ and $\theta$, so that in full notation, we may write $q_s(z)$ as $q_{s,\theta}(z|x)$.

By change of variable,

$$z_K \sim q_s(z) = p(F^{-1}(z)|\det(dF^{-1}(z)/dz)|.$$

(14)

We may treat $q_s(z)$ as a flow-like variational inference model.

### 4.4. Variational optimization of step size

We want to optimize the step size $s$ so that $q_s(z)$ best approximates the true posterior $p_\theta(z|x)$. This can be accomplished by

$$\min_s \text{KL}(q_s(z)\|p_\theta(z|x)).$$

(15)

This is similar to variational approximation, with step size $s$ being the variational parameter.

$$\text{KL}(q_s(z)||p_\theta(z|x)) = E_{q_s(z)}[\log q_s(z) - \log p_\theta(x, z)] + \log p_\theta(x),$$

(16)

where the last term $\log p_\theta(x)$ is independent of $s$, and for the first two terms on the right hand side,

$$E_{q_s(z)}[\log p_\theta(x, z)] = E_{p(z_0)}[\log p_\theta(x, F(z_0))],$$

(17)

and

$$E_{q_s(z)}[\log p_\theta(z)] = E_{p(z_0)}[\log p(z_0)] - \log |\det(dF(z_0)/dz_0)|.$$  

(18)

In the above two equations, $E_{p(z_0)}$ can be approximated by random samples from $z_0 \sim p(z)$, e.g., $N(0, I_d)$ in the case of generator network.

In the above computations, we do not need to invert $F$, as is typical in flow-based variational approximation, but we need to compute the log determinant of the Jacobian $dF(z_0)/dz_0$. Fortunately, on modern deep learning platforms, such computation is easily feasible even if the dimension of $z_0$ is very high. For a sampled $z_0 \sim p(z)$, after computing the matrix $dF(z_0)/dz_0$, we can compute the eigenvalues of $dF(z_0)/dz_0$, so that the log-determinant is the sum of the log of the eigenvalues. Then we can optimize the step size $s$ by minimizing $\text{KL}(q_s(z)||p_\theta(z|x))$ via a grid search or gradient descent.

While we can optimize the step size $s$ for each example $x$, in our work, we optimize over an overall $s$ that is shared by all the examples. Reverting to the full notation $q_{s,\theta}(z|x)$ for $q_s(z)$, this means we minimizes

$$\frac{1}{n} \sum_{i=1}^{n} \text{KL}(q_{s,\theta}(z_i|x_i)||p_\theta(z_i|x_i))$$

(20)

over $s$.

Instead of using a constant step size $s$, gradient descent with respect to $s$ may also be generalized to optimize over varying step sizes $s_k, k = 1, ..., K$. We leave it to future work.

### 4.5. Learning with short run inference dynamics

Each learning iteration consists of the following two steps. (1) Update $s$ by minimizing (20). (2) Update $\theta$ by

$$\theta_{t+1} = \theta_t + \eta_t \frac{1}{n} \sum_{i=1}^{n} E_{q_{s,\theta}(z_i|x_i)} \left( \frac{\partial}{\partial \theta} \log p_\theta(x_i, z_i) \bigg|_{\theta=\theta_t} \right),$$

(21)

where $\eta_t$ is the learning rate, $E_{q_{s,\theta}(z_i|x_i)}$ there we use the full notation $q_{s,\theta}(z|x)$ instead of the abbreviated notation
$q_s(z)$ can be approximated by sampling from $q_{s,\theta}(z_i|x_i)$ using the noise initialized $K$-step gradient descent. Compared to MLE learning algorithm (8), we replace $p_{s,\theta}(z|x)$ by $q_{s,\theta}(z|x)$, and Monte Carlo samples from $q_{s,\theta}(z|x)$ can be obtained exactly.

Given $\theta_t$, the above iteration seeks to maximize

$$Q_s(\theta) = \frac{1}{n} \sum_{i=1}^{n} E_q s, \theta (z_i|x_i) \left[ \log p_{\theta}(x_i, z_i) \right],$$  \tag{22}

by a single gradient ascent step in $\theta$. In fact, in an approximate Monte Carlo EM algorithm, we may maximize $Q_s(\theta)$ with multiple gradient ascent steps. $Q_s(\theta)$ is an approximation to the complete-data log-likelihood in the EM algorithm [5, 37].

Compared to the log-likelihood function in MLE learning, $L(\theta) = \frac{1}{n} \sum_{i=1}^{n} \log p_{\theta}(x)$, we have

$$Q_s(\theta) = L(\theta) + \frac{1}{n} \sum_{i=1}^{n} E_q s, \theta (z_i|x_i) \left[ \log p_{\theta}(z_i|x_i) \right] - \frac{1}{n} \sum_{i=1}^{n} KL(q_{s,\theta}(z_i|x_i)\|p_{\theta}(z_i|x_i)) \tag{23}$$

$$= L(\theta) - \frac{1}{n} \sum_{i=1}^{n} KL(q_{s,\theta}(z_i|x_i)\|p_{\theta}(z_i|x_i)) \tag{24}$$

$$+ \frac{1}{n} \sum_{i=1}^{n} E_q s, \theta (z_i|x_i) \left[ \log q_{s,\theta}(z_i|x_i) \right]. \tag{25}$$

Since the last term has nothing to do with $\theta$, thus maximizing $Q_s(\theta)$ is equivalent to maximizing $L(\theta) - \frac{1}{n} \sum_{i=1}^{n} KL(q_{s,\theta}(z_i|x_i)\|p_{\theta}(z_i|x_i))$, which is a lower bound of $L(\theta)$.

Thus each learning iteration can be interpreted as a joint maximization of $Q_s(\theta)$ over $s$ and $\theta$. Specifically, step (1) maximizes $Q_s(\theta)$ over $s$ given $\theta = \theta_t$, and step (2) seeks to maximize $Q_s(\theta)$ over $\theta$ given $s$. This is similar to variational inference with $s$ being the variational parameter. The learning procedure is summarized in Algorithm 1.

### 4.6. Objective and estimating equation

The objective $-Q_s(\theta)$ is equivalent to

$$KL(p_{data}(x)q_{s,\theta}(z|x)\|p(z)p_{\theta}(z|x)), \tag{26}$$

up to constant independent of $\theta$ and $s$. At $\theta = \theta_t$, optimizing $s$ is to make the left hand side to be close to the right hand side. Fixing $s$, gradient descent on $\theta$ is to make the right hand side to get closer to the left-hand side. This may have the effect to push $p_{\theta}(z|x)$ to be close to $q_{s,\theta}(z|x)$, so that the short run inference is close to the posterior.

The learning algorithm (21) solves the following estimating equation:

$$\frac{1}{n} \sum_{i=1}^{n} E_{q_{s,\theta}(z|x_i)} \left[ \frac{\partial}{\partial \theta} \log p_{\theta}(x_i, z_i) \right] = 0. \tag{27}$$

### Algorithm 1: Learning with short run inference dynamics.

**input**: Learning iterations $T$, step size interval $T_s$, learning rate $\eta$, initial weights $\theta_0$, observed examples $\{x_i\}_{i=1}^{n}$, batch size $m$, number of steps $K$, initial step size $s$.

**output**: Weights $\theta_{T+1}$.

**for** $t = 0 : T$ **do**

1. Draw observed examples $\{x_i\}_{i=1}^{m}$.
2. Draw latent vectors $\{z_{i,0} \sim p(z)\}_{i=1}^{m}$.
3. Infer $\{z_{i,K}\}_{i=1}^{m}$ by $K$-steps of dynamics (11) with step size $s$.
4. Update $\theta$ according to (21).
5. Every $T_s$ iterations, update $s$ by minimizing (20).

The learning algorithm is a Robbins-Monro algorithm for stochastic approximation [36]. For fixed $s$, its convergence follows from regular conditions of Robbins-Monro. We expect that the optimized $s$ will also converge to a fixed value. Unlike the original maximum likelihood learning, $q_{s,\theta}(z|x)$ can be sampled exactly so that Robbins-Monro theory applies.

The bias of the learned $\theta$ based on the short run inference dynamics relative to the MLE depends on the gap between $q_{s,\theta}(z|x)$ and $p_{\theta}(z|x)$.

### 5. General theoretical formulation for short run inference and synthesis

To put our work in the big picture of generative modeling and computing, let us consider a latent EBM model $p_{\theta}(x, z)$, which includes generator model and its multi-layer version as well as regular EBM as special cases. The maximum likelihood learning is to minimize $KL(p_{data}(x)\|p_{\theta}(x))$, where $p_{\theta}(x) = \int p_{\theta}(x, z)dz$, and $p_{data}$ is the data distribution that generates the data $\{x_{i}, i = 1, ..., n\}$. Expectation with respect to $q_{data}$ can be approximated by the average over $\{x_{i}\}$.

The learning gradient is based on

$$- \frac{\partial}{\partial \theta} KL(p_{data}(x)\|p_{\theta}(x)) \tag{28}$$

$$= E_{p_{data}(x)} E_{p_{\theta}(z|x)} \left[ \frac{\partial}{\partial \theta} \log p_{\theta}(x, z) \right] \tag{29}$$

$$= E_{p_{data}(x)} E_{p_{\theta}(z|x)} \left[ \frac{\partial}{\partial \theta} f_{\theta}(x, z) \right] \tag{30}$$

$$- E_{p_{\theta}(x, z)} \left[ \frac{\partial}{\partial \theta} f_{\theta}(x, z) \right]. \tag{31}$$

$E_{p_{\theta}(z|x)}$ requires the inference sampling from $p_{\theta}(z|x)$ in the so-called positive or wake phase (or clamped sampling) in
the terminology of Boltzmann machine [4] and Helmholtz machine [4], while $E_{p_{th}(x,z)}$ requires the synthesis sampling from $p_{th}(x,z)$ in the so-called negative or sleep phase (or unclamped sampling) [17]. Both can be replaced by short run dynamics. Let $q_{a,b}(z|x)$ be the sort-run inference dynamics with tuning parameters $a$, and let $q_{b}(x,z)$ be the short run synthesis dynamics with tuning parameters $b$, then at learning iteration $t$ with $\theta_t$, the learning gradient for $\theta$ seeks to minimize the following generalized version of contrastive divergence:

$$C_{a,b}(\theta) = \text{KL}(p_{data}(x)q_{a,b}(z|x)||p_{\theta}(x,z)) - \text{KL}(q_{b}(x,z)||p_{\theta}(x,z)).$$

Compared to maximum likelihood,

$$C_{a,b}(\theta) = \text{KL}(p_{data}(x)||p_{\theta}(x)) + \Delta(\theta),$$

where

$$\Delta(\theta) = \text{KL}(q_{a,b}(z|x)||p_{\theta}(z|x)) - \text{KL}(q_{b}(x,z)||p_{\theta}(x,z)).$$

$C_{a,b}(\theta)$ is an approximation to $\text{KL}(p_{data}(x)||p_{\theta}(x))$. The learning gradient is

$$-\frac{\partial}{\partial \theta}C_{a,b}(\theta) = E_{p_{data}(x)}E_{p_{\theta}(x,z)}\left[\frac{\partial}{\partial \theta}f_{\theta}(x,z)\right] - E_{p_{\theta}(x,z)}\left[\frac{\partial}{\partial \theta}f_{\theta}(x,z)\right].$$

Compared to (38) with (31), we replace $p_{\theta}(z|x)$ by the short run inference $q_{a,b}(z|x)$, and we replace $p_{\theta}(x,z)$ by the short run synthesis $q_{b}(x,z)$. In fact, (31) can be derived based on (38).

As to $a$ and $b$, we seek to solve $\min_a \max_b C_{a,b}(\theta_t)$, which amounts to

$$\min_a \text{KL}(q_{a,b}(z|x)||p_{\theta}(z|x)), \quad \min_b \text{KL}(q_{b}(x,z)||p_{\theta}(x,z)).$$

Both are variational optimizations with respect to the tuning parameters in the short run inference and short run synthesis respectively. Overall, the learning iteration seeks to solve $\min_{\theta} \min_a \max_b C_{a,b}(\theta)$. Compared to the original contrastive divergence [16], we initialize the short run synthesis from a fixed noise distribution, instead of the observed examples.

For generator model or a purely top-down model, the second KL-divergence in the above generalized contrastive divergence disappears, since synthesis sampling can be accomplished by direct ancestral sampling. This is the case treated in this paper. For regular EBM, $z$ disappears, and with it the short run inference, so that we only have a short run synthesis $q_{b}(x)$, and the learning is based on $C_b(\theta) = \text{KL}(p_{data}(x)||p_{\theta}(x)) - \text{KL}(q_{b}(x)||p_{\theta}(x))$, and the learning seeks to solve $\min_{\theta} \max_b C_b(\theta)$. See the recent work [32] for short run synthesis for regular EBM. See also the recent work [13] for a divergence triangle formulation that is related to the above generalized contrastive divergence formulation.

6. Experiments

In this section, we will demonstrate (1) realistic synthesis, (2) faithful reconstructions of observed examples, (3) inpainting of occluded images, (4) variational grid search and gradient descent on the step size, and (5) ablation on the number of latent layers and Langevin steps. We emphasize the simplicity of the short run inference algorithm.

All the training image datasets are resized and scaled to $[-1, 1]$ with no further pre-processing. We train the models with $T = 3 \times 10^5$ parameter updates optimized by Adam [22]. The learning rate $\eta$ decays step-wise ($1 \times 10^{-4}$, $5 \times 10^{-5}$, $1 \times 10^{-5}$) for each $1 \times 10^5$ iterations. If not stated otherwise, we use $K = 20$ short run inference steps and $\sigma$ is gradually annealed from 2 to .05.

The baselines are trained with ladder variational autoencoder [39] to improve the performance of multi-layer latent variable models. We refer to the supplementary material for detailed model specifications.

6.1. Synthesis

We evaluate the learned generator $g_{\theta}(z)$ fidelity of generated examples quantitatively on various datasets, each reduced to 40,000 observed examples. Figure 3 depicts generated samples of size $32 \times 32$ pixels for various datasets with $K = 20$ short run inference steps. Figure 1 depicts generated samples of size $64 \times 64$ pixels on the CelebA dataset (see generated samples from a VAE with the same generator architecture in Figure 2). Table 1 (a) compares the Fréchet Inception Distance (FID) [15] with Inception v3 classifier [40] on 40,000 generated examples. Despite its simplicity, short run inference dynamics is competitive to elaborate means of inference in VAE models.

6.2. Reconstruction

We evaluate the accuracy of the learned inference dynamics $q_{a,b}(z|x_i)$ by reconstructing test images. In contrast to traditional MCMC posterior sampling with persistent chains, short run inference with small $K$ allows not only for efficient learning on training examples, but also the same dynamics can be recruited for testing examples.

Figure 4 compares the reconstructions of learned generators with $L = 5$ layers by VAE and short run inference on CelebA ($64 \times 64 \times 3$). The fidelity of reconstructions by short run inference appears qualitatively improved over
Table 1. Comparison of generators $g_\theta(z)$ with varied number of latent layers $L$ learned by VAE and short run inference with respect to MSE of reconstructions and FID of generated samples of size for MNIST (28 × 28), SVHN (32 × 32 × 3), and CelebA (32 × 32 × 3) datasets. (FID on MNIST is not considered meaningful or reflecting human judgment of synthesis quality and hence omitted.)

| Models | MNIST MSE | MNIST FID | SVHN MSE | SVHN FID | CelebA MSE | CelebA FID |
|--------|-----------|-----------|----------|----------|------------|------------|
| VAE, L=1 | 0.020 | - | 0.019 | 46.78 | 0.031 | 69.90 |
| VAE, L=3 | 0.018 | - | 0.015 | 41.72 | 0.029 | 58.33 |
| VAE, L=5 | 0.018 | - | 0.014 | 39.26 | 0.028 | 53.40 |
| Ours, L=1 | 0.019 | - | 0.018 | 44.86 | 0.019 | 45.80 |
| Ours, L=3 | 0.017 | - | 0.015 | 39.02 | 0.018 | 41.20 |
| Ours, L=5 | 0.015 | - | 0.011 | 35.23 | 0.011 | 37.29 |

6.3. Inpainting

Our method can “inpaint” occluded image regions. To recover the occluded pixels, the only required modification of (11) involves the computation of $\|x - g_\theta(z)\|^2/\sigma^2$. For a fully observed image, the term is computed by the summation over all pixels. For partially observed images, we only compute the summation over the observed pixels. Figure 5 depicts test images taken from the CelebA dataset (64 × 64 × 3) for which a mask randomly occludes pixels in various patterns.

6.4. Variational optimization of step size

The step size $s$ in (11) may be optimized such that $q_s(z)$ best approximates the true posterior $p_\theta(z|x)$. That is, we can optimize the step size $s$ by minimizing $\text{KL}(q_s(z)||p_\theta(z|x))$ via a grid search or gradient descent. As outlined in Section 4.4, we require $dF(z_0)/dz_0$. In reverse-mode auto-differentiation, we construct the Jacobian one row at a time by evaluating vector-Jacobian products. Then, we evaluate the eigenvalues of $dF(z_0)/dz_0$. As both steps are computed in a differentiable manner, we may compute the gradient with respect to step size $s$.

Figure 6 depicts the optimal step size $s$ over learning iterations $t$ determined by grid-search with $s \in \{0.01, 0.02, \ldots, 0.15\}$ and gradient descent on (20). For both grid-search and gradient descent the step size settles near 0.05 after a few learning iterations. Figure 7 details the optimization objective of $s$, $E_{q_s(z)}[\log q_s(z) - \log p_\theta(x, z)]$, with respect to individual step sizes $s$.

6.5. Influence of number of layers and steps

Finally, Tables 2 and 3 show the influence of the number of latent layers $L$ for the generator network $g_\theta(z)$ and the number of steps $K$ in the short run inference dynamics (11), respectively. Increasing the number of layers $L$ im-
proves the quality of synthesis and reconstruction. Increasing the number of inference steps $K$ up to 20 steps results in significant improvements, while $K > 20$ appears to affect the scores only marginally.

![Figure 3](image1.png)  
Figure 3. Generated samples for $K = 20$ short run inference steps with $L = 5$ layers. From left to right: (1) MNIST ($28 \times 28$), (2) SVHN ($32 \times 32 \times 3$), (3) CelebA ($32 \times 32 \times 3$).

![Figure 4](image2.png)  
Figure 4. Comparison of reconstructions between VAE samples and our method on CelebA ($64 \times 64 \times 3$) with $L = 5$. Top: original test images. Middle: reconstructions from VAE. Bottom: reconstructions by short run inference.

![Figure 5](image3.png)  
Figure 5. Inpainting on CelebA ($64 \times 64 \times 3$) with $L = 5$ for varying occlusion masks. Top: original test images. Middle: occluded images. Bottom: inpainted test images by short run inference.

![Figure 6](image4.png)  
Figure 6. Variational optimal step size $s$ over epochs $T$ for three individual runs with varying random seed. Top: Grid-search. Bottom: Gradient-descent.

| $L$ | FID | MSE |
|-----|-----|-----|
| 1   | 61.03 | 0.020 |
| 3   | 52.19 | 0.018 |
| 5   | 47.95 | 0.015 |

Table 2. Influence of number of layers $L$ with $K = 20$ for CelebA ($64 \times 64 \times 3$).
| $K$ | 5   | 10  | 20  | 40  |
|-----|-----|-----|-----|-----|
| FID | 83.03 | 67.58 | 37.29 | 35.41 |
| MSE | 0.045 | 0.037 | 0.011 | 0.010 |

Table 3. Influence of number of short run inference steps $K$ on models with $L = 5$ for CelebA ($32 \times 32 \times 3$).

### 7. Conclusion

This paper proposes to use short run inference dynamics to infer latent variables in deep generative models. The inference dynamics is always initialized from the prior noise distribution, followed by a small number (e.g., 20) of updates. It can be viewed as a residual network or an RNN. Similar to the variational inference, the tuning parameters such as step size of the short run inference dynamics are optimized by a variational criterion. Unlike the variational inference, there is no need to design an extra inference model, which is usually a challenging task with multiple layers of latent variables. In fact, the short run dynamics is guided by the log-posterior distribution to regulate the explaining-away competitions and top-down feedbacks between the latent variables. The short run inference dynamics is easily affordable on the current computing platforms and can be easily scaled up to big training data. It will enable the researchers to design more sophisticated latent variable models without worrying about designing inference models.

The following are the directions that we shall explore in our future work.

1. In this paper, we focus on gradient descent update, and we optimize the step size. We shall explore more general updates and other tuning parameters. A simple extension is to consider varying step sizes, i.e., difference step sizes at different iterations of the short run dynamics. Another extension is gradient descent with momentum, where the tuning parameters can be optimized. We may also consider second order optimization algorithm.

2. In this paper, we focus on continuous latent variables or latent vectors. Continuous vector representations are commonly used in deep learning models. Discrete variables can be obtained from continuous variables. In our future work, we shall also explore short run inference for discrete latent variables explicitly.

3. In this paper, we focus on top-down generative models. Our method can be applied to graphical models in general, including the latent energy-based models. We shall also study these models using short run inference as well as short run synthesis in our future work.

### Acknowledgments

The work is supported by DARPA XAI project N66001-17-2-4029; ARO project W911NF1810296; and ONR MURI project N00014-16-1-2007; and XSEDE grant ASC170063. We thank NVIDIA for hardware donations. We thank Eric Fischer for assistance with experiments.

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8. Appendix

8.1. Model Specification

For the multi-layer generator model, we have $z = (z_l, l = 1, \ldots, L)$ for which layer $L$ is the top layer, and layer 1 is the bottom layer close to $x$. For simplicity, let $x = z_0$. Then, $p_0(z) = p_L(z_L) \prod_{l=0}^{L-1} p_l(z_l | z_{l+1})$. In our case, we have $z_L \sim \mathcal{N}(0, I)$, $[z_l | z_{l+1}] \sim \mathcal{N}(\mu_l(p_l(z_{l+1}))), \sigma_l^2(p_l(z_{l+1})))$, $l = 0, \ldots, L - 1$. where $\mu_l(\cdot)$ and $\sigma_l^2(\cdot)$ are the mean vector and the diagonal variance-covariance matrix of $z_l$ respectively, and they are functions of $d_l(p_l(z_{l+1}))$ where $d_l$ are deterministic layers and $p_l$ are projection layer to preserve dimensionality. $d_l$ is defined as two subsequent $conv2d$ layers with $GeLU$ activation functions and skip connection. $p_l$ is a linear layer with subsequent $transpose_{conv2d}$. $\mu_l$ and $\sigma_l$ are a pair of $conv2d$ and linear layers to project to dimensionality of $z_l$. Then, $z_l = \mu_l(d_l(p_l(z_{l+1}))) + \sigma_l(d_l(p_l(z_{l+1}))) \otimes \epsilon_l$ where $\epsilon_l \sim \mathcal{N}(0, I_{d_l})$. The final deterministic block $o_0$ is a $transpose_{conv2d}$ layer projecting to the desired dimensionality of $x$. The range of $x$ is bounded by $\tanh(\cdot)$.

Table 4 illustrates a specification with $L = 3$ layers, latent dimensions $d_3 = 32$, $d_2 = 64$, $d_1 = 128$ for $z_3$, $z_2$, $z_1$, respectively, and $n_f = 64$ channels.

| $l$ | operation | dimensions |
|-----|-----------|------------|
| $3$ | $z_3 \sim \mathcal{N}(0, I_{d_3})$ | $[n, d_3, 1, 1]$ |
| $2$ | $z_{3,p} = p_2(z_3)$ | $[n, n_f, 16, 16]$ |
| $2$ | $z_{3,d} = d_2(z_{3,p})$ | $[n, n_f, 16, 16]$ |
| $2$ | $z_2 = \mu_2(z_{3,d}) + \sigma_2(z_{3,d}) \otimes \epsilon_2$ | $[n, d_2, 1, 1]$ |
| $1$ | $z_{2,p} = p_1(z_2)$ | $[n, n_f, 16, 16]$ |
| $1$ | $z_{2,d} = d_1(z_{2,p}) + z_{3,d}$ | $[n, n_f, 16, 16]$ |
| $1$ | $z_1 = \mu_1(z_{2,d}) + \sigma_1(z_{2,d}) \otimes \epsilon_1$ | $[n, d_1, 1, 1]$ |
| $0$ | $z_{1,p} = p_0(z_1)$ | $[n, n_f, 16, 16]$ |
| $0$ | $z_{1,d} = d_0(z_{1,p}) + z_{2,d}$ | $[n, n_f, 16, 16]$ |
| $0$ | $x = \tanh(o_0(z_{1,d}))$ | $[n, 3, 32, 32]$ |

Table 4. Specification of multi-layer generator model with $L = 3$ layers, latent dimensions $d_3 = 32$, $d_2 = 64$, $d_1 = 128$ for $z_3$, $z_2$, $z_1$, respectively, and $n_f = 64$ channels.