Iterative Refinement of Approximate Posteriors for Training Directed Belief Networks

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Abstract

Deep directed graphical models, while a potentially powerful class of generative representations, are challenging to train due to difficult inference. Recent advances in variational inference that make use of an inference or recognition network have advanced well beyond traditional variational inference and Markov chain Monte Carlo methods. While these techniques offer higher flexibility as well as simpler and faster inference, they are still limited by approximate posterior inference and require variance reduction techniques. Less focus has been given to improving or refining the approximate posterior beyond what is provided by variational inference. We show that iterative refinement of an approximate posterior can provide notable gains in maximizing the lower bound of the log likelihood, either by using adaptive importance sampling or by applying gradient descent as inference during the E-step of a variational expectation-maximization algorithm. We show our approach achieves state of the art for training directed belief networks with binary latent variables, and provides a unique means of refining the posterior for directed belief networks with Gaussian latent variables.

1 Introduction

Deep generative models offer the capacity for rich representations of complex data as they can capture multimodal properties of the distribution of interest and generalize better than models based purely on deterministic processes. Deep directed graphical models in particular have some advantage over their undirected cousins such as deep Boltzmann machines (DBMs, Salakhutdinov & Hinton, 2009) as they do not suffer from learning and evaluation difficulties arising from an intractable partition function. Despite their representational power, directed graphical models are often difficult to train, as the true posterior is generally intractable.

Methods for training variants of the Helmholtz machine (Dayan et al., 1995), such as wake-sleep (Hinton et al., 1995, Bornschein & Bengio, 2014) and neural variational inference and learning (NVIL, Mnih & Gregor, 2014), and methods for training the variational autoencoder (VAE, Kingma & Welling, 2013) variant have supplanted more traditional Markov chain Monte Carlo (MCMC) (Neal, 1993) and variational inference based methods such as mean-field coordinate ascent inference (Saul et al., 1996) in training deep generative models. The gains offered by these methods are due to
parameterizing the approximate posterior with a recognition network in addition to clever learning algorithms. As opposed to traditional methods, this general approach provides a fast and effective means of performing inference and learning which scales well to large datasets.

While advances have been clear, these methods are still limited by the choice of approximate posterior, which translates to a looseness in the lower bound. Some recent work has begun to address this limitation by either relaxing the factorial assumption [Burda et al., 2015] on the approximate posterior or through the introduction of auxiliary inference networks [Rezende & Mohamed, 2015].

There has been recent focus on refining the variational posterior by applying gradient descent to variational inference [Honkela et al., 2010; Hoffman et al., 2013] or by applying additional MCMC transitions [Salimans et al., 2015]. We demonstrate two different, yet fundamentally related methods to refine the approximate posterior from the recognition network during the E-step of an expectation-maximization (EM, Dempster et al., 1977; Neal & Hinton, 1998) algorithm to improve the variational lower bound. We show that adaptive importance sampling (AdIS, Oh & Berger, 1992) can be used to give an asymptotically unbiased estimate of the lower bound, and demonstrate this approach with binary latent variables where no good unbiased solutions exist. We also show that, given lower bound can be reinterpreted as a deterministic function with auxiliary noise, we can use stochastic gradient descent to refine the approximate posterior.

2 Directed Belief Networks and Variational Inference

In this work, we use directed belief network to refer to a generative directed graphical model consisting of a conditional density \( p(x|h) \) and a prior \( p(h) \), such that the joint density can be expressed as \( p(x, h) = p(x|h)p(h) \). In particular, the conditional density factorizes into a hierarchy of conditional densities: \( p(x|h) = p(x|h_1) \prod_{l=1}^{L-1} p(h_l|h_{l+1}) \), where each layer \( i \) is conditionally independent on the layer above with density \( p(h_l|h_{l+1}) \) and \( p(h_L) \) is a prior distribution of the top layer. This latent variable structure is meant to improve model capacity, but inference can still be intractable. This is especially the case in deep directed networks, such as deep sigmoid belief networks (SBN, Neal, 1992), deep belief networks (DBN, Hinton et al., 2006), and other models in which each of the conditional distributions involves complex nonlinear functions.

Directed belief networks can be trained by maximizing likelihood estimation (MLE), but this is difficult due to the necessary marginalization over the latent density. If we had the posterior \( p(h|x) = p(x, h)/p(x) \), then learning would be straightforward, but in general this is not possible and requires more advanced techniques. One solution is to use MCMC sampling to iteratively approximate the posterior distribution over the latent variables, which can be exact given an unbound number of steps under certain conditions. However, this approach is not practical in large-scale applications due to slow mixing and high computational costs.

2.1 Variational Lowerbound of Directed Belief Network

Another popular method, variational inference, introduces an approximate posterior \( q(h|x; \theta) \) with variational parameters \( \theta \), such that:

\[
\log p(x) = \log \sum_h p(x, h) = \log \sum_h q(h|x) \frac{p(x, h)}{q(h|x)} \\
\geq \sum_h q(h|x) \log \frac{p(x, h)}{q(h|x)} = \sum_h q(h|x) \log p(x, h) + H(q) = \mathcal{L},
\]

where \( H(q) \) is the entropy of the approximate posterior. This introduces lower bound, \( \mathcal{L} \), of the exact likelihood.

Variational inference rephrases inference as choosing the variational parameters \( \theta \) to maximize this bound, rather than choosing the latent variables directly. The bound is tight (e.g., \( \mathcal{L} = \log p(x) \)) when the KL divergence between the approximate and true posterior is 0 (e.g., \( D_{KL}(q(h|x; \theta)||p(h|x)) = 0 \)); or equivalently when the approximate matches the true posterior. Optimization then is dependent on the choice of a parametric form for the posterior that can best approximate the exact posterior, and models generally vary in choice of parameterization followed by a learning algorithm which efficiently maximizes its lower bound.
2.2 Training a Directed Belief Network

Given a means for inferring an approximate posterior, \( q(h|x; \theta) \), learning is done by an expectation-maximization (EM, Dempster et al., 1977; Neal & Hinton, 1998). In the expectation (E) step, the variational parameters of the approximate posterior, \( \theta \), are chosen/updated such that the KL-divergence between the approximate posterior and true posterior is minimized. In the maximization (M) step, the model parameters \( \phi \) are chosen/updated to maximize the likelihood function.

In general, the gradient of the lower bound w.r.t. the model parameters can be estimated using the following Monte Carlo approximation:

\[
\nabla_{\phi} L \approx \frac{1}{N} \sum_{n} \nabla_{\phi} \log p(x, h^{(n)}; \phi),
\]

where \( h^{(n)} \sim q(h|x) \).

Most of the difficulty in training directed networks lies in inferring the approximate posterior. It is often convenient to assume that the posterior distribution factorizes, that is \( q(h|x) = \prod_i q(h_i|x) \), an approach known as mean-field inference. However, mean-field variational inference for directed networks is non-trivial, as the exact mean-field equations often do not have a closed form. Coordinate ascent mean field inference is expensive, though in limited settings the natural gradient can be used (Honkela et al., 2010; Hoffman et al., 2013). For sigmoid belief networks, introducing additional variational parameters can help (Saul et al., 1996), but this has had very limited success.

2.3 Recognition Network

Recently, it has been found that approximate posterior inference can be done quickly by using a feed forward, often deep, recognition network composed of global variational parameters, \( \psi \), the output of which are local variational parameters for the approximate posterior \( q(h|x; \theta) \) (see, e.g., Salakhutdinov & Larochelle, 2010; Kingma & Welling, 2013; Mnih & Gregor, 2014; Rezende et al., 2014), trading time and complexity for overall model size:

\[
\theta(x) = f(x; \psi).
\]

It is very common to assume the output parameters, \( \theta \), parameterize a factorized approximate posterior, such that the recognition network output is an estimate of the mean-field parameters. Generally known as a “Helmholtz machine” (Dayan et al., 1995) in the context of variational inference of directed belief networks, a “sufficiently flexible” recognition network is necessary to better approximate the true posterior, the limits of which are not well understood. In addition, these approaches often require additional tricks to train, as the gradients of the lower bound from the expected reconstruction loss, \( E_{q(z|x)} \log p(x, h) \), do not back-propagate naturally through the latent variables, and most of the off-the-shelf approximations, such as Monte Carlo gradient estimator, have high variance (Mnih & Gregor, 2014).

A special case of a Helmholtz machine known as a variational autoencoder (VAE, Kingma & Welling, 2013) solves this problem by making use of a clever parameterization trick so that the stochastic variables \( h \sim q(h|x; \theta) \) can be rephrased as a deterministic function of \( \theta \) with some auxiliary noise:

\[
\bar{h}(\theta) = \mu + \epsilon \odot \sigma
\]

\[
\epsilon \sim \mathcal{N}(0, 1),
\]

where \((\mu, \sigma) = \theta\) are the mean and variance parameters for the posterior density and our auxiliary noise variables, \( \epsilon \), are sampled from a unit-variance, zero-mean normal distribution. While this type of parameterization works well certain families of distributions, re-parameterizations of this sort are not available with discrete latent variables. Instead, inference with discrete variables relies on creative methodology. For instance, the wake-sleep algorithm uses samples from the joint density \( p(z, h) \) to optimize the variational parameters, effectively making the algorithm an optimization over two cost functions (Hinton et al., 1995). Neural variational inference and learning (NVIL) uses REINFORCE (Williams, 1992) along with a baseline predicted from a deep neural network to make lower variance MCMC estimates of the gradient.
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Figure 1: Iterative refinement for variational inference. An initial mean-field estimate of the approximate posterior is made through a recognition network. The mean-field parameters are then updated iteratively, maximizing the lower bound. The final approximate posterior is used to train the generative model by sampling. The recognition network parameters are trained using the KL divergence between the refined posterior \( q_k \) and the output of the recognition network \( q_0 \).

3 ITERATIVE REFINEMENT FOR VARIATIONAL INFERENCE (IRVI)

3.1 ITERATIVE REFINEMENT OF THE APPROXIMATE POSTERIOR

With deep Boltzmann machines, mean-field inference is instrumental to estimating the log-likelihood, and an inference network can be used to initialize the local variational parameters to speed up inference (DBMs, Salakhutdinov & Larochelle [2010]). For directed nets, given a transition whose stationary state is the true posterior, we can use mean-field inference, initializing inference on the output of the recognition network.

For the remainder of this paper, we will distinguish the generative parameters \( \phi \) from the variation parameters of the recognition network, \( \psi \), and the local parameters of the approximate posterior, \( \theta \).

We assume the generative model is composed of a factorized prior \( p(h) = \prod_i p(h_i) \) along with the hierarchal conditional likelihood.

The basic principle behind iterative refinement for variational inference (IRVI) is the use of an efficient transition operator to iteratively refine the approximate posterior, either through:

1. a stochastic transition operator \( g(\theta, x, \epsilon) \) for which the true posterior is a stationary state,

or

2. a deterministic function \( G(\theta, x, \epsilon) \) with transition operator, \( g(\theta, x, \epsilon) = \theta + \gamma \nabla_{\theta} G(\theta, x, \epsilon) \), such that \( \arg \min_{\theta} \mathbb{E}_{p(\epsilon)} [G(\theta, x, \epsilon)] \approx \arg \min_{\theta} \mathcal{L}(\theta, x) \) and \( \gamma \) is a scalar hyperparameter, where \( \epsilon \) is some auxiliary noise variables not dependent on the parameters \( \theta \).

An overview of IRVI is available in Figure 1. For the E-step, we apply \( K \) steps of the transformation, \( \theta_{k+1} = g(\theta_k, x) \), iterating through \( K \) parameterizations of the approximate posterior \( q_0(h|x), q_1(h|x), \ldots, q_K(h|x) \) to update the mean-field equations for the lower bound. With the final set of parameters, \( \theta_K \), the gradients with respect to \( \phi \) and \( \psi \) in the M-step become:

\[
\nabla_{\phi} \mathcal{L} = \mathbb{E}_{q_K(h|x)} [\nabla_{\phi} \log p(x, h; \phi)] \\
\nabla_{\psi} \mathcal{L} = -\nabla_{\psi} D_{KL}(q_K(h|x)||q_0(h|x; \psi)),
\]

(5)

where the KL divergence term can be solved either by MCMC or analytically, depending on the model.
The general IRVI algorithm then follows Algorithm 1. While the iterative refinement may reduce the variance in our stochastic gradient estimates and speed up the optimization, it comes at a computational cost, as each update is $K$ times more expensive than fixed approximations. However, in addition to potential learning benefits, IRVI can also be applied to improve approximate posterior to an already trained Helmholtz machine (VAE or otherwise) at test only.

**Algorithm 1 IRVI**

**Require:** An already trained Helmholtz machine (VAE or otherwise) at test only.

**Require:** Number of iterations $K$

**Require:** Gradient $\nabla_{\theta } q_0(\theta _h, \epsilon )$ and inference rate $\gamma$

Calculate initial local variational parameters $\theta _0 = f(x; \psi)$ for $q_0(z|x)$

For $k = 1:K$

- $(E$-step for training or test) $\theta _k = g(\theta _{k-1}, x)$

- $(M$-step for training only) $\Delta \phi \propto \mathbb{E}_{q_K(h|x)}[\nabla \phi \log p(x, h; \phi)]$

- $\Delta \psi \propto -\nabla \psi D_{KL}(q_K(h|x)||q_0(h|x; \psi))$

3.1.1 Adaptive Importance Sampling Iterative Refinement (AIR)

Adaptive importance sampling (AdIS, Oh & Berger [1992]) provides a general approach to iteratively refining the local variational parameters. Adaptive importance sampling "recalibrates" the proposed distribution using a weighted average of samples, $h^{(n)} \sim q(h|x)$, weighted by the importance weights:

$$w(n) = p(x, h^{(n)}) / q(h^{(n)}|x)$$

$$\tilde{w}(n) = w(n) / \sum_n w(n).$$

The true posterior is a stationary state, as the unnormalized importance weights become $p(x, h^{(n)}) / q(h^{(n)}|x) = p(x)$, making the weights uniform across samples.

For binary stochastic variables with the Bernoulli centers $\mu = \theta$ at each inference step, $k$:

$$h^{(n)} \sim \text{Bernoulli}(\mu_k)$$

$$\mu_{k+1} = g(\mu_k, x) = (1 - \gamma)\mu_k + \gamma \sum_n \tilde{w}(n)h^{(n)},$$

where $\gamma$ is the inference rate and $(1 - \gamma)$ can be thought of as the adaptive "damping" rate. This is an asymptotically unbiased estimate of the lower bound that works very well in practice with a finite number of samples. The approach outlined above should work with any discrete parametric distribution, and we use Bernoulli variables as an exemplar here. Although AIR should be applicable with continuous Gaussian variables, which have both mean and covariance, we were able to make reasonable gains using gradient-descent iterative refinement below (GDIR), leaving applying AIR to continuous latent variables for future work.

3.1.2 Gradient Descent Iterative Refinement (GDIR)

If we can rephrase the lower bound as a deterministic differentiable function $G(\theta, x, \epsilon)$ of the local variational parameters and some optional auxiliary noise variables, $\epsilon$, then we are guaranteed to improve the approximate posterior by applying iterative steps of gradient ascent. The success of this approach will depend on the choice of approximation, which we will show.

Gaussian Latent Variables Rather than use the re-parameterization to pass gradients to the global variational parameters, $\psi$, as in VAE, we can apply the gradients iteratively at the local parameters, $\theta$, improving the initial estimate provided by $q_0(h|x; \psi)$.
The iterative transition follows the stochastic gradient of the lower bound w.r.t. $\theta$, which can be approximated easily by Monte Carlo method:

$$g(\theta, x, \epsilon) = \theta + \gamma \frac{1}{N} \sum_n \nabla \theta \left( \log p(x, h^{(n)}) - \log q_K(h^{(n)}|x) \right),$$  \hspace{1cm} (8)

where $\gamma$ is the inference rate. To more efficiently refine the posterior, we can use any of the more sophisticated families of gradient-based learning available, such as momentum, RMS prop [Hinton, 2012], or Adam [Kingma & Ba, 2014]. In the limit of $K = 0$, we do not arrive at VAE, as the gradients are never passed through the approximate posterior during learning.

**Bernoulli Latent Variables** Unfortunately, a suitable re-parameterization as above is not available to us with binary latent variables. In order to use gradient descent to back-propagate the gradients of the lower bound, we need to make a stronger approximation.

There has been some recent work into passing gradients through binary latent variables [Bengio et al., 2013; Raiko et al., 2014]. Instead of approximating the partial derivatives w.r.t. the latent variables in back-propagation, we instead push the centers of the Bernoulli distribution (mu-push), avoiding sampling overall. Our lower bound becomes:

$$g(\mu, x) = \mu + \gamma \nabla \mu \left( \log p(x|\mu) - D_{KL}(q_K(h|x)||p(h)) \right),$$  \hspace{1cm} (9)

where $\log p(x|\mu)$ is the log-output of the generation network using the variational parameters $\mu = \text{sigmoid}(z)$ as input. However, this approximation is likely highly biased, and expect this approximation to be best when the entropy, $\mathcal{H}(q_K)$, is small. In general, mu-push outperformed other approximate gradient methods, such as straight-through, but was greatly out-performed by AIR.

4 **Related Work**

Iterative refinement for variational inference (IRVI) is a hybrid method, combining concepts from variational inference and MCMC. In spirit, it is closest to the refinement procedure of hybrid MCMC for variational inference (HVI, Salimans et al., 2015) and normalizing flows for VAE (NF, Rezende & Mohamed, 2015). HVI uses Hamiltonian MCMC to extend the posterior along a directed graph corresponding to a periodic solution to a Hamiltonian with the use of auxiliary momentum variables. HVI is the same complexity as IRVI, as it requires passing the gradients of the reconstruction error at every step. NF extends the posterior with invertible transformations with a Jacobian that is reasonably easy to compute. Despite the extra complexity involved with computation of the Jacobian and inverse, NF is typically cheaper than both IRVI and HVI. While IRVI refines the posterior by adjusting the mean-field parameters, HVI and NF depart from the mean-field approximation in whole by adjusting the form of the approximate posterior, are fundamentally deeper latent models, and thus should provide superior solutions to IRVI when applied to mean-field. However, they come with two limitations compared to IRVI. First, they rely on the VAE re-parameterization to work, and thus cannot be applied to discrete variables. Second, their refinement cannot be applied to already-trained models to improve the posterior.

GDIR also shares similarities with stochastic variational inference (SVI, Hoffman et al., 2013), which also uses gradient descent to improve on the variational inference algorithm. SVI, however, requires global latent variables with carefully chosen relationships with the local latent variables (our equivalent of $h$) to do inference.

Neural variational inference and learning (NVIL, Mnih & Gregor, 2014) and re-weighted wake-sleep (RWS, Bornschein & Bengio, 2014), like adaptive importance sampling iterative refinement (AIR), offer arguably the best solution for inference and learning in directed belief networks with discrete variables, though NVIL is biased, and RWS (like AIR) is asymptotically so. While NVIL generally works, the variance is still not low enough to be practical, and convergence takes much longer in terms of epochs and wall clock time than AIR, despite lower complexity. RWS is very successful at training SBNs, but its complex objective function means that convergence properties cannot be proven.
AIR also shares similarities with RWS in the use of importance sampling, as with importance-weighted autoencoders (IWAE, Burda et al., 2015) and recent work on stochastic feed-forward networks (SFFN, Tang & Salakhutdinov, 2013; Raiko et al., 2014). Iterative refinement, however, takes a distinctly orthogonal approach, as it uses importance sampling instead to achieve a better posterior through refinement. While the end result may be a reduction of variance during training, none of these methods can refine the posterior further at test.

Finally, IRVI is not entirely orthogonal to many of the inference and learning methods above, and could be combined to enhance results, particularly with variational inference methods that follow an EM training procedure.

5 Experiments

5.1 Settings

We test the two versions of iterative refinement for variational inference (IRVI): adaptive importance sampling iterative refinement (AIR) and gradient descent iterative refinement (GDIR), on the MNIST handwritten digit dataset, using the benchmark binarized dataset found in Salakhutdinov & Murray (2008), with a standard train, validation, and test split of 50k, 10k, and 10k samples. We centered the entire MNIST dataset by subtracting the mean digit over the corresponding dataset (train, valid, and test) for inference only. Unfortunately, recent papers on variational autoencoders (VAE) (Mnih & Gregor, 2014) have used different, non-standard splits, or actively sample from continuous MNIST (Burda et al., 2015), making it difficult to compare performance or compete. We, however, make sure that our results are from the most conservative setting (having the least amount of training examples and binarizing only once), thereby making any comparison as meaningful as possible.

All models used a recognition network for comparison to similar models, with the number of parameters and deterministic layers (if present) matching the generation network. Models were trained using the RMSprop algorithm (Hinton, 2012), with a batch size of 100, with early stopping by recording best validation lowerbound. All models were tested using 1000 posterior samples to estimate the lower bounds and log-likelihoods.

5.2 Discrete Variables

For the discrete case, we use Bernoulli variables, which have been widely used in previous related work. We used two different model parameterizations in order compare to results from wake-sleep, re-weighted wake-sleep (RWS), and neural variational inference and learning (NVIL) on 1-layer and 2-layer sigmoid belief networks (SBNs) against both GDIR (mu-push) and AIR. For comparison to wake-sleep and RWS, we used a shallow feed-forward network with 200 output neurons, $z$, for the local variational parameters as $\theta = \mu = \text{sigmoid}(z)$, with no additional deterministic units for neither the recognition nor generation nets. As NVIL uses an additional feed forward network for baseline prediction, we trained an additional model with an intermediate deterministic layer with 240 softplus units in both the recognition and generation networks to roughly match the total number of parameters to NVIL. Models were trained using 20 samples during inference and 20 posterior samples to estimate the lower bound during the M-step.

To demonstrate IRVI with multiple layers, we used an SBN with a generation network with a structure of 200-200 binary latent layers and a recognition network with a matched parameterization. However, for our approximate posterior we used a completely deterministic network, treating the outputs of each layer as the factors of the complete approximate posterior, that is $q(h1, h2|x) = q(h1|x)q(h2|x)$, where $q(h2|x)$ shares the lower-level parameters with those of $q(h1|x)$, allowing us to adapt the Bernoulli means of $h1$ and $h2$ simultaneously.

Single-layer AIR and GDIR models were trained with 1, 5, 10, 20, and 50 inference steps, while the 2-layer SBN was trained only with 50 inference steps. Single-layer SBNs (with and without intermediate deterministic layer) were trained for 500 epochs with a learning rate of $1 \times 10^{-4}$, while the 2-layer SBN was trained with a learning rate of $2 \times 10^{-4}$. For AIR, an adaptive damping rate of 0.9 was used, as lower damping rates proved unstable, though these models often gave competitive results. During test, more inference samples were needed to ensure stable inference, and more steps
Model & $\leq -\log p(x)$ & $\approx -\log p(x)$ \\
Wake-sleep & 120.7 & 116.3 \\
WS (200-200) & 109.4 & 106.9 \\
RWS & & 103.1 \\
RWS (200-200) & & 93.4 \\
NVIL & 113.1 & 99.8 \\
NVIL (200-200) & & \\
AIR$_{50}$ & & \\
$AIR_{20}$ (240 det sp) & 97.16 & 93.31 \\
AIR$_{50}$ (200-200) & 96.62 & 92.26 \\
$GDIR_{20}$ & 129.94 & 113.6 \\
$GDIR_{20}$ (240 det sp) & 118.28 & 104.22 \\

Table 1: Results for GDIR and AIR for a single-layer SBN with and without an intermediate softplus layer of 240 units and a 2-layer SBN compared to similar models trained on the same MNIST dataset. All models have 100 latent variables.

200 steps were used during inference for the single-layer SBN and 1000 steps were used for the 2-layer SBN. However, while these step numbers proved sufficient for our analysis (Figure 2), neither model converged completely at test, so we are confident we are underestimating the log-likelihood.

Table 2: Results for models without intermediate deterministic layer trained with AIR with $n$ inference steps. Each model above was evaluated using 200 steps and 1000 samples during inference.

The comparative results are compiled in Table 1. While mu-push GDIR does not perform nearly as well, AIR greatly outperforms NVIL with a single-layer SBN, whether parameter-matched or not, and also outperforms NVIL in 2-layer SBN. In addition, AIR outperforms RWS in log-likelihood estimates with a single-layer SBN, and slightly outperforms with 2 layers, despite the extremely simple deterministic recognition network. As with continuous variables, we observe that higher number of inference steps during training (Table 2) and during test (Figure 2) improves and tightens the lower bound.

5.3 Continuous Variables

For continuous latent variables, we used the same network structure as in [Kingma & Welling, 2013; Salimans et al., 2015], with 200 latent variables and a generation and recognition network with 500 intermediate deterministic softplus ($\log(1 + \exp(x))$) units. We excluded the mean and variance of the prior distribution from learning, keeping the prior at zero-mean, unit-variance. Each of our models were trained using an inference rate of $3 \times 10^{-3}$, 20 or 50 samples during inference using GDIR to refine output of the recognition network, and 20 or 50 samples to approximate the lower bound during the M-step; with all hyper-parameters chosen from validation runs. We used momentum for each GDIR step, with a coefficient of 0.9. In order to demonstrate the effect of inference steps on learning, we varied the number of inference steps from 1, 5, 10, 20, and 50.

All models were trained for 1000 epochs with an initial learning rate of $1 \times 10^{-4}$, followed by 100 epochs at a learning rate of $1 \times 10^{-5}$, and finished with 100 epochs of $1 \times 10^{-6}$. We also used $L2$ weight decay with a decay coefficient of $2 \times 10^{-4}$. During test, all models were evaluated using 100 inference steps and 300 inference samples during the E-step when refining the approximate posterior.
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| Model                  | ≤-log p(x) | ≈-log p(x) |
|------------------------|------------|------------|
| VAE                    | 94.48      | 89.31      |
| VAE (w/ refinement)    | 90.57      | 88.53      |
| GDIR$_{50,20}$         | 90.60      | 88.54      |
| VAE†                   | 94.18      | 88.95      |
| HV/1†                  | 91.70      | 88.08      |
| HV/8†                  | 88.30      | 85.51      |
| VAE§                   | 89.9       |            |
| DLGM + NFI$_{10}$§     | 87.5       |            |
| DLGM + NFI$_{80}$§     | 85.1       |            |
| VAE‡                   | 86.35      |            |
| IWAE (K = 50)$‡$       |            | 84.78      |

Table 3: Lower bounds and NLL for various continuous latent variable models and training algorithms along with the corresponding VAE estimates. We use 200 latent Gaussian variables. *Approximate value from Kingma & Welling (2013) with 200 latent variables. †Using 200 latent variables with an inference network for the initial posterior and an addition network for the reverse dynamics. §With multiple maxout layers and 40 latent variables. ‡Sampling from continuous MNIST at each update with 2 deterministic layers with 200 units and 50 latent units.

| n  | 1      | 5      | 10     | 20     | 50     |
|----|--------|--------|--------|--------|--------|
| ≤-log p(x) | 95.15 | 92.74  | 92.33  | 90.75  | 91.31  |
| ≈-log p(x) | 94.34 | 90.74  | 89.98  | 88.65  | 88.71  |

Table 4: Results for models trained with n GDIR inference steps. Each model above was evaluated using 100 steps and 300 samples during inference. We report the lower bounds and estimated marginal probabilities on the test set.

Our test results with continuous latent variables (GDIR) are presented in Table 3 with the number of posterior samples, $K$, and inference steps, $n$, specified as GDIR$_{K,n}$, with $K = 50$ and $n = 20$ chosen from validation. For comparison are deep latent gaussian models with normalizing flow (DLGM+NF, Rezende & Mohamed, 2015) with the number of flow layers specified, hybrid MCMC for variational inference (HVI) with the number of leapfrog steps specified, and importance-weighted autoencoders (IWAE). Included in Table 4 is the effect of inference steps during training on the lower bound and log likelihood. Included for each model is their results for VAE, the baseline.

GDIR shows improvement over VAE, and equally to VAE when the posterior of VAE is refined using GDIR at test. While showing comparable performance to HVI with 1 leapfrog step, GDIR falls short of HVI with 8 leap from steps, DLGM+NF, and IWAE, though differences in model and training specification make a direct comparison difficult. Worth noting is while our unrefined VAE results are similar to those reported with the HVI results, thus are the most comparable, the VAE results for DLGM+NF and IWAE are much lower, possibly due to better optimization. Overall, GDIR provides an alternative to VAE during training (though at a higher complexity), but also provides a means of refining VAE otherwise unavailable. We also believe that the gains offered by HVI, NF, and IWAE reflect the non-factorial posteriors, which will not be realized in mean-field GDIR.

We observe that the number of inference steps during training improves lower bound and log-likelihood estimates, though there is a slight increase of the lower bound at 50 inference steps. In addition, the bound becomes tighter and the log-likelihood estimate improves as the number of inference steps increases, both during training (Table 4) and during evaluation (Figure 3).
6 Conclusion

We have introduced iterative refinement for variational inference (IRVI), an unsophisticated, yet powerful and flexible approach for improving variational inference. We introduced through two variants: adaptive importance sampling iterative refinement (AIR), which uses importance sampling at each iterative step, and gradient descent iterative refinement (GDIR), which uses gradient descent to refine the posterior. With AIR, we achieve state-of-the-art results with a single- or two-layer sigmoid belief networks (SBN), notably against reweighted wake-sleep (RWS) and neural variational inference and learning (NVIL). With GDIR, we show that IRVI can be used to train a directed belief network with gaussian latent variables that at least matches variational autoencoders (VAE), though GDIR is outperformed by methods which move away from a factorized approximate posterior. Finally, IRVI can be used to refine an already-trained VAE posterior at test, providing a tighter lower bound and better log-likelihood estimates.

We can also achieve better results than RWS with a less-sophisticated recognition network, indicating that we can initiate inference with IRVI with a less complex recognition network than existing methods and achieve similar or better performance. While we applied IRVI with simple approximate posteriors parameterized by deterministic feed-forward networks, this is not a limitation of the method. Iterative refinement should be applicable to numerous formulations of variational inference, making it a potentially valuable means of general improvement.

As the results show definite improvement over NVIL, this indicates that IRVI may be used as an alternative to REINFORCE in reinforcement learning tasks, such as applications of Q-learning (Watkins & Dayan [1992] Mnih et al. [2013]). Finally, many real-world applications in latent factor analysis, such as intrinsic networks from fMRI (Hjelm et al. [2014]), require additional regularization to improve “interpretability” of results. By modifying the cost function at inference, IRVI indicates a principled way to regularize or have control of the the final form of latent variables.

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