Neural Variational Inference and Learning in Belief Networks

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Abstract

Highly expressive directed latent variable models, such as sigmoid belief networks, are difficult to train on large datasets because exact inference in them is intractable and none of the approximate inference methods that have been applied to them scale well. We propose a fast non-iterative approximate inference method that uses a feedforward network to implement efficient exact sampling from the variational posterior. The model and this inference network are trained jointly by maximizing a variational lower bound on the log-likelihood. Although the naive estimator of the inference network gradient is too high-variance to be useful, we make it practical by applying several straightforward model-independent variance reduction techniques. Applying our approach to training sigmoid belief networks and deep autoregressive networks, we show that it outperforms the wake-sleep algorithm on MNIST and achieves state-of-the-art results on the Reuters RCV1 document dataset.

1. Introduction

Compared to powerful globally-normalized latent variable models, such as deep belief networks (Hinton et al., 2006) and deep Boltzmann machines (Salakhutdinov & Hinton, 2009a), which can now be trained on fairly large datasets, their purely directed counterparts have been left behind due to the lack of efficient learning algorithms. This is unfortunate, because their modularity and ability to generate observations efficiently make them better suited for integration into larger systems.

Training highly expressive directed latent variable models on large datasets is a challenging problem due to the difficulties posed by inference. Although the generality

of Markov Chain Monte Carlo (MCMC) methods makes them straightforward to apply to models of this type (Neal, 1992), they tend to suffer from slow mixing and are usually too computationally expensive to be practical in all but the simplest models. Such methods are also difficult to scale to large datasets because they need to store the current state of the latent variables for all the training observations between parameter updates.

Variational methods (Jordan et al., 1999) provide an optimization-based alternative to the sampling-based Monte Carlo methods, and tend to be more efficient. They involve approximating the exact posterior using a distribution from a more tractable family, often a fully factored one, by maximizing a variational lower bound on the log-likelihood w.r.t. the parameters of the distribution. For a small class of models, using such variational posteriors allows the expectations that specify the parameter updates to be computed analytically. However, for highly expressive models such as the ones we are interested in, these expectations are intractable even with the simplest variational posteriors. This difficulty is usually dealt with by lower bounding the intractable expectations with tractable one by introducing more variational parameters, as was done for sigmoid belief nets by Saul et al. (1996). However, this technique increases the gap between the bound being optimized and the log-likelihood, potentially resulting in a poorer fit to the data. In general, variational methods tend to be more model-dependent than sampling-based methods, often requiring non-trivial model-specific derivations.

We propose a new approach to training directed graphical models that combines the advantages of the sampling-based and variational methods. Its central idea is using a feedforward network to implement efficient exact sampling from the variational posterior for the given observation. We train this inference network jointly with the model by maximizing the variational lower bound on the log-likelihood, estimating all the required gradients using samples from the inference network. Although naive estimate of the gradient for the inference network parameters is unusable due to its high variance, we make the approach practical by applying several straightforward and general variance reduc-

tion techniques. The resulting training procedure for the inference network can be seen as an instance of the RE-INFORCE algorithm (Williams, 1992). Due to our use of stochastic feedforward networks for performing inference we call our approach Neural Variational Inference and Learning (NVIL).

Compared to MCMC methods, where many iterations over the latent variables are required to generate a sample from the exact posterior and successive samples tend to be highly correlated, NVIL does not suffer from mixing issues as each forward pass through the inference network generates an independent exact sample from the variational posterior. In addition to being much faster than MCMC, our approach has the additional advantage of not needing to store the latent variables for each observation and thus is not only more memory efficient but also applicable to the pure online learning setting, where each training case is seen once before being discarded.

In contrast to other work on scaling up variational inference, NVIL can handle both discrete and continuous latent variables (unlike Kingma & Welling (2013); Rezende et al. (2014)) as well variational posteriors with complex dependency structures (unlike Ranganath et al. (2013)). Moreover, the variance reduction methods we employ are simple and model-independent, unlike the more sophisticated model-specific control variates of Paisley et al. (2012).

Though the idea of training an inference model by following the gradient of the variational bound has been considered before, it was dismissed as infeasible (Dayan & Hinton, 1996). Our primary contribution is to show how to reduce the variance of the naive gradient estimator to make it practical without narrowing its range of applicability. We also show that the resulting method trains sigmoid belief networks better than the wake-sleep algorithm (Hinton et al., 1995), which is the only algorithm we are aware of that is capable of training the same range of models efficiently. Finally, we demonstrate the effectiveness and scalability of NVIL by using it to achieve state-of-the-art results on the Reuters RCV1 document dataset.

2. Neural variational inference and learning

2.1. Variational objective

Suppose we are interested in training a latent variable model $P_\theta(x, h)$ with parameters θ. We assume that exact inference in the model is intractable and thus maximum likelihood learning is not an option. For simplicity, we will also assume that all the latent variables in the model are discrete, though essentially the same approach applies if some or all of the variables are continuous.

We will train the model by maximizing a variational lower bound on the marginal log-likelihood. Following the standard variational inference approach (Jordan et al., 1999), given an observation x, we introduce a distribution $Q_\phi(h|x)$ with parameters ϕ, which will serve as an approximation to its exact posterior $P_\theta(h|x)$. The variational posterior Q will have a simpler form than the exact posterior and thus will be easier to work with.

The contribution of x to the log-likelihood can then be lower-bounded as follows (Jordan et al., 1999):

$$\log P_\theta(x) = \log \sum_h P_\theta(x, h)$$
$$\geq \sum_h Q_\phi(h|x) \log \frac{P_\theta(x, h)}{Q_\phi(h|x)}$$
$$= E_Q[\log P_\theta(x, h) - \log Q_\phi(h|x)] \quad (1)$$
$$= \mathcal{L}(x, \theta, \phi).$$

By rewriting the bound as

$$\mathcal{L}(x, \theta, \phi) = \log P_\theta(x) - KL(Q_\phi(h|x), P_\theta(h|x)), \quad (2)$$

we see that its tightness is determined by the Kullback-Leibler (KL) divergence between the variational distribution and the exact posterior. Maximizing the bound with respect to the parameters ϕ of the variational distribution makes the distribution a better approximation to the posterior (w.r.t. the KL-divergence) and tightens the bound.

In contrast to most applications of variational inference where the variational posterior for each observation is defined using its own set of variational parameters, our approach does not use any local variational parameters. Instead, we use a flexible feedforward model to compute the variational distribution from the observation. We call the model mapping x to $Q_\phi(h|x)$ the *inference network*. The architecture of the inference network is constrained only by the requirement that $Q_\phi(h|x)$ it defines has to be efficient to evaluate and sample from. Using samples from the inference network we will be able to compute gradient estimates for the model and inference network parameters for a large class of highly expressive architectures, without having to deal with architecture-specific approximations.

Given a training set $\mathcal{D}$, consisting of observations $x_1, ..., x_D$, we train the model by (locally) maximizing $\mathcal{L}(\mathcal{D}, \theta, \phi) = \sum_i \mathcal{L}(x_i, \theta, \phi)$ using gradient ascent w.r.t. to the model and inference network parameters. To ensure scalability to large datasets, we will perform stochastic optimization by estimating gradients on small minibatches of randomly sampled training cases.

2.2. Parameter gradients

The gradient of the variational bound for a single observation x w.r.t. to the model parameters is straightforward to

derive and has the form

$$\nabla_\theta \mathcal{L}(x) = E_Q \left[\nabla_\theta \log P_\theta(x, h) \right], \quad (3)$$

where we left θ and ϕ off the list of the arguments of $\mathcal{L}$ to simplify the notation. The corresponding gradient w.r.t. to the inference network parameters is somewhat more involved:

$$\nabla_\phi \mathcal{L}(x) = E_Q[(\log P_\theta(x, h) - \log Q_\phi(h|x)) \\ \times \nabla_\phi \log Q_\phi(h|x)], \quad (4)$$

We give its derivation in the supplementary material.

As both gradients involve expectations which are intractable in all but a handful of special cases, we will estimate them with Monte Carlo integration, using samples from the inference network. Having generated n samples $h^{(1)}, ..., h^{(n)}$ from $Q_\phi(h|x)$, we compute

$$\nabla_\theta \mathcal{L}(x) \approx \frac{1}{n} \sum_{i=1}^{n} \nabla_\theta \log P_\theta(x, h^{(i)}) \quad (5)$$

and

$$\nabla_\phi \mathcal{L}(x) \approx \frac{1}{n} \sum_{i=1}^{n} (\log P_\theta(x, h^{(i)}) - \log Q_\phi(h^{(i)}|x)) \\ \times \nabla_\phi \log Q_\phi(h^{(i)}|x). \quad (6)$$

The above gradient estimators are unbiased and thus can be used to perform stochastic maximization of the variational objective using a suitable learning rate annealing schedule. The speed of convergence of this procedure, however, depends heavily on the variance of the estimators used, as we will see in Section 4.2.

The model gradient estimator (5) is well-behaved and does not pose a problem. The variance of the inference network gradient estimator (6), however, can be very high due to the scaling of the gradient inside the expectation by a potentially large term. As a result, learning variational parameters with updates based on this estimator can be unacceptably slow. In fact, it is widely believed that learning variational parameters using gradient estimators of the form (6) is infeasible (Hinton & Zemel, 1994; Dayan & Hinton, 1996; Kingma & Welling, 2013). In the next section we will show how to make this approach practical by applying variance reduction techniques.

2.3. Variance reduction techniques

Though gradient estimates computed using Eq. 6 are usually too noisy to be useful in practice, it is easy to reduce their variance to a manageable level with the following model-independent techniques.

2.3.1. CENTERING THE LEARNING SIGNAL

Inspecting Eq. 4, we see that we are using

$$l_\phi(x, h) = \log P_\theta(x, h) - \log Q_\phi(h|x) \quad (7)$$

as the learning signal for the inference network parameters, and thus are effectively fitting $\log Q_\phi(h|x)$ to $\log P_\theta(x, h)$. This might seem surprising, given that we want the inference network $Q_\phi(h|x)$ to approximate the posterior distribution $P_\theta(x|h)$, as opposed to the joint distribution $P_\theta(x, h)$. It turns out however that using the joint instead of the posterior distribution in Eq. 4 does not affect the value of the expectation. To see that we start by noting that

$$E_Q[\nabla_\phi \log Q_\phi(h|x)] = E_Q \left[\frac{\nabla_\phi Q_\phi(h|x)}{Q_\phi(h|x)} \right] \\ = \nabla_\phi E_Q[1] = 0. \quad (8)$$

Therefore we can subtract any c that does not depend on h from the learning signal in Eq. 4 without affecting the value of the expectation:

$$E_Q[(l_\phi(x, h) - c)\nabla_\phi \log Q_\phi(h|x)] \\ = E_Q[l_\phi(x, h)\nabla_\phi \log Q_\phi(h|x)] - cE_Q[\nabla_\phi \log Q_\phi(h|x)] \\ = E_Q[l_\phi(x, h)\nabla_\phi \log Q_\phi(h|x)]. \quad (9)$$

And as $\log P_\theta(x, h) = \log P_\theta(h|x) + \log P_\theta(x)$ and $\log P_\theta(x)$ does not depend on h, using $P_\theta(h|x)$ in Eq. 4 in place of $P_\theta(x, h)$ does not affect the value of the expectation.

This equivalence allows us to compute the learning signal efficiently, without having to evaluate the intractable $P_\theta(h|x)$ term. The price we pay for this tractability is the much higher variance of the estimates computed using Eq. 6. Fortunately, Eq. 9 suggests that we can reduce the variance by subtracting a carefully chosen c from the learning signal. The simplest option is to make c a parameter and adapt it as learning progresses. However, c will not be able capture the systematic differences in the learning signal for different observations x, which arise in part due to the presence of the $\log P_\theta(x)$ term. Thus we can reduce the gradient variance further by subtracting an observation-dependent term $C_\psi(x)$ to minimize those differences. Doing this does not affect the expected value of the gradient estimator because $C_\psi(x)$ does not depend on the latent variables. Borrowing a name from the reinforcement learning literature we will refer to c and $C_\psi(x)$ as *baselines*. We will elaborate on this connection in Section 3.4.

We implement the input-dependent baseline $C_\psi(x)$ using a neural network and train it to minimize the expected square of the centered learning signal $E_Q[(l_\phi(x, h) - C_\psi(x) - c)^2]$. Though this approach to fitting the baseline does not result in the maximal variance reduction, it is simpler and in

our experience works as well as the optimal approach of Weaver & Tao (2001) which requires taking into account the magnitude of the gradient of the inference network parameters. We also experimented with per-parameter baselines but found that they did not improve on the global ones. Finally, we note that incorporating baselines into the learning signal can be seen as using simple control variates. In contrast to the more elaborate control variates (e.g. of Paisley et al. (2012)), baselines do not depend on the form of the model or of the variational distribution and thus are easier to use.

2.3.2. VARIANCE NORMALIZATION

Even after centering, using $l_\phi(x, h)$ as the learning signal is non-trivial as its average magnitude can change dramatically, and not necessarily monotonically, as training progresses. This variability makes training an inference network using a fixed learning rate difficult. We address this issue by dividing the centered learning signal by a running estimate of its standard deviation. This normalization ensures that the signal is approximately unit variance, and can be seen as a simple and efficient way of adapting the learning rate. To ensure that we stop learning when the magnitude of the signal approaches zero, we apply variance normalization only when the estimate of the standard deviation is greater than 1. The algorithm for computing NVIL parameter updates using the variance reduction techniques described so far is provided in the supplementary material.

2.3.3. LOCAL LEARNING SIGNALS

So far we made no assumptions about the structure of the model or the inference network. However, by taking advantage of their conditional independence properties we can train the inference network using simpler and less noisy local learning signals instead of the monolithic global learning signal $l_\phi(x, h)$. Our approach to deriving a local signal for a set of parameters involves removing all the terms from the global signal that do not affect the value of the resulting gradient estimator.

We will derive the layer-specific learning signals for the common case of both the model and the inference network having n layers of latent variables. The model and the variational posterior distributions then naturally factor as

$$P_\theta(x, h) = P_\theta(x|h^1) \prod_{i=1}^{n-1} P_\theta(h^i|h^{i+1}) P_\theta(h^n), \quad (10)$$

$$Q_\phi(h|x) = Q_{\phi^1}(h^1|x) \prod_{i=1}^{n-1} Q_{\phi^{i+1}}(h^{i+1}|h^i), \quad (11)$$

where h^i denotes the latent variables in the ith layer and ϕ^i the parameters of the variational distribution for that layer. We will also use $h^{i:j}$ to denote the latent variables in layers i through j.

To learn the parameters of the the variational distribution for layer i, we need to compute the following gradient:

$$\nabla_{\phi_i} \mathcal{L}(x) = E_{Q(h|x)}[l_\phi(x, h) \nabla_{\phi_i} \log Q_{\phi_i}(h^i|h^{i-1})].$$

Using the law of iterated expectation we can rewrite the expectation w.r.t. $Q(h|x)$ as

$$\nabla_{\phi_i} \mathcal{L}(x) = E_{Q(h^{1:i-1}|x)}[$$
$$E_{Q(h^{i:n}|h^{i-1})}[l_\phi(x, h) \nabla_{\phi_i} \log Q_{\phi_i}(h^i|h^{i-1})]|h^{i-1}]],$$

where we also used the fact that under the variational posterior, $h^{i:n}$ is independent of $h^{1:i-2}$ and x, given h^{i-1}. As a consequence of Eq. 9, when computing the expectation w.r.t. $Q(h^{i:n}|h^{i-1})$, all the terms in the learning signal that do not depend on $h^{i:n}$ can be safely dropped without affecting the result. This gives us the following local learning signal for layer i:

$$l_\phi^i(x, h) = \log P_\theta(h^{i-1:n}) - \log Q_\phi(h^{i:n}|h^{i-1}). \quad (12)$$

To get the signal for the first hidden layer we simply use x in place of h^0, in which case we simply recover the global learning signal. For hidden layers $i > 1$, however, the local signal involves fewer terms than $l_\phi(x, h)$ and thus can be expected to be less noisy. As we do not assume any within-layer structure, Eq. 12 applies to models and inference networks whether or not $Q_\phi(h^i|h^{i-1})$ and $P_\theta(h^i|h^{i+1})$ are factorial.

Since local signals can be significantly different from each other, we use separate baselines and variance estimates for each signal. For layers $i > 1$, the input-dependent baseline $C_\psi(x)$ is replaced by $C_{\psi_i}^i(h^{i-1})$.

In some cases, further simplification of the learning signal is possible, yielding a different signal per latent variable. We leave exploring this as future work.

3. Related work

3.1. Feedforward approximations to inference

The idea of training an approximate inference network by optimizing a variational lower bound is not new. It goes back at least to Hinton & Zemel (1994), who derived the variational objective from the Minimum Description Length (MDL) perspective and used it to train linear autoencoders. Their probabilistic encoder and decoder correspond to our inference network and model respectively. However, they computed the gradients analytically, which was possible due to the simplicity of their model, and dismissed the sampling-based approach as infeasible due to noise.

Salakhutdinov & Larochelle (2010) proposed using a feedforward "recognition" model to perform efficient input-dependent initialization for the mean field inference algorithm in deep Boltzmann machines. As the recognition

model is trained to match the marginal probabilities produced by mean field inference, it inherits the limitations of the inference procedure, such as the inability to model structured posteriors. In contrast, in NVIL the inference net is trained to match the true posterior directly, without involving an approximate inference algorithm, and thus the accuracy of the fit is limited only by the expressiveness of the inference network itself.

Recently a method for training nonlinear models with continuous latent variables, called Stochastic Gradient Variational Bayes (SGVB), has been proposed by Kingma & Welling (2013) and Rezende et al. (2014). Like NVIL, it involves using feedforward models to perform approximate inference and trains them by optimizing a sampling-based estimate of the variational bound on the log-likelihood. However, SGVB is considerably less general than NVIL, because it uses a gradient estimator obtained by taking advantage of special properties of real-valued random variables and thus is not applicable to models with discrete random variables. Moreover, unlike NVIL, SGVB method cannot handle inference networks with nonlinear dependencies between latent variables. The ideas of the two methods are complementary however, and NVIL is likely to benefit from the SGVB-style treatment of continuous-valued variables, while SGVB might converge faster using the variance reduction techniques we proposed.

Gregor et al. (2013) have recently proposed a related algorithm for training sigmoid belief network like models based on the MDL framework. They also use a feedforward model to perform approximate inference, but concentrate on the case of a deterministic inference network and can handle only binary latent variables. The inference network is trained by backpropagating through binary thresholding units, ignoring the thresholding nonlinearities, to approximately minimize the coding cost of the joint latent-visible configurations. This approach can be seen as approximately maximizing a looser variational lower bound than (2) due to the absence of the entropy term.

An inference network for efficient generation of samples from the approximate posterior can also be seen as a probabilistic generalization of the approximate feedforward inference methods developed for sparse coding models in the last few years (Kavukcuoglu et al., 2008; Bradley & Bagnell, 2008; Gregor & LeCun, 2010).

3.2. Sampling-based variational inference

Like NVIL, Black Box Variational Inference (BBVI, Ranganath et al., 2013) learns the variational parameters of the posterior by optimizing the variational bound using sampling-based gradient estimates, which makes it applicable to a large range of models. However, unlike NVIL, BBVI follows the traditional approach of learning a sepa-

rate set of variational parameters for each observation and does not use an inference network. Moreover, BBVI uses a fully-factorized mean field approximation to the posterior, which limits its power.

3.3. The wake-sleep algorithm

NVIL shares many similarities with the wake-sleep algorithm (Hinton et al., 1995), which enjoys the same scalability and applicability to a wide range of models. This algorithm was introduced for training Helmholtz machines (Dayan et al., 1995), which are multi-layer belief networks augmented with recognition networks. These recognition networks are used for approximate inference and are directly analogous to NVIL inference networks. Wake-sleep alternates between updating the model parameters in the wake phase and the recognition network parameters in the sleep phase. The model parameter update is based on the samples generated from the recognition network on the training data and is identical to the NVIL one (Eq. 5). However, in contrast to NVIL, the recognition network parameters are learned from samples generated by the model. In other words, the recognition network is trained to recover the hidden causes corresponding to the samples from the model distribution by following the gradient

$$\nabla_\phi \mathcal{L}(x) = E_{P_\theta(x,h)} \left[\nabla_\phi \log Q_\phi(h|x) \right]. \quad (13)$$

Unfortunately, this update does not optimize the same objective as the model parameter update, which means that the wake-sleep algorithm does not optimize a well-defined objective function and is not guaranteed to converge. This is the algorithm's main weakness, compared to NVIL, which optimizes a variational lower bound on the log-likelihood.

The wake-sleep gradient for recognition network parameters does have the advantage of being much easier to estimate than the corresponding gradient of the variational bound. In fact, the idea of training the recognition networks using the gradient of the bound was mentioned in (Hinton & Zemel, 1994) and (Dayan & Hinton, 1996) but not seriously considered due concerns about the high variance of the estimates. In Section 4.2 we show that while the naive estimator of the gradient given in Eq. 6 does exhibit high variance, the variance reduction techniques from Section 2.3 improve it dramatically and make it practical.

3.4. REINFORCE

Using the gradient (4) to train the inference network can be seen as an instance of the REINFORCE algorithm (Williams, 1992) from reinforcement learning (RL), which adapts the parameters of a stochastic model to maximize the external reward signal which depends on the model's output. Given a model $P_\theta(x)$ and a reward signal $r(x)$,

REINFORCE updates the model parameters using the rule

$$\Delta\theta \propto E_P[(r(x) - b)\nabla_\theta \log P_\theta(x)]. \qquad (14)$$

We can view NVIL as an application of REINFORCE on the per-training-case basis, with the inference network corresponding to the stochastic model, latent state h to the output, and the learning signal $l_\phi(x, h)$ to the reward. The term b in Eq. 14, called a *baseline* in the RL literature, is a hyperparameter that can be adapted to reduce the variance of the parameter update. Thus it serves the same function as c and $C_\psi(x)$ that we subtract from the learning signal to center it in Section 2.3.1. The considerable body of work on baselines and other variance reduction methods done in the RL community (e.g. Greensmith et al., 2004) is likely to contain additional techniques relevant for training inference networks.

4. Experimental results

We performed two sets of experiments, with the first set intended to evaluate the effectiveness of our variance reduction techniques and to compare NVIL's performance to that of the wake-sleep algorithm. In the second set of experiments, we demonstrate NVIL's ability to handle larger real-world datasets by using it to train generative models of documents.

4.1. Experimental protocol

We trained all models using stochastic gradient ascent using minibatches of 20 observations sampled randomly from the training data. The gradient estimates were computed using a single sample from the inference network. For each dataset, we created a validation set by removing a random subset of 100 observations from the training set. The only form of regularization we used was early stopping based on the validation bound, implemented by keeping track of the parameter configuration with the best validation score seen so far. We implemented each input-dependent baseline using a neural network with a single hidden layer of 100 tanh units.

We used fixed learning rates because we found them to produce superior results to the annealing schedules we experimented with. The learning rates we report were selected based on the validation set performance in preliminary experiments with smaller models. We always make the learning rate for inference network five times smaller than for the model (which is the one we report), as we found this to improve performance. We used inference networks with layered structure given by Eq. 11, without dependencies within each layer except in the experiment with autoregressive inference networks. All multi-layer inference networks were trained using layer-specific learning signals from Section 2.3.3.

As the models we train are intractable, we cannot compute the exact log-likelihoods for them. Instead we report the estimates of the variational bound (2) computed using 10 samples from the inference network, which we found to be sufficient to get the accurate bound estimates. We expect this approach to underestimate the log-likelihood considerably, but leave finding more direct and thus less pessimistic evaluation methods as future work.

4.2. Modelling images of digits

Our first set of experiments was performed on the binarized version of the MNIST dataset, which has become the standard benchmark for evaluating generative models of binary data. The dataset consists of $70,000$ 28×28 binary images of handwritten digits, partitioned into a 60,000-image training set and 10,000-image test set. We used the binarization of Salakhutdinov & Murray (2008), which makes our scores directly comparable to those in the literature.

We used 3×10^{-4} as the learning rate for training models with NVIL on this dataset. Centering the input vectors by subtracting the mean vector was essential for making the inference networks and input-dependent baselines work well.

To demonstrate the importance of variance reduction techniques, we trained two SBNs using a range of variance control settings. The first SBN had a single layer of 200 latent variables, while the second one had two layers of 200 variables each. Figure 1 shows the estimate of the variational objective on the validation set plotted against the number of parameter updates. For both models, it is clear that using all three techniques – the input-dependent and input-independent baselines along with variance normalization – is essential for best performance. However, of the three techniques, the input-dependent baseline appears to be the least important. Comparing the plots for the two models suggests that variance reduction becomes more important for larger models, with the gap between the best combination and the others (excluding the very worst one) widening. For both models, learning with all three variance reduction techniques disabled makes barely any progress and is clearly infeasible.

We found that disabling layer-specific learning signals had little effect on the performance of the resulting model. The difference was about 0.4 nats for an SBN with two or three layers of latent variables.

We next compared NVIL to the wake-sleep algorithm, which is its closest competitor in terms of scalability and breadth of applicability, by training a range of models using both algorithms. Wake-sleep training used a learning rate of 1×10^{-4}, as we found this algorithm to be more sensitive to the choice of the learning rate than NVIL, per-
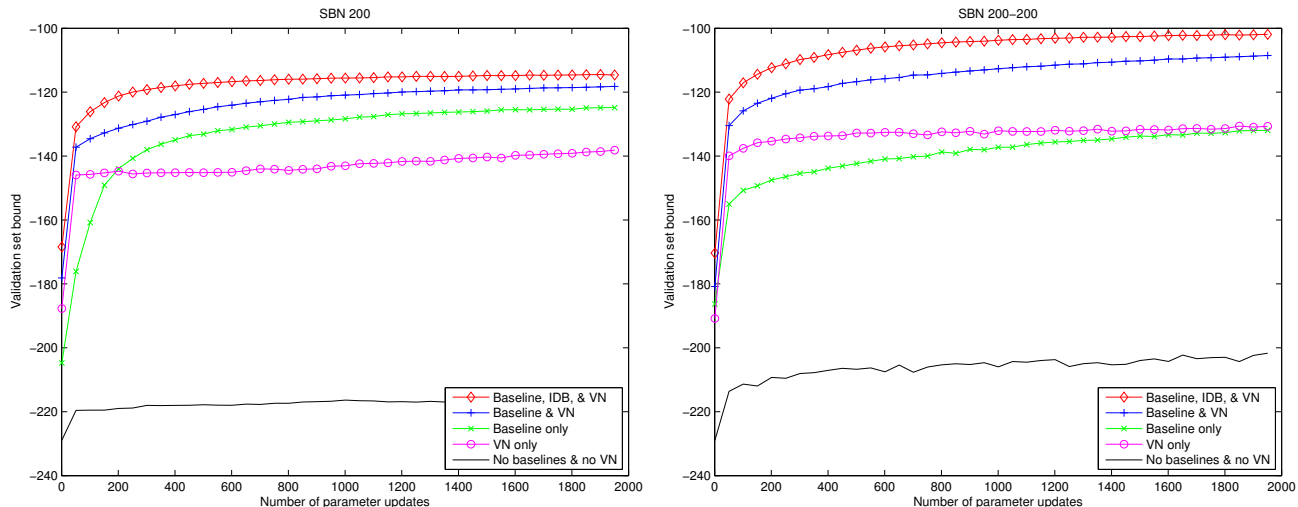
Figure 1. Bounds on the validation set log-likelihood for an SBN with (Left) one and (Right) two layers of 200 latent variables. Baseline and IDB refer to the input-independent and the input-dependent baselines respectively. VN is variance normalization.

Table 1. Results on the binarized MNIST dataset. "Dim" is the number of latent variables in each layer, starting with the deepest one. NVIL and WS refer to the models trained with NVIL and wake-sleep respectively. NLL is the negative log-likelihood for the tractable models and an estimate of it for the intractable ones.

MODEL	DIM	TEST NLL	
		NVIL	WS
SBN	200	113.1	120.8
SBN	500	112.8	121.4
SBN	200-200	99.8	107.7
SBN	200-200-200	96.7	102.2
SBN	200-200-500	97.0	102.3
FDARN	200	92.5	95.9
FDARN	500	90.7	97.2
FDARN	400	96.3	
DARN	400	93.0	
NADE	500	88.9	
RBM (CD3)	500	105.5	
RBM (CD25)	500	86.3	
MOB	500	137.6	

forming considerably better with lower learning rates. The results, along with some baselines from the literature, are shown in Table 1. We report only the means of the bound estimates as their standard deviations were all very small, none exceeding 0.1 nat. We can see that models trained with NVIL have considerably better bounds on the log-likelihood, compared to their wake-sleep counterparts, with the difference ranging from 3.4 to 8.6 nats. Additional layers make SBNs perform better, independently of the training method. Interestingly, single-layer fDARN (Gregor et al., 2013) models, which have autoregressive connections between the latent variables, perform better than any of the SBN models trained using the same algorithm. Comparing to results from the literature, we see that all the SBN

and fDARN models we trained perform much better than a mixture of 500 factorial Bernoulli distributions (MoB) but not as well as the deterministic Neural Autoregressive Distribution Estimator (NADE) (Larochelle & Murray, 2011). The NVIL-trained fDARN models with 200 and 500 latent variables also outperform the fDARN (as well as the more expressive DARN) model with 400 latent variables from (Gregor et al., 2013), which were trained using an MDL-based algorithm. The fDARN and multi-layer SBN models trained using NVIL also outperform a 500-hidden-unit RBM trained with 3-step contrastive divergence (CD), but not the one trained with 25-step CD (Salakhutdinov & Murray, 2008). However, both sampling and CD-25 training in an RBM is considerably more expensive than sampling or NVIL training for any of our models.

The sampling-based approach to computing gradients allows NVIL to handle variational posteriors with complex dependencies. To demonstrate this ability, we retrained several of the SBN models using inference networks with autoregressive connections within each layer. These networks can capture the dependencies between variables within layers and thus are considerably more expressive than the ones with factorial layers. Results in Table 2 indicate that using inference networks with autoregressive connections produces better models, with the single-layer models exhibiting large gains.

4.3. Document modelling

We also applied NVIL to the more practical task of document modelling. The goal is to train a generative model of documents which are represented as vectors of word counts, also known as bags of words. We trained two sim-

Table 2. The effect of using autoregressive connections in the inference network. "Dim" is the number of latent variables in each layer, starting with the deepest one. "Test NLL" is an estimate of the lower bound on the log-likelihood on the MNIST test set. "Autoreg" and "Factorial" refer to using inference networks with and without autoregressive connections respectively.

MODEL	DIM	TEST NLL	
		AUTOREG	FACTORIAL
SBN	200	103.8	113.1
SBN	500	104.4	112.8
SBN	200-200-200	94.5	96.7
SBN	200-200-500	96.0	97.0

Table 3. Document modelling results. "Dim" is the number of latent variables in the model. The third and the fourth columns report the estimated test set perplexity on the 20 Newsgroups and Reuters RCV1 datasets respectively.

MODEL	DIM	20 NEWS	REUTERS
SBN	50	909	784
FDARN	50	917	724
FDARN	200		598
LDA	50	1091	1437
LDA	200	1058	1142
REPSOFTMAX	50	953	988
DOCNADE	50	896	742

ple models on the 20 Newsgroups and Reuters Corpus Volume I (RCV1-v2) datasets, which have been used to evaluate similar models in (Salakhutdinov & Hinton, 2009b; Larochelle & Lauly, 2012). 20 Newsgroups is a fairly small dataset of Usenet newsgroup posts, consisting of about 11K training and 7.5K test documents. RCV1 is a much larger dataset of Reuters newswire articles, with about 794.4K training and 10K test documents. We use the standard preprocessed versions of the datasets from Salakhutdinov & Hinton (2009b), which have vocabularies of 2K and 10K words respectively.

We experimented with two simple document models, based on the SBN and DARN architectures. Both models had a single layer of latent variables and a multinomial visible layer and can be seen as directed counterparts of the Replicated Softmax model (Salakhutdinov & Hinton, 2009b). We used the same training procedure as on MNIST with the exception of the learning rates which were 3×10^{-5} on 20 Newsgroups and 10^{-3} on RCV1.

The established evaluation metric for such models is the perplexity per word, computed as $\exp\left(-\frac{1}{N}\sum_n \frac{1}{L_n}\log P(x_n)\right)$, where N is the number of documents, L_n is the length of document n, and $P(x_n)$ the probability of the document under the model. As we cannot compute $\log P(x_n)$, we use the variational lower bound in its place and thus report an upper bound on perplexity.

The results for our models, along with ones for the Replicated Softmax and DocNADE models from (Salakhutdinov & Hinton, 2009b) and (Larochelle & Lauly, 2012) respectively, are shown in Table 3. We can see that the SBN and fDARN models with 50 latent variables perform well, producing better scores than LDA and Replicated Softmax on both datasets. Their performance is also competitive with that of DocNADE on 20 Newsgroups. The score of 724 for fDARN with 50 latent variables on RCV1 is already better than DocNADE's 742, the best published result on that dataset. fDARN with 200 hidden units, however, performs

even better, setting a new record with 598.

5. Discussion and future work

We developed, NVIL, a new training method for intractable directed latent variable models which is general and easy to apply to new models. We showed that NVIL consistently outperforms the wake-sleep algorithm at training sigmoid-belief-network-like models. Finally, we demonstrated the potential of our approach by achieving state-of-the-art results on a sizable dataset of documents (Reuters RCV1).

As the emphasis of this paper is on the training method, we applied it to some of the simplest possible model and inference network architectures, which was sufficient to obtain promising results. We believe that considerable performance gains can be made by using more expressive architectures, such as those with nonlinearities between layers of stochastic variables. Applying NVIL to models with continuous latent variables is another promising direction since binary latent variables are not always appropriate.

We expect NVIL to be also applicable to training conditional latent variable models for modelling the distribution of observations given some context, which would require making the inference network take both the context and the observation as input. This would make it an alternative to the importance-sampling training method of Tang & Salakhutdinov (2013) for conditional models with structured high-dimensional outputs.

We hope that the generality and flexibility of our approach will make it easier to apply powerful directed latent variable models to real-world problems.

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A. Algorithm for computing NVIL gradients

Algorithm 1 provides an outline of our implementation of NVIL gradient computation for a minibatch of n randomly chosen training cases. The exponential smoothing factor α used for updating the estimates of the mean c and variance v of the inference network learning signal was set to 0.8 in our experiments.

Algorithm 1 Compute gradient estimates for the model and the inference network

---

$\Delta\theta \leftarrow 0, \Delta\phi \leftarrow 0, \Delta\psi \leftarrow 0$
$\mathcal{L} \leftarrow 0$
{Compute the learning signal and the bound}
for $i \leftarrow 1$ to n **do**
  $x_i \leftarrow$ random training case
  {Sample from the inference model}
  $h_i \sim Q_\phi(h_i|x_i)$
  {Compute the unnormalized learning signal}
  $l_i \leftarrow \log P_\theta(x_i, h_i) - \log Q_\phi(h_i|x_i)$
  {Add the case contribution to the bound}
  $\mathcal{L} \leftarrow \mathcal{L} + l_i$
  {Subtract the input-dependent baseline}
  $l_i \leftarrow l_i - C_\psi(x_i)$
end for
{Update the learning signal statistics}
$c_b \leftarrow \text{mean}(l_1, ..., l_n)$
$v_b \leftarrow \text{variance}(l_1, ..., l_n)$
$c \leftarrow \alpha c + (1 - \alpha)c_b$
$v \leftarrow \alpha v + (1 - \alpha)v_b$
for $i \leftarrow 1$ to n **do**
  $l_i \leftarrow \frac{l_i - c}{\max(1, \sqrt{v})}$
  {Accumulate the model parameter gradient}
  $\Delta\theta \leftarrow \Delta\theta + \nabla_\theta \log P_\theta(x_i, h_i)$
  {Accumulate the inference net gradient}
  $\Delta\phi \leftarrow \Delta\phi + l_i\nabla_\phi \log Q_\phi(h_i|x_i)$
  {Accumulate the input-dependent baseline gradient}
  $\Delta\psi \leftarrow \Delta\psi + l_i\nabla_\psi C_\psi(x_i)$
end for

B. Inference network gradient derivation

Differentiating the variational lower bound w.r.t. to the inference network parameters gives

$$
\begin{aligned}
\nabla_\phi\mathcal{L}(x) =& \nabla_\phi E_Q[\log P_\theta(x, h) - \log Q_\phi(h|x)] \\
=& \nabla_\phi \sum_h Q_\phi(h|x) \log P_\theta(x, h) - \\
& \nabla_\phi \sum_h Q_\phi(h|x) \log Q_\phi(h|x) \\
=& \sum_h \log P_\theta(x, h)\nabla_\phi Q_\phi(h|x) - \\
& \sum_h \left(\log Q_\phi(h|x) + 1\right)\nabla_\phi Q_\phi(h|x) \\
=& \sum_h \left(\log P_\theta(x, h) - \log Q_\phi(h|x)\right)\nabla_\phi Q_\phi(h|x),
\end{aligned}
$$

where we used the fact that $\sum_h \nabla_\phi Q_\phi(h|x) = \nabla_\phi \sum_h Q_\phi(h|x) = \nabla_\phi 1 = 0$. Using the identity $\nabla_\phi Q_\phi(h|x) = Q_\phi(h|x)\nabla_\phi \log Q_\phi(h|x)$, then gives

$$
\begin{aligned}
\nabla_\phi\mathcal{L}(x) =& \sum_h \left(\log P_\theta(x, h) - \log Q_\phi(h|x)\right) \\
& \times Q_\phi(h|x)\nabla_\phi \log Q_\phi(h|x) \\
=& E_Q\left[\left(\log P_\theta(x, h) - \log Q_\phi(h|x)\right)\nabla_\phi \log Q_\phi(h|x)\right].
\end{aligned}
$$