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# Auto-Encoding Variational Bayes

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## Abstract

Can we efficiently learn the parameters of directed probabilistic models, in the presence of continuous latent variables with intractable posterior distributions? We introduce an unsupervised on-line learning method that efficiently optimizes the variational lower bound on the marginal likelihood and that, under some mild conditions, even works in the intractable case. The method optimizes a probabilistic encoder (also called a recognition network) to approximate the intractable posterior distribution of the latent variables. The crucial element is a reparameterization of the variational bound with an independent noise variable, yielding a stochastic objective function which can be jointly optimized w.r.t. variational and generative parameters using standard gradient-based stochastic optimization methods. Theoretical advantages are reflected in experimental results.

## 1 Introduction

How to efficiently learn the parameters of directed probabilistic models whose continuous latent variables have intractable posterior distributions? The variational approach to approximate Bayesian inference involves the introduction of an approximate posterior to the intractable posterior, used to maximize the variational lower bound on the marginal likelihood. Unfortunately, the common mean-field approach requires analytical solutions to expectations w.r.t. the approximate posterior, which are also intractable in the general case. We show how for continuous latent variables, a reparameterization of the expectation w.r.t. the approximate posterior yields a novel and practical estimator of the variational lower bound that can be differentiated and jointly optimized w.r.t. all parameters, i.e. both the variational parameters and regular parameters, using standard stochastic gradient ascent techniques.

The objective contains, in addition to regularization terms dictated by the variational bound, a noisy data reconstruction term, exposing a novel connection between auto-encoders and stochastic variational inference. In contrast to a typical objective for auto-encoders [BCV13], all parameters updates, including those of the noise distribution, correspond to optimization of the variational lower bound on the marginal likelihood. From the learned generative model it is straightforward to generate samples, without the typical requirement of running Markov chains. The probabilistic encoder can be used for fast approximate inference of latent variables, i.e. for recognition, representation or visualization purposes. Furthermore, the lower bound estimator can be used for unsupervised inference tasks such as denoising and inpainting.

## 2 Method

The strategy in the following section can be used to derive a lower bound estimator (a stochastic objective function) for a variety of directed graphical models with continuous latent variables. We will restrict ourselves here to the common case where we have an i.i.d. dataset with latent variables per datapoint, and where we like to perform ML or MAP inference on the (global) parameters, and

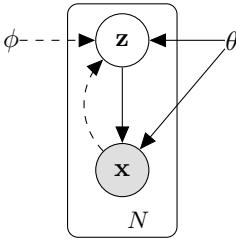


Figure 1: The type of directed graphical model under consideration. Solid lines denote the generative model  $p_\theta(\mathbf{z})p_\theta(\mathbf{x}|\mathbf{z})$ , dashed lines denote the variational approximation  $q_\phi(\mathbf{z}|\mathbf{x})$  to the intractable posterior  $p_\theta(\mathbf{z}|\mathbf{x})$ . The variational parameters  $\phi$  are learned jointly with the generative model parameters  $\theta$ .

variational inference on the latent variables. It is, for example, straightforward to extend this scenario to the case where we also perform variational inference on the global parameters; that algorithm is put in the appendix, but experiments with that case are left to future work. Note that our method can be applied to online, non-stationary settings, e.g. streaming data, but here we assume a fixed dataset for simplicity.

## 2.1 Problem scenario

Let us consider some dataset  $\mathbf{X} = \{\mathbf{x}^{(i)}\}_{i=1}^N$  consisting of  $N$  i.i.d. samples of some continuous or discrete variable  $\mathbf{x}$ . We assume that the data are generated by some random process, involving an unobserved continuous random variable  $\mathbf{z}$ . The process consists of two steps: (1) a value  $\mathbf{z}^{(i)}$  is generated from some prior distribution  $p_{\theta^*}(\mathbf{z})$ ; (2) a value  $\mathbf{x}^{(i)}$  is generated from some conditional distribution  $p_{\theta^*}(\mathbf{x}|\mathbf{z})$ . We assume that the prior  $p_{\theta^*}(\mathbf{z})$  and likelihood  $p_{\theta^*}(\mathbf{x}|\mathbf{z})$  come from parametric families of distributions  $p_\theta(\mathbf{z})$  and  $p_\theta(\mathbf{x}|\mathbf{z})$ , and that their PDFs are differentiable almost everywhere w.r.t. both  $\theta$  and  $\mathbf{z}$ . Unfortunately, a lot of this process is hidden from our view: the true parameters  $\theta^*$  as well as the values of the latent variables  $\mathbf{z}^{(i)}$  are unknown to us.

Very importantly, we *do not* make the usual simplifying assumptions common in the literature. Conversely, we are here interested in a general algorithm that even works in the case of:

1. *Intractability*: the case where the integral of the marginal likelihood  $p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{z})p_\theta(\mathbf{x}|\mathbf{z}) d\mathbf{z}$  is intractable (so we cannot evaluate or differentiate the marginal likelihood), where the true posterior density  $p_\theta(\mathbf{z}|\mathbf{x}) = p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})/p_\theta(\mathbf{x})$  is intractable (so the EM algorithm cannot be used), and where the required integrals for any reasonable mean-field Variational Bayes are also intractable. These intractabilities are quite common and already appear in case of moderately complicated likelihood functions  $p_\theta(\mathbf{x}|\mathbf{z})$ , e.g. a neural network with a nonlinear hidden layer.
2. *A large dataset*: we have so much data that batch optimization is too costly; we would like to make parameter updates using small minibatches or even single datapoints. Sampling-based solutions, e.g. Monte Carlo EM, would in general be too slow, since it involves a typically expensive sampling loop per datapoint.

We are interested in, and propose a solution to, three related problems in the above scenario:

1. Efficient approximate maximum likelihood (ML) or maximum a posteriori (MAP) estimation for the parameters  $\theta$ . The parameters can be of interest themselves, e.g. if we are analyzing some natural process. They also allow us to mimic the hidden random process and generate artificial data that resembles the real data.
2. Efficient approximate posterior inference of the latent variable  $\mathbf{z}$  given an observed value  $\mathbf{x}$  for a choice of parameters  $\theta$ . This is useful for coding or data representation tasks.
3. Efficient approximate marginal inference of the variable  $\mathbf{x}$ . This allows us to perform all kinds of inference tasks where a prior over  $\mathbf{x}$  is required. Common applications in computer vision include image denoising, inpainting and super-resolution.

For the purpose of solving the above problems, let us introduce the parametric variational approximation  $q_\phi(\mathbf{z}|\mathbf{x})$ : an approximation to the intractable true posterior  $p_\theta(\mathbf{z}|\mathbf{x})$ . Note that in contrast with the approximate posterior in mean-field variational inference, it is not necessarily factorial and its parameters are not computed from some closed-form expectation. Instead, its parameters  $\phi$  are learned jointly with the parameters of the generative model.

From a coding theory perspective, the unobserved variables  $\mathbf{z}$  have an interpretation as a latent representation or *code*. In this paper we will therefore also refer to  $q_\phi(\mathbf{z}|\mathbf{x})$  as a (*variational*) *encoder* or *recognition model*, since given a datapoint  $\mathbf{x}$  it produces a distribution (e.g. a Gaussian) over the possible values of the code  $\mathbf{z}$  from which the datapoint  $\mathbf{x}$  could have been generated. In a similar vein we will refer to  $p_\theta(\mathbf{x}|\mathbf{z})$  as a (*generative*) *decoder*, since given a code  $\mathbf{z}$  it produces a distribution over the possible corresponding values of  $\mathbf{x}$ .

## 2.2 The variational bound

The marginal likelihood is composed of a sum over the marginal likelihoods of individual datapoints  $\log p_\theta(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}) = \sum_{i=1}^N \log p_\theta(\mathbf{x}^{(i)})$ , which can each be rewritten as:

$$\log p_\theta(\mathbf{x}^{(i)}) = D_{KL}(q_\phi(\mathbf{z}|\mathbf{x}^{(i)})||p_\theta(\mathbf{z}|\mathbf{x}^{(i)})) + \mathcal{L}(\theta, \phi; \mathbf{x}^{(i)}) \quad (1)$$

The first RHS term is the KL divergence of the approximate from the true posterior, which is non-negative. The second RHS term  $\mathcal{L}(\theta, \phi; \mathbf{x}^{(i)})$  denotes the variational lower bound on the marginal likelihood of datapoint  $i$ :

$$\log p_\theta(\mathbf{x}^{(i)}) \geq \mathcal{L}(\theta, \phi; \mathbf{x}^{(i)}) = \int q_\phi(\mathbf{z}|\mathbf{x}) (\log p_\theta(\mathbf{x}^{(i)}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})) d\mathbf{z} \quad (2)$$

Note that the bound equals the true marginal when the divergence of the approximate from true posterior distribution is zero.

The expectation on the RHS of eq. (2) can obviously be written as a sum of three separate expectations, of which the second and third component can sometimes be analytically solved, e.g. when both  $p_\theta(\mathbf{x})$  and  $q_\phi(\mathbf{z}|\mathbf{x})$  are Gaussian. For generality we will here assume that each of these expectations are intractable.

We would like to optimize the lower bound  $\mathcal{L}(\theta, \phi; \mathbf{x}^{(i)})$  (eq. (2)) using stochastic gradients. Note that following these gradients would either decrease the KL divergence between the approximate and true posterior distributions, or increase the marginal likelihood, or both. A naïve attempt to compute a stochastic gradient would be to draw samples  $\{\mathbf{z}^{(l)}\}_{l=1}^L$  from  $q_\phi$  and then differentiate the following Monte Carlo estimate of the lower bound:

$$\mathcal{L}(\theta, \phi; \mathbf{x}^{(i)}) \simeq \frac{1}{L} \sum_{l=1}^L (\log p_\theta(\mathbf{x}^{(i)}|\mathbf{z}^{(l)}) + \log p_\theta(\mathbf{z}^{(l)}) - \log q_\phi(\mathbf{z}^{(l)}|\mathbf{x}^{(i)})) \quad \text{where } \mathbf{z}^{(l)} \sim q_\phi(\mathbf{z}|\mathbf{x})$$

While the above expression is an unbiased estimator of the marginal likelihood (i.e. it will equal the lower bound in the limit  $L \rightarrow \infty$ ), differentiating it w.r.t. the parameters  $\phi$  will not result in an unbiased gradient: the variational parameters  $\phi$  indirectly influence the estimate through the samples  $\mathbf{z}^{(l)} \sim q_\phi(\mathbf{z}|\mathbf{x})$ , and it is impossible to differentiate through this sampling process. Existing work on stochastic variational bayes provide workarounds [BJP12], but not a solution to this problem.

## 2.3 Our estimator of the lower bound

Under certain mild conditions outlined in section 2.4 for a chosen approximate posterior  $q_\phi(\mathbf{z}|\mathbf{x})$  we can reparameterize its conditional samples  $\tilde{\mathbf{z}} \sim q_\phi(\mathbf{z}|\mathbf{x})$  as

$$\tilde{\mathbf{z}} = g_\phi(\epsilon, \mathbf{x}) \quad \text{with } \epsilon \sim p(\epsilon) \quad (3)$$

where we choose a prior  $p(\epsilon)$  and a function  $g_\phi(\epsilon, \mathbf{x})$  such that the following holds:

$$\begin{aligned} \mathcal{L}(\theta, \phi; \mathbf{x}^{(i)}) &= \int q_\phi(\mathbf{z}|\mathbf{x}) (\log p_\theta(\mathbf{x}^{(i)}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})) d\mathbf{z} \\ &= \int p(\epsilon) (\log p_\theta(\mathbf{x}^{(i)}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})) \Big|_{\mathbf{z}=g_\phi(\epsilon, \mathbf{x}^{(i)})} d\epsilon \end{aligned} \quad (4)$$

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162   **Algorithm 1** Pseudocode for computing a stochastic gradient using our estimator. See section 2.3  
 163   for meaning of the functions  $f_{\theta, \phi}$  and  $g_\phi$ . The minibatch  $\mathbf{X}^M = \{\mathbf{x}^{(i)}\}_{i=1}^M$  is a randomly drawn  
 164   subset of the full dataset  $\mathbf{X}$ . We use settings  $M = 100$  and  $L = 1$  in experiments.

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165   **Require:**  $\theta, \phi$  (Current value of parameters)

```

166   g ← 0
167    $\mathbf{X}^M$  ← Random subset (minibatch) of  $M$  datapoints from dataset
168   for each  $\mathbf{x} \in \mathbf{X}^M$  do
169     for  $l$  is 1 to  $L$  do
170        $\epsilon$  ← Random sample from  $p(\epsilon)$ 
171        $g \leftarrow g + \nabla_{\theta, \phi} f_{\theta, \phi}(\mathbf{x}, g_\phi(\epsilon, \mathbf{x}))$ 
172     end for
173   end for
174   return  $(N/(M \cdot L)) \cdot g$ 
```

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175  
 176   For notational conciseness we introduce a shorthand notation  $f_{\theta, \phi}(\mathbf{x}, \mathbf{z})$  for the sum of three PDFs:

$$f_{\theta, \phi}(\mathbf{x}, \mathbf{z}) = \log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x}) \quad (5)$$

180   Using eq. (4), the Monte Carlo estimate of the variational lower bound, given datapoint  $\mathbf{x}^{(i)}$ , is:

$$\mathcal{L}(\theta, \phi; \mathbf{x}^{(i)}) \simeq \frac{1}{L} \sum_{l=1}^L f_{\theta, \phi}(\mathbf{x}^{(i)}, g_\phi(\epsilon^{(l)}, \mathbf{x}^{(i)})) \quad \text{where } \epsilon^{(l)} \sim p(\epsilon) \quad (6)$$

185   The estimator only depends on samples from  $p(\epsilon)$  which are obviously not influenced by  $\phi$ , therefore  
 186   we can use it as an objective function that can be differentiated and jointly optimized w.r.t. both  $\theta$  and  
 187    $\phi$ . Given multiple datapoints from the dataset  $\mathbf{X}$ , we can easily construct a minibatch-based version  
 188   of the estimator:  $\mathcal{L}(\theta, \phi; \mathbf{X}) \simeq \frac{N}{M} \sum_{i=1}^M \mathcal{L}(\theta, \phi; \mathbf{x}^{(i)})$  where the minibatch  $\mathbf{X}^M = \{\mathbf{x}^{(i)}\}_{i=1}^M$  is  
 189   a randomly drawn subset of the full dataset  $\mathbf{X}$ . In our experiments we found that the number of  
 190   samples  $L$  per datapoint can be set to 1 as long as the minibatch size  $M$  was large enough, e.g.  $M =$   
 191   100. Derivatives  $\nabla_{\theta, \phi} \tilde{\mathcal{L}}(\theta; \mathbf{X}^M)$  can be taken, and the resulting gradients can be used in conjunction  
 192   with stochastic optimization methods such as SGD or Adagrad [DHS10]. See algorithm 1 for a basic  
 193   approach to compute the stochastic gradients.

194   A connection with auto-encoders becomes clear when looking at the objective function given at  
 195   eq. (6). The variational approximation  $q_\phi(\mathbf{z}|\mathbf{x}^{(i)})$  (the encoder) maps a datapoint  $\mathbf{x}^{(i)}$  to a distribution  
 196   over latent variables  $\mathbf{z}$  from which the datapoint could have been generated. The function  $g_\phi(\cdot)$   
 197   is chosen such that it maps a datapoint  $\mathbf{x}^{(i)}$  and a random noise vector  $\epsilon^{(l)}$  to a sample from the  
 198   approximate posterior for that datapoint:  $\mathbf{z}^{(i,l)} = g_\phi(\epsilon^{(l)}, \mathbf{x}^{(i)})$  where  $\mathbf{z}^{(i,l)} \sim q_\phi(\mathbf{z}|\mathbf{x}^{(i)})$ . Subse-  
 199   quently, the sample  $\mathbf{z}^{(i,l)}$  is then input to function  $f_{\theta, \phi}(\cdot)$ , which consists of three parts. The first  
 200   part ( $\log p_\theta(\mathbf{x}^{(i)}|\mathbf{z}^{(i,l)})$ ) can be interpreted as the *negative reconstruction error* in neural network  
 201   parlance. The second and third part can be interpreted as regularization terms that make sure the  
 202   code activations have high entropy due to the term  $\log q_\phi(\mathbf{z}|\mathbf{x})$ , while not being too far from the  
 203   prior due to the term  $\log p_\theta(\mathbf{z})$ .

## 2.4 The deterministic parameterization trick

204   In order to solve the problem we invoked a reparameterization trick that is perhaps best known in  
 205   literature for a different application, namely an efficient Gibbs sampling technique going under the  
 206   name of *non-centered parameterization* [PRS07] or *ancillary augmentation* (AA) [YM11].

207   The essential parameterization trick is quite simple. Let  $q_\phi(\mathbf{z}|\mathbf{x})$  be some conditional distribution  
 208   parameterized by  $\phi$ . It is then often possible to express the random variable  $\mathbf{z}$  given  $\mathbf{x}$  as a deter-  
 209   ministic variable  $\mathbf{z} = g_\phi(\epsilon, \mathbf{x})$ , where  $\epsilon$  is an auxiliary variable with independent marginal  $p(\epsilon)$ , and  
 210    $g_\phi(\cdot)$  is some vector-valued function parameterized by  $\phi$ .

211   This reparameterization is useful for our case since it can be used to rewrite an expectation w.r.t.  
 212    $q_\phi(\mathbf{z}|\mathbf{x})$  such that the Monte Carlo estimate of the expectation is differentiable w.r.t.  $\phi$ . A proof  
 213   is as follows. Given the deterministic mapping  $\mathbf{z} = g_\phi(\epsilon, \mathbf{x})$  we know that  $q_\phi(\mathbf{z}|\mathbf{x}) \prod_i dz_i =$

216  $p(\epsilon) \prod_i d\epsilon_i$ . Therefore<sup>1</sup>,  $\int q_\phi(\mathbf{z}|\mathbf{x})f(\mathbf{z}) d\mathbf{z} = \int p(\epsilon)f(\mathbf{z}) d\epsilon = \int p(\epsilon)f(g_\phi(\epsilon, \mathbf{x})) d\epsilon$ . It follows  
 217 that a differentiable estimator can be constructed:  $\int q_\phi(\mathbf{z}|\mathbf{x})f(\mathbf{z}) d\mathbf{z} \simeq \frac{1}{L} \sum_{l=1}^L f(g_\phi(\mathbf{x}, \epsilon^{(l)}))$   
 218 where  $\epsilon^{(l)} \sim p(\epsilon)$ . In section 2.3 we applied this trick to obtain a differentiable estimator of the  
 219 variational lower bound.  
 220

221 Take, for example, the univariate Gaussian case: let  $z$  be distributed as  $p(z|x) = \mathcal{N}(z, \sigma)$ . The  
 222 random variable  $z$  is partially explained by  $x$ , but there is some uncertainty left indicated by  $\sigma$ .  
 223 In this case, a deterministic parameterization is  $z = x + \sigma\epsilon$ , where  $\epsilon$  is an independent auxiliary  
 224 variable  $\epsilon \sim \mathcal{N}(0, 1)$ . In this univariate Gaussian case,  $\phi = \{\sigma\}$  and  $g_\phi(\epsilon, y) = y + \sigma\epsilon$ .

225 When can we do this, i.e., for which  $q_\phi(\mathbf{z}|\mathbf{x})$  can we choose such a  $g_\phi(\cdot)$  and  $p(\epsilon)$ ? There are three  
 226 basic approaches:  
 227

- 228 1. Tractable inverse CDF. In this case, let  $\epsilon \sim \mathcal{U}(\mathbf{0}, \mathbf{I})$ , and let  $g_\phi(\epsilon, \mathbf{x})$  be the inverse CDF of  
 229  $q_\phi(\mathbf{z}|\mathbf{x})$ . Examples: Exponential, Cauchy, Logistic, Rayleigh, Pareto, Weibull, Reciprocal,  
 230 Gompertz, Gumbel and Erlang distributions.
- 231 2. Analogous to the Gaussian example, for any "location-scale" family of distributions (with  
 232 differentiable log-PDF) we can choose the standard distribution (with location = 0, scale =  
 233 1) as the auxiliary variable  $E$ , and let  $g(\cdot) = \text{location} + \text{scale} \cdot \epsilon$ . Examples: Laplace,  
 234 Elliptical, Student's t, Logistic, Uniform, Triangular and Gaussian distributions.
- 235 3. Composition: It is often possible to express variables as functions of component variables  
 236 with distributions that are reparameterizable using either of the above two approaches. Ex-  
 237 amples: Log-Normal (exponentiation of normally distributed variable), Gamma (a sum  
 238 over exponentially distributed variables), Dirichlet (weighted sum of Gamma variates),  
 239 Beta, Chi-Squared, and F distributions.

240 When all three approaches fail, good approximations to the inverse CDF exist requiring computa-  
 241 tions with time complexity comparable to the PDF (see e.g. [Dev86] for some methods).  
 242

### 243 3 Example

244 Here we'll give an example generative model and posterior approximation used in experiments.

245 Let the prior over the latent variables be the centered isotropic Gaussian  $p_\theta(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I})$ . Note  
 246 that in this case, the prior lacks parameters. Let  $p_\theta(\mathbf{x}|\mathbf{z})$  (the decoder) be a multivariate Bernoulli  
 247 whose probabilities are computed from  $\mathbf{z}$  with a fully-connected neural network with a single hidden  
 248 layer:  
 249

$$250 \log p_\theta(\mathbf{x}|\mathbf{z}) = \sum_{i=1}^D x_i \log y_i - (1 - x_i) \cdot \log(1 - y_i) \\ 251 \text{where } \mathbf{y} = \exp(\mathbf{W}_2 \tanh(\mathbf{W}_1 \mathbf{z} + \mathbf{b}_1) + \mathbf{b}_2) \quad (7)$$

252 While there is much freedom in the choice of  $q_\phi(\mathbf{z}|\mathbf{x})$  (the decoder), we'll for a moment assume a  
 253 relatively simple case: let's assume that the true posterior  $p_\theta(\mathbf{z}|\mathbf{x})$  takes on a approximate Gaussian  
 254 form with an approximately diagonal covariance. In this case, we can let the variational approximate  
 255 posterior be a multivariate Gaussian with a diagonal covariance structure<sup>2</sup>:  
 256

$$257 \log q_\phi(\mathbf{z}|\mathbf{x}) = \log \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2 \mathbf{I}) \quad (8)$$

258 where  $\boldsymbol{\mu}$  and  $\boldsymbol{\sigma}$  are yet unspecified functions of  $\mathbf{x}$ . We can sample from  $q_\phi(\mathbf{z}|\mathbf{x})$  using  $\tilde{\mathbf{z}} =$   
 259  $h_\phi(\mathbf{x}, \epsilon) = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \epsilon$  where  $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ . With  $\odot$  we signify an element-wise product. Therefore,  
 260 given a minibatch  $\mathbf{X}^M$  of data, and using the  $f_{\theta, \phi}(\cdot)$  abbreviation of eq. (5), our estimator of the  
 261 lower bound is:  
 262

$$263 \mathcal{L}(\boldsymbol{\theta}, \phi; \mathbf{x}^{(i)}) \simeq \frac{1}{L} \sum_{l=1}^L f_{\theta, \phi}(\mathbf{x}^{(i)}, \mathbf{z}^{(i, l)}) \Big|_{\mathbf{z}^{(i, l)} = \boldsymbol{\mu}^{(i)} + \boldsymbol{\sigma}^{(i)} \odot \epsilon^{(l)}} \quad \text{where } \epsilon^{(l)} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad (9)$$

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264 <sup>1</sup>Note that for infinitesimals we use the notational convention  $d\mathbf{z} = \prod_i dz_i$

265 <sup>2</sup>Note that this is just a (simplifying) choice, and not a limitation our method.

270 where  $\mu^{(i)}$  and  $\sigma^{(i)}$  denote the mean and s.d. of the approximation of the posterior  $q_\phi(\mathbf{z}|\mathbf{x}^{(i)})$ , which  
 271 we didn't yet specify. Let the mean  $\mu^{(i)}$  and variance  $\sigma^{(i)}$  of the Gaussian encoding distribution be  
 272 the following nonlinear function of  $\mathbf{x}$ , (a neural network):  
 273

$$274 \log q_\phi(\mathbf{z}|\mathbf{x}) = \log \mathcal{N}(\mathbf{z}; \mu, \sigma^2 \mathbf{I})$$

$$275 \text{ where } \mu = \mathbf{W}_4 \mathbf{h} + \mathbf{b}_4, \text{ and } \log \sigma^2 = \mathbf{W}_5 \mathbf{h} + \mathbf{b}_5, \text{ and } \mathbf{h} = \tanh(\mathbf{W}_3 \mathbf{x} + \mathbf{b}_3) \quad (10)$$

277 Note that the generative (decoding) parameters are  $\theta = \{\mathbf{W}_j, \mathbf{b}_j\}_{j=1}^2$  and the variational (encoding)  
 278 parameters are  $\phi = \{\mathbf{W}_j, \mathbf{b}_j\}_{j=3}^5$ . These definitions for the encoder and decoder can be plugged in  
 279 eq. 6, and the lower bound can subsequently be differentiated and optimized w.r.t. the parameters.

280 In this model both  $p_\theta(\mathbf{z})$  and  $q_\phi(\mathbf{z}|\mathbf{x})$  are Gaussian; in this special case, the second and third term  
 281 of  $f_{\theta,\phi}$  (eq. (5)) can be solved analytically. This results in an estimator with a lower variance than  
 282 the generic estimator given in eq. (9). The resulting estimator is:  
 283

$$284 \mathcal{L}(\theta, \phi; \mathbf{x}^{(i)}) \simeq \frac{1}{2} \sum_{j=1}^J \left( 1 + \log((\sigma_j^{(i)})^2) - (\mu_j^{(i)})^2 - (\sigma_j^{(i)})^2 \right) + \frac{1}{L} \sum_{l=1}^L \log p_\theta(\mathbf{x}^{(i)}|\mathbf{z}^{(i,l)}) \quad (11)$$

287 See the appendix for the derivation.  
 288

## 289 4 Related work

291 Perhaps the most relevant related method is the Wake-Sleep algorithm [HDFN95]. Like AEVB,  
 292 the wake-sleep algorithm employs an encoder (called a recognition network) that approximates the  
 293 true posterior. A well-known drawback of the wake-sleep algorithm is that it lacks a theoretically  
 294 justified method for learning the parameters of the recognition network: its updates correspond  
 295 to optimization of the divergence  $KL(p||q)$  instead of the divergence  $KL(q||p)$  dictated by the  
 296 lower bound. A theoretical advantage of the wake-sleep algorithm is that it also applies to models  
 297 with discrete latent variables. Wake-Sleep has the same computational complexity as AEVB per  
 298 datapoint.

299 AEVB corresponds to the optimization of a type of auto-encoder, exposing a connection between  
 300 generative models and auto-encoders. A connection between *linear* auto-encoders and a certain  
 301 class of generative linear-Gaussian models has long been known. In [Row98] it was shown that PCA  
 302 corresponds to the maximum-likelihood (ML) solution of a special case of the linear-Gaussian model  
 303 with a prior  $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$  and a conditional distribution  $p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \mathbf{W}\mathbf{z}, \epsilon\mathbf{I})$ , specifically the  
 304 case with infinitesimally small  $\epsilon$ .

305 In relevant recent work on autoencoders [VLL<sup>+</sup>10] it was shown that the training criterion of un-  
 306 regularized autoencoders corresponds to maximization of a lower bound (see the infomax princi-  
 307 ple [Lin89]) of the mutual information between input  $X$  and latent representation  $Z$ . Maximiz-  
 308 ing (w.r.t. parameters) of the mutual information is equivalent to maximizing the conditional en-  
 309 tropy, which is lower bounded by the expected loglikelihood of the data under the autoencoding  
 310 model [VLL<sup>+</sup>10], i.e. the negative reconstruction error. However, it is well known that this recon-  
 311 struction criterion is in itself not sufficient for learning useful representations [BCV13]. Regular-  
 312 ization techniques have been proposed to make autoencoders learn useful representations, such as  
 313 denoising, contractive and sparse autoencoder variants [BCV13]. Related are also encoder-decoder  
 314 architectures such as the predictive sparse decomposition (PSD) [KRL08] from which we drew some  
 315 inspiration. In contrast to our method, these methods fall under the umbrella of either unnormalized  
 316 (or energy-based) models or sparse coding. Our objective function contains (hyper-parameter free)  
 317 regularization terms dictated by the variational bound (eq. (5)).

## 318 5 Experiments

321 We trained generative models of images from the MNIST and Frey Face datasets<sup>3</sup> and compared  
 322 learning algorithms in terms of the variational lower bound, and the estimated marginal likelihood.  
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<sup>3</sup>Available at <http://www.cs.nyu.edu/~roweis/data.html>

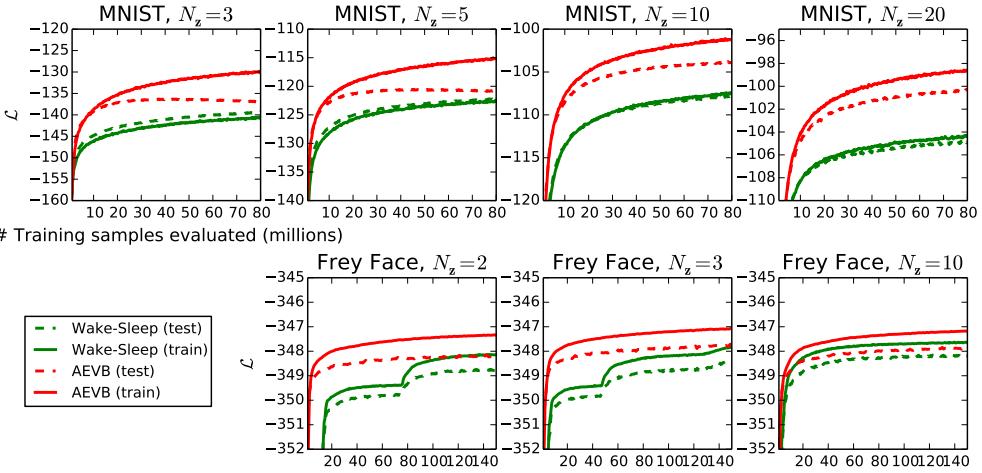


Figure 2: Comparison of our AEVB method to the wake-sleep algorithm, in terms of optimizing the lower bound, for different dimensionality of latent space ( $N_z$ ). Our method converged considerably faster and reached a better solution in all experiments. Vertical axis: the estimated average variational lower bound per datapoint. The estimator variance was small ( $< 1$ ) and omitted. Horizontal axis: amount of training points evaluated. Computation took around 20 minutes per million training samples with a dated quad-core Xeon CPU.

The generative model (encoder) and variational approximation (decoder) from section 3 were used, where the described encoder and decoder have an equal number of hidden units. Note that with *hidden units* we denote the neural-network units in the hidden layer of the neural networks of the encoder and decoder.

All parameters were updated according to the MAP criterion  $\nabla_{\theta, \phi} \log p(\theta, \phi | \mathbf{X}) = \nabla_{\theta, \phi} \log p_\theta(\mathbf{X}) + \nabla_{\theta, \phi} \log p(\theta, \phi)$ , with a prior  $p(\theta, \phi) = \mathcal{N}(0, \mathbf{I})$ . Optimization of this MAP objective is equivalent to plain likelihood maximization with the addition of a weight decay term. The likelihood gradient was approximated by the gradient of the lower bound:  $\nabla_{\theta, \phi} \log p_\theta(\mathbf{X}) \approx \nabla_{\theta, \phi} \mathcal{L}(\theta, \phi; \mathbf{X})$ . We compared performance of AEVB to the wake-sleep algorithm [HDFN95]. We employed the same encoder (also called recognition network) for the wake-sleep algorithm and the variational auto-encoder. All parameters, both variational and generative, were initialized by random sampling from  $\mathcal{N}(0, 0.01)$ , and were jointly stochastically optimized using the MAP criterion. Stepsizes were adapted with Adagrad [DHS10]; the Adagrad global stepsize parameters were chosen from  $\{0.01, 0.02, 0.1\}$  based on performance on the training set in the first few iterations. Minibatches of size  $M = 100$  were used, with  $L = 1$  samples per datapoint.

**Likelihood lower bound** We trained generative models (decoders) and corresponding encoders (a.k.a. recognition networks) having 500 hidden units in case of MNIST, and 200 hidden units in case of the Frey Face dataset (to prevent overfitting, since it is a considerably smaller dataset). Figure 2 shows the results when comparing the lower bounds.

**Marginal likelihood** For very low-dimensional latent space it is possible to estimate the marginal likelihood of the learned generative models using an MCMC estimator. More information about the marginal likelihood estimator is available in the appendix. For the encoder and decoder we again used neural networks, this time with 100 hidden units, and 3 latent variables; for higher dimensional latent space the estimates became unreliable. The AEVB and Wake-Sleep methods were compared to Monte Carlo EM (MCEM) with a Hybrid Monte Carlo (HMC) [DKPR87] sampler; details are in the appendix. We compared the convergence speed for the three algorithms, for a small and large training set size. Results are in figure 3.

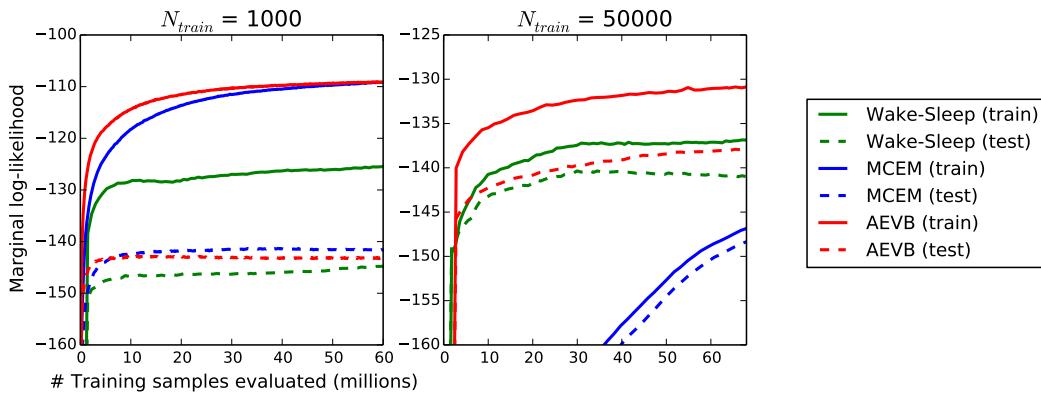
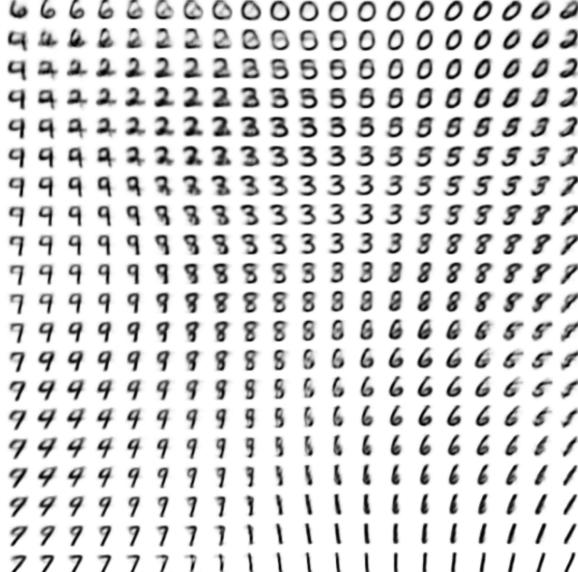


Figure 3: Comparison of AEVB to the wake-sleep algorithm and Monte Carlo EM, in terms of the estimated marginal likelihood, for a different number of training points. The Monte Carlo EM algorithm is (unlike AEVB and the wake-sleep method) asymptotically unbiased but cannot be applied online such that it becomes inefficient for large datasets (right figure).



(a) Learned Frey Face manifold



(b) Learned MNIST manifold

Figure 4: Visualisations of learned data manifold for generative models with two-dimensional latent space, learned with AEVB. Since the prior of the latent space is Gaussian, linearly spaced coordinates on the unit square were transformed through the inverse CDF of the Gaussian to produce values of the latent variables  $\mathbf{z}$ . For each of these values  $\mathbf{z}$ , we plotted the corresponding generative  $p_{\theta}(\mathbf{x}|\mathbf{z})$  with the learned parameters  $\theta$ .

## 6 Conclusion

We have introduced a novel online learning and approximate inference method for models with continuous latent variables, that works for the case where mean-field VB and EM methods are intractable. The proposed estimator can be straightforwardly differentiated and optimized w.r.t. all parameters, resulting in stochastic gradients that are easily plugged into existing stochastic gradient optimization methods. The method learns an encoder, or variational approximation to the posterior, that can be used for fast approximate inference of the distribution of the latent variables. The theoretical advantages are reflected in experimental results.

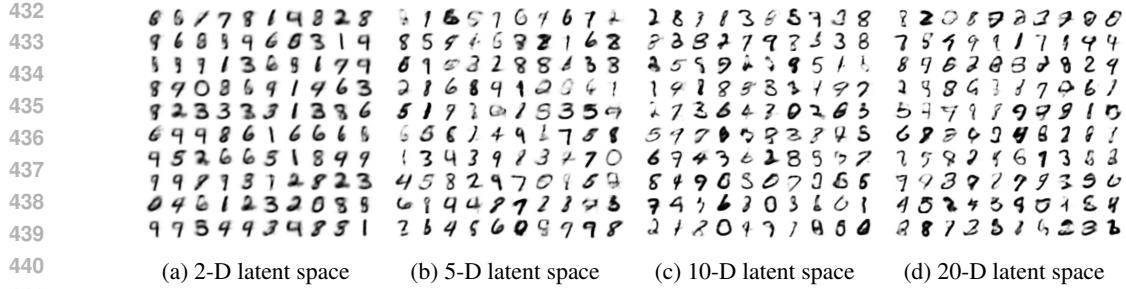


Figure 5: Random samples from learned generative models of MNIST for different dimensionalities of latent space.

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