Auto-Encoding Variational Bayes

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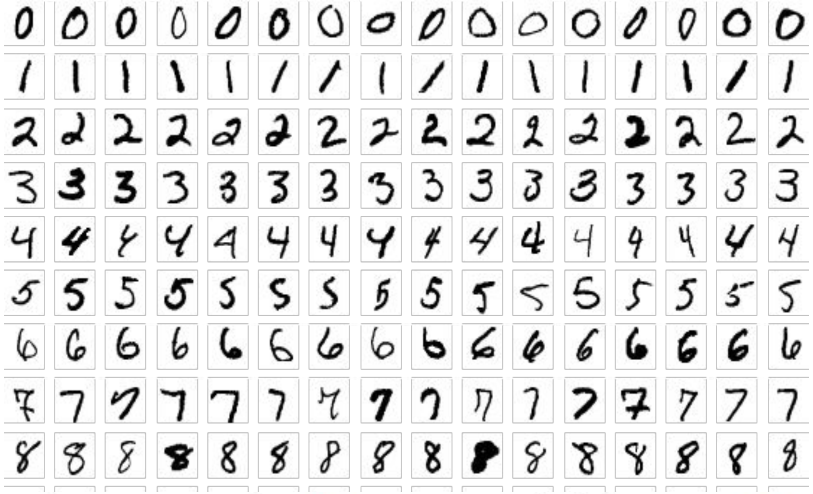
Problem scenario

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 $p_{\boldsymbol{\theta}^*}(\mathbf{z})$; (2) a value $\mathbf{x}^{(i)}$ is generated from some conditional distribution $p_{\boldsymbol{\theta}^*}(\mathbf{x}|\mathbf{z})$.

$$\begin{pmatrix}0.3\\0.5\\0.2\end{pmatrix} \mathbf{z} \longrightarrow \mathbf{X}$$

Marginal likelihood

$$\begin{pmatrix} 0.3 \\ 0.5 \\ 0.2 \end{pmatrix} \mathbf{z} \longrightarrow \mathbf{x}$$



Given a set of independent identically distributed data points $\mathbf{X} = (x_1, \ldots, x_n)$, where $x_i \sim p(x|\theta)$ according to some probability distribution parameterized by θ, where θ itself is a random variable described by a distribution, i.e. $\theta \sim p(\theta \mid \alpha)$, the marginal likelihood in general asks what the probability $p(\mathbf{X} \mid \alpha)$ is, where θ has been marginalized out (integrated out):

$$p(\mathbf{X} \mid \alpha) = \int_\theta p(\mathbf{X} \mid \theta)\, p(\theta \mid \alpha)\ \mathrm{d}\theta$$

In our case:

$$\int p_{\boldsymbol{\theta}}(\mathbf{z}) p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})\, d\mathbf{z}$$

Problems with existing methods

1. *Intractability*: the case where the integral of the marginal likelihood $p_{\boldsymbol{\theta}}(\mathbf{x}) = \int p_{\boldsymbol{\theta}}(\mathbf{z}) p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) \, d\mathbf{z}$ is intractable (so we cannot evaluate or differentiate the marginal likelihood), where the true posterior density $p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}) = p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) p_{\boldsymbol{\theta}}(\mathbf{z}) / p_{\boldsymbol{\theta}}(\mathbf{x})$ is intractable (so the EM algorithm cannot be used), and where the required integrals for any reasonable mean-field VB algorithm are also intractable. These intractabilities are quite common and appear in cases of moderately complicated likelihood functions $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$, 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.

Method

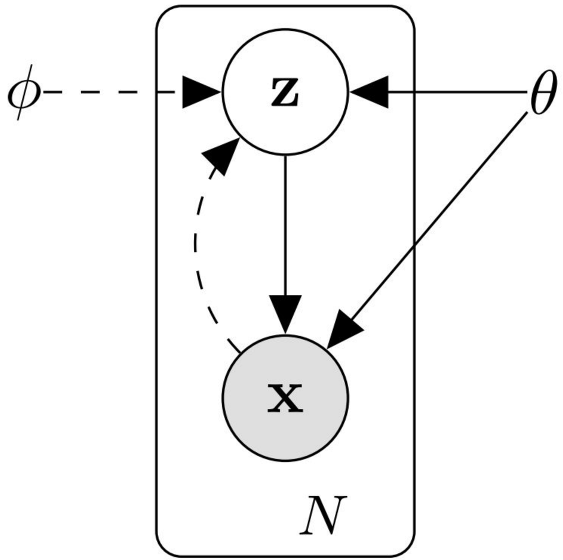


Figure 1: The type of directed graphical model under consideration. Solid lines denote the generative model $p_{\boldsymbol{\theta}}(\mathbf{z})p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$, dashed lines denote the variational approximation $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ to the intractable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

Probabilistic encoder definition

$$p_\theta(z|x) \longrightarrow q_\phi(z|x)$$

Probabilistic decoder definition

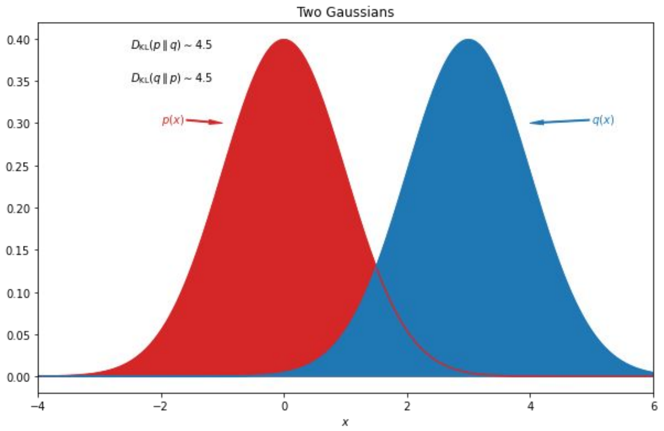
$$p_\theta(x|z)$$

This solves intractability!

Kullback–Leibler divergence

The Kullback-Leibler divergence is a measure of the dissimilarity between two probability distributions.

$$D_{\mathrm{KL}}(p \parallel q) + H(p) = H(p, q)$$



Variational lower bound

marginal likelihood

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

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) \geq \mathcal{L}(\boldsymbol{\theta}, \phi; \mathbf{x}^{(i)})$$

Now we can optimize $\mathcal{L}(\boldsymbol{\theta}, \phi; \mathbf{x}^{(i)})$ instead!

But the gradient of L can't be approximated well with Monte-Carlo methods 😞

Idea of reparametrization

$$\widetilde{\mathbf{z}} \sim q_\phi(\mathbf{z}|\mathbf{x}) \Rightarrow \widetilde{\mathbf{z}} = g_\phi(\boldsymbol{\epsilon}, \mathbf{x}) \quad \text{with} \quad \boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$$

1. Tractable inverse CDF. In this case, let $\boldsymbol{\epsilon} \sim \mathcal{U}(\mathbf{0}, \mathbf{I})$, and let $g_\phi(\boldsymbol{\epsilon}, \mathbf{x})$ be the inverse CDF of $q_\phi(\mathbf{z}|\mathbf{x})$. Examples: Exponential, Cauchy, Logistic, Rayleigh, Pareto, Weibull, Reciprocal, Gompertz, Gumbel and Erlang distributions.
2. Analogous to the Gaussian example, for any "location-scale" family of distributions we can choose the standard distribution (with location $= 0$, scale $= 1$) as the auxiliary variable $\boldsymbol{\epsilon}$, and let $g(.) = \text{location} + \text{scale} \cdot \boldsymbol{\epsilon}$. Examples: Laplace, Elliptical, Student's t, Logistic, Uniform, Triangular and Gaussian distributions.
3. Composition: It is often possible to express random variables as different transformations of auxiliary variables. Examples: Log-Normal (exponentiation of normally distributed variable), Gamma (a sum over exponentially distributed variables), Dirichlet (weighted sum of Gamma variates), Beta, Chi-Squared, and F distributions.

Stochastic Gradient Variational Bayes estimator

We can now form Monte Carlo estimates of expectations of some function $f(\mathbf{z})$ w.r.t. $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ as follows:

$$\mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}^{(i)})}\left[f(\mathbf{z})\right] = \mathbb{E}_{p(\boldsymbol{\epsilon})}\left[f(g_{\boldsymbol{\phi}}(\boldsymbol{\epsilon}, \mathbf{x}^{(i)}))\right] \simeq \frac{1}{L}\sum_{l=1}^{L} f(g_{\boldsymbol{\phi}}(\boldsymbol{\epsilon}^{(l)}, \mathbf{x}^{(i)})) \quad \text{where} \quad \boldsymbol{\epsilon}^{(l)} \sim p(\boldsymbol{\epsilon}) \tag{5}$$

We apply this technique to the variational lower bound (eq. (2)), yielding our generic Stochastic Gradient Variational Bayes (SGVB) estimator $\widetilde{\mathcal{L}}^{A}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}^{(i)}) \simeq \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}^{(i)})$:

$$\widetilde{\mathcal{L}}^{A}(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{x}^{(i)}) = \frac{1}{L}\sum_{l=1}^{L} \log p_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}, \mathbf{z}^{(i,l)}) - \log q_{\boldsymbol{\phi}}(\mathbf{z}^{(i,l)}|\mathbf{x}^{(i)})$$

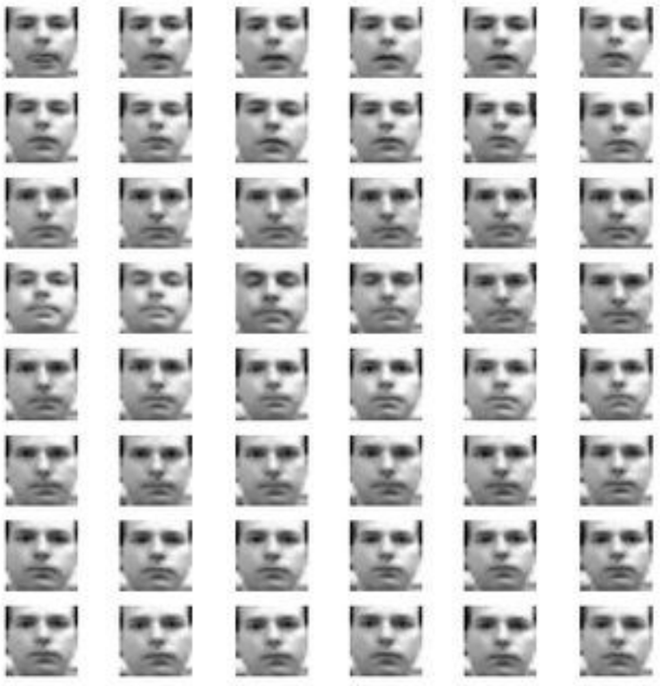
$$\text{where} \quad \mathbf{z}^{(i,l)} = g_{\boldsymbol{\phi}}(\boldsymbol{\epsilon}^{(i,l)}, \mathbf{x}^{(i)}) \quad \text{and} \quad \boldsymbol{\epsilon}^{(l)} \sim p(\boldsymbol{\epsilon}) \tag{6}$$

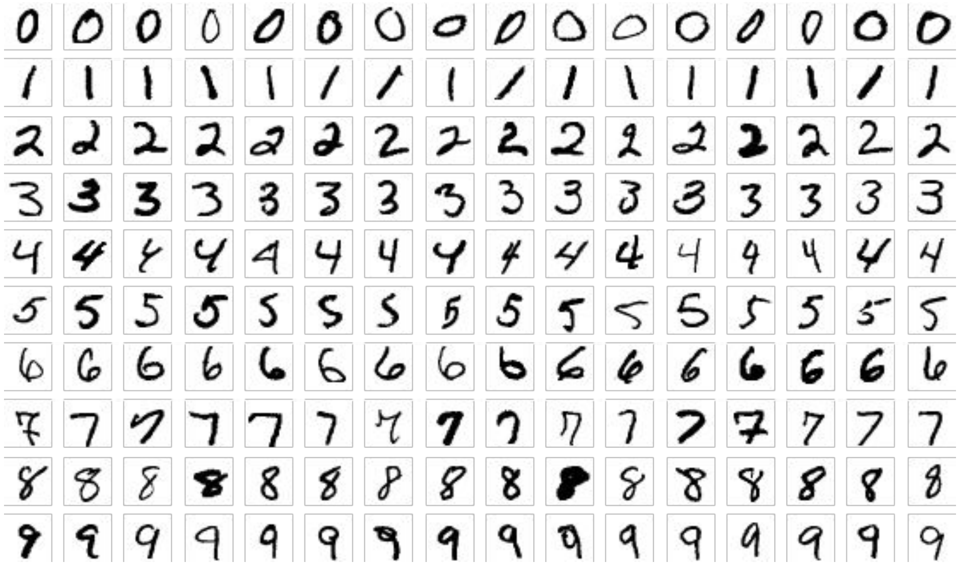
Auto-Encoding Variational Bayesian algorithm

Algorithm 1 Minibatch version of the Auto-Encoding VB (AEVB) algorithm. Either of the two SGVB estimators in section 2.3 can be used. We use settings $M = 100$ and $L = 1$ in experiments.

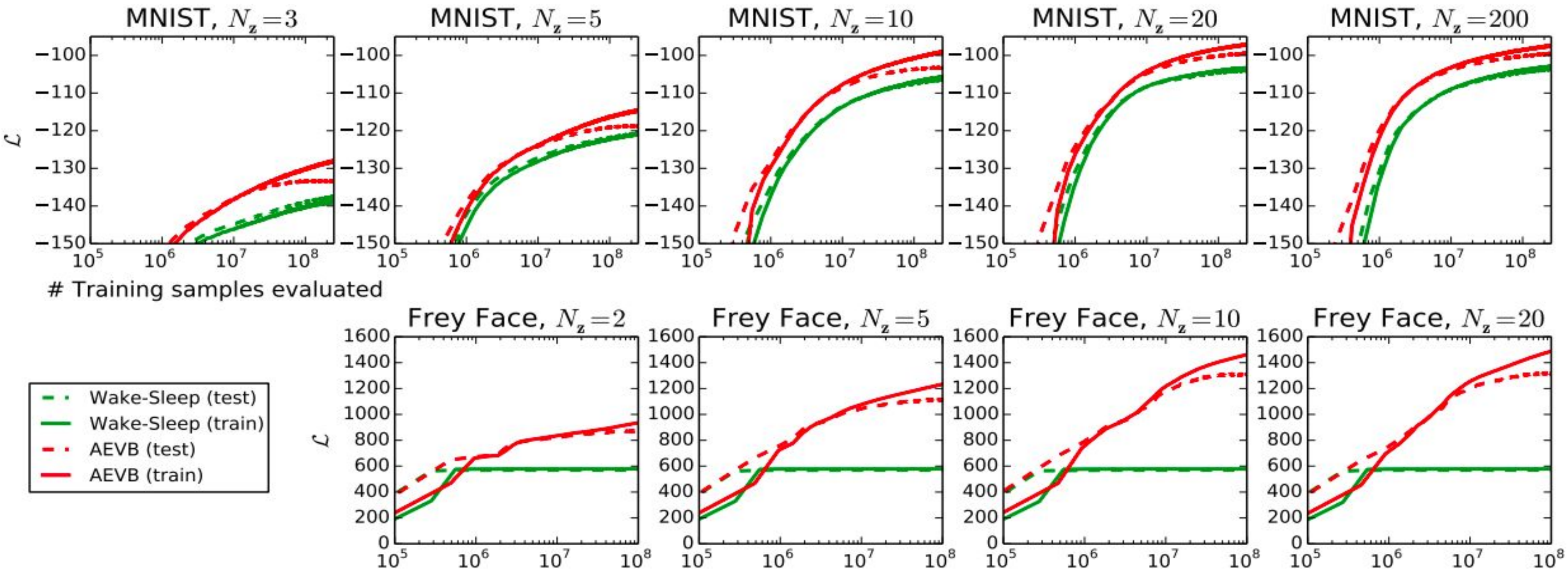
$\boldsymbol{\theta}, \boldsymbol{\phi} \leftarrow$ Initialize parameters
repeat
    $\mathbf{X}^M \leftarrow$ Random minibatch of M datapoints (drawn from full dataset)
    $\boldsymbol{\epsilon} \leftarrow$ Random samples from noise distribution $p(\boldsymbol{\epsilon})$
    $\mathbf{g} \leftarrow \nabla_{\boldsymbol{\theta},\boldsymbol{\phi}} \widetilde{\mathcal{L}}^M(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{X}^M, \boldsymbol{\epsilon})$ (Gradients of minibatch estimator (8))
    $\boldsymbol{\theta}, \boldsymbol{\phi} \leftarrow$ Update parameters using gradients $\mathbf{g}$ (e.g. SGD or Adagrad [DHS10])
until convergence of parameters $(\boldsymbol{\theta}, \boldsymbol{\phi})$
return $\boldsymbol{\theta}, \boldsymbol{\phi}$

Frey Face and MNIST Datasets





Results for Frey Face and MNIST:



Visualisations of learned data manifold for generative models with two-dimensional latent space, learned with AEVB.

(a) 2-D latent space (b) 5-D latent space (c) 10-D latent space (d) 20-D latent space

Thank you for attention