Variational Bayes

Lecture 11

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Outline

- Latent Variable Model and Variational Autoencoders
- Improving the representation power of the variational posterior
- Discrete latent variables and Concrete distribution
- Black-box gradient estimation
- Vector-Quantized Variational Autoencoder

Discriminative vs Generative modeling[1]

Discriminative: $p(y|\mathbf{x})$

Advantages:

1. Solve the problem you are evaluating on
2. Very accurate given a sufficiently large amount of data
3. Effective training procedure

Generative: $p(y, \mathbf{x})$

Advantages:

1. Injection of expert knowledge
2. Could be turned to a discriminator with Bayes rule
3. Facilitates semi/un-supervised learning

[1] Kingma D. et. al, An Introduction to Variational Autoencoders, 2019

Latent Variable Model

Probalistic model:
Given an observed $\mathbf{x} \sim \pi(\mathbf{x})$, where $\pi(\mathbf{x})$ is unknown. We attempt to approximate $\pi(.)$ with a parametric model $p_{\boldsymbol{\theta}}(.)$.

Latent variable model:
Introduce a latent variable $\mathbf{z}$:

$$p_{\boldsymbol{\theta}}(\mathbf{x}) = \int p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) dz.$$

The most common approach:

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

where $p_{\boldsymbol{\theta}}(\mathbf{z})$ is the *prior* distribution.

Example:

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I}), \;\; p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) = \prod_{j=1}^{D} \mathrm{Bern}(x_j | f^j_{\boldsymbol{\theta}}(\mathbf{z})),$$

$$f^j_{\boldsymbol{\theta}}(\mathbf{z}) = \sigma(\mathrm{MLP}(\mathbf{z})_j).$$

Maximul Likelihood Learning:
Given a set of N i.i.d. datapoints $\mathfrak{D} = \{\mathbf{x}_i\}_{i=1}^N$

$$\log p_{\boldsymbol{\theta}}(\mathfrak{D}) = \sum_{\mathbf{x} \in \mathfrak{D}} \log p_{\boldsymbol{\theta}}(\mathbf{x}) \to \max_{\boldsymbol{\theta}} .$$

Intractabilities: the marginal likelihood $p_{\boldsymbol{\theta}}(\mathbf{x})$ is intractable due to the integral.
Note: while $\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\mathbf{x}) = (p_{\boldsymbol{\theta}}(\mathbf{x}))^{-1} \nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) p(\mathbf{z})$ is intractable ($p_{\boldsymbol{\theta}}(\mathbf{z}) = p(\mathbf{z})$ for simplicity)

Evidence Lower Bound (ELBO)

Challenge: the intractability of $\log p_{\theta}(\mathbf{x})$.
Solution: variational lower bound. First, note that $p_{\theta}(\mathbf{x})$ is tractable $\Leftrightarrow$ $p_{\theta}(\mathbf{z}|\mathbf{x}) = p_{\theta}(\mathbf{x}, \mathbf{z}) / p_{\theta}(\mathbf{x})$ is tractable.
Second, introduce a parametric *variational distribution* $q_{\phi}(\mathbf{z}|\mathbf{x})$, where ϕ is the vector of *variational parameters*. So, derive the lower bound

$$
\begin{aligned}
\log p_{\theta}(\mathbf{x}) &= \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \log p_{\theta}(\mathbf{x}) \\
&= \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \log \frac{p_{\theta}(\mathbf{x}, \mathbf{z}) q_{\phi}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x}) p_{\theta}(\mathbf{z}|\mathbf{x})} \\
&= \underbrace{\mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \log \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})}}_{\mathcal{L}_{\theta,\phi}(\mathbf{x})} + \underbrace{\mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\theta}(\mathbf{z}|\mathbf{x})}}_{\mathrm{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) || p_{\theta}(\mathbf{z}|\mathbf{x})) \geq 0}
\end{aligned}
$$

Here $\mathcal{L}_{\theta,\phi}(\mathbf{x})$ is the *variational lower bound*.

Proposition (Evidence Lower Bound)

$$
p_{\theta}(\mathbf{x}) \geq \mathcal{L}_{\theta,\phi}(\mathbf{x}) = \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \log \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})}
$$

Note 1: The gap between ELBO and the marginal likelihood is called the *tightness of the bound*. The better $q_{\phi}(\mathbf{z}|\mathbf{x})$ approximates the true posterior $p_{\theta}(\mathbf{z}|\mathbf{x})$ (in terms of KL), the closer the gap.
Note 2: We will show that there are tractable gradients of ELBO w.r.t. $\boldsymbol{\theta}, \boldsymbol{\phi}$.

Stochastic Gradient-Based optimization of the ELBO

Unbiased gradient of ELBO w.r.t the generative model parameters

$$
\begin{aligned}
&\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\boldsymbol{\theta},\phi}(\mathbf{x}) \\
&= \nabla_{\boldsymbol{\theta}} \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})] \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z}) \\
&\approx \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\mathbf{x},\hat{\mathbf{z}}),\ \hat{\mathbf{z}} \sim q_\phi(\mathbf{z}|\mathbf{x}).
\end{aligned}
$$

Reparametrization trick: First, assume that we can express $\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})$ as $\mathbf{z} = \mathbf{g}(\epsilon,\phi,\mathbf{x})$, $\epsilon \sim p(\epsilon)$, where $\mathbf{g}$ is differentiable w.r.t. ϕ, i.e. $q_\phi(\mathbf{z}|\mathbf{x})$ is *reparametrizable*. Also assume that $f(.)$ is differentiable. Let $\hat{\epsilon} \sim p(\epsilon)$.

$$
\begin{aligned}
&\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} f(\mathbf{z}) = \nabla_\phi \mathbb{E}_{p(\epsilon)} f(\mathbf{g}(\epsilon,\phi,\mathbf{x})) \\
&= \mathbb{E}_{p(\epsilon)} \nabla_\phi f(\mathbf{g}(\epsilon,\phi,\mathbf{x})) \approx \nabla_\phi f(\mathbf{g}(\hat{\epsilon},\phi,\mathbf{x}))
\end{aligned}
$$

Unbiased gradient of ELBO w.r.t. the variational parameters

$$
\begin{aligned}
&\nabla_\phi \mathcal{L}_{\boldsymbol{\theta},\phi}(\mathbf{x}) \\
&= \nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})] \\
&= \mathbb{E}_{p(\epsilon)}[\nabla_\phi \log p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z}) - \nabla_\phi \log q_\phi(\mathbf{z}|\mathbf{x})]\big|_{\mathbf{z}=\mathbf{g}(\epsilon,\phi,\mathbf{x})} \\
&\approx [\nabla_\phi \log p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z}) - \nabla_\phi \log q_\phi(\mathbf{z}|\mathbf{x})]\big|_{\mathbf{z}=\mathbf{g}(\hat{\epsilon},\phi,\mathbf{x}),\ \hat{\epsilon}\sim p(\epsilon)}
\end{aligned}
$$

Note: also assume that we have access to $q_\phi(\mathbf{z}|\mathbf{x})$, $\nabla_{\mathbf{z}} \log q_\phi(\mathbf{z}|\mathbf{x})$, and $\nabla_\phi \log q_\phi(\mathbf{z}|\mathbf{x})$.
Example: $q_\phi(\mathbf{z}|\mathbf{x}) = \prod_{i=1}^{\dim \mathbf{z}} \mathcal{N}(z_i|\mu_i,\sigma_i^2)$.

Optimimazion of the ELBO

Factorized Gaussian posterior: a common choice of $q_\phi(\mathbf{z}|\mathbf{x})$ is a factorized Gaussian

$$(\boldsymbol{\mu}, \log \boldsymbol{\sigma}) = \mathrm{MLP}_\phi(\mathbf{x}), \; q_\phi(\mathbf{z}|\mathbf{x}) = \prod_{i=1}^{\dim \mathbf{z}} \mathcal{N}(z_i|\mu_i, \sigma_i^2),$$

$$\mathbf{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\epsilon}.$$

Limitation: factorized distribuions are not flexible. By increasing the flexibility of $q_\phi(\mathbf{z}|\mathbf{x})$, we improve the tightness of the ELBO $(\mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})))$.

Optimization problem

$$\log p_\theta(\mathfrak{D}) \geq \sum_{\mathbf{x} \in \mathfrak{D}} \mathcal{L}_{\theta,\phi}(\mathbf{x}) \to \max_{\theta,\phi}.$$

Data: $\mathfrak{D} = \{\mathbf{x}_i\}_{i=1}^N$
Result: learned $\boldsymbol{\theta}, \boldsymbol{\phi}$
$\boldsymbol{\theta}, \boldsymbol{\phi} \leftarrow$ initialization;
while *not converged* **do**
- $\mathbf{x}_{1:M} \leftarrow$ random minibatch of M datapoints;
- $\boldsymbol{\epsilon} \leftarrow$ sample random noise from $p(\boldsymbol{\epsilon})$;
- $\hat{\mathbf{g}} \leftarrow$ stochastic gradients of $\mathcal{L}_{\theta,\phi}(\mathbf{x})$ w.r.t $\boldsymbol{\theta}, \boldsymbol{\phi}$;
- $\boldsymbol{\theta}, \boldsymbol{\phi} \leftarrow$ update parameters using $\hat{\mathbf{g}}$

end

Algorithm 1: Minibatch version of the Auto-Encoding VB

Estimation of the Marginal Likelihood

Theorem

For all $k \geq 1$ the following is true:

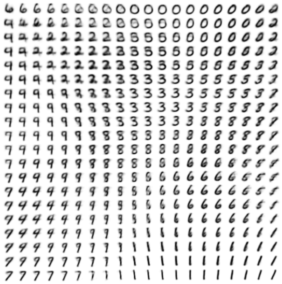
$$\log p(\mathbf{x}) \geq \mathcal{L}_{k+1}(\mathbf{x}) \geq \mathcal{L}_k(\mathbf{x}),$$

$$\mathcal{L}_k(\mathbf{x}) := \mathbb{E}_{\mathbf{z}_{1:k} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \log \left(\frac{1}{k} \sum_{i=1}^{k} \frac{p_{\theta}(\mathbf{x}, \mathbf{z}_i)}{q_{\phi}(\mathbf{z}_i|\mathbf{x})} \right).$$

Moreover, if $p_{\theta}(\mathbf{x}, \mathbf{z}) / q_{\phi}(\mathbf{z}|\mathbf{x})$ is bounded, then $\mathcal{L}_k(\mathbf{x})$ approaches $\log p(\mathbf{x})$ as k goes to infinity.

Sampling[a]

$$\mathbf{x} \sim p_{\theta}(\mathbf{x}) \Leftrightarrow \mathbf{z} \sim p_{\theta}(\mathbf{z}), \ \mathbf{x} \sim p_{\theta}(\mathbf{x}|\mathbf{z}).$$



[a]Kingma D. et. al, Auto-Encoding Variational Bayes, 2014

[2]Burda Y. et. al, Importance Weighted Autoencoders, 2016

Semi-Implicit Variational Inference[3]

Challenge: the representation power of the variational family is limited by the assumption that $q(\mathbf{z}|\mathbf{x})$ is factorizable.
Solution: introduce a mixing distribution on the parameters on the original $q(\mathbf{z}|\mathbf{x})$.

$$
\begin{aligned}
&\mathcal{H} := \{h_{\phi}(\mathbf{z}) \; : \; h_{\phi}(\mathbf{z}) = \mathbb{E}_{q_{\phi}(\boldsymbol{\psi})} q(\mathbf{z}|\boldsymbol{\psi})\}, \\
&q(\mathbf{z}|\boldsymbol{\psi}) \quad \text{explicit and reparametrizable}, \\
&q_{\phi}(\boldsymbol{\psi}) \quad \text{implicit and reparametrizable}, \\
&\Rightarrow h_{\phi}(\mathbf{z}) \quad \text{implicit in the general case}
\end{aligned}
$$

Lower bound of ELBO:

$$
\mathrm{ELBO} = \mathbb{E}_{\mathbf{z} \sim h_{\phi}(\mathbf{z})} \log \frac{p(\mathbf{x}, \mathbf{z})}{h_{\phi}(\mathbf{z})} =
$$

$$
\log p(\mathbf{x}) - \mathrm{KL}(\mathbb{E}_{\boldsymbol{\psi} \sim q_{\phi}(\boldsymbol{\psi})} q(\mathbf{z}|\boldsymbol{\psi}) || p(\mathbf{z}|\mathbf{x})) \geq
$$

$$
- \mathbb{E}_{\boldsymbol{\psi} \sim q_{\phi}(\boldsymbol{\psi})} \mathrm{KL}(q(\mathbf{z}|\boldsymbol{\psi}) || p(\mathbf{z}|\mathbf{x})) + \log p(\mathbf{x}) =
$$

$$
\mathbb{E}_{\boldsymbol{\psi} \sim q_{\phi}(\boldsymbol{\psi})} \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\boldsymbol{\psi})} \log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\boldsymbol{\psi})} =: \underline{\mathcal{L}}(q(\mathbf{z}|\boldsymbol{\psi}), q_{\phi}(\boldsymbol{\psi}))
$$

Theorem

Let $\boldsymbol{\psi}^* = \arg\max_{\boldsymbol{\psi}} \mathbb{E}_{q(\mathbf{z}|\boldsymbol{\psi})} \frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z}|\boldsymbol{\psi})}$. *Then*

$$
\max_{q_{\phi}(\boldsymbol{\psi})} \underline{\mathcal{L}}(q(\mathbf{z}|\boldsymbol{\psi}), q_{\phi}(\boldsymbol{\psi})) = \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\boldsymbol{\psi}^*)} \log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\boldsymbol{\psi}^*)},
$$

$$
\arg\max_{q_{\phi}(\boldsymbol{\psi})} \underline{\mathcal{L}}(q(\mathbf{z}|\boldsymbol{\psi}), q_{\phi}(\boldsymbol{\psi})) = \delta(\boldsymbol{\psi} - \boldsymbol{\psi}^*)
$$

Therefore, SIVI degenerates to vanilla VI.

[3]Yin M. et. al, Semi-Implicit Variational Inference, 2018

Introduce a regularizer:

$$B_K := \mathbb{E}_{\psi, \psi^{(1:K)} \sim q_\phi(\psi)} \mathrm{KL}(q(\mathbf{z}|\psi) || \tilde{h}_K(\mathbf{z})),$$

$$\tilde{h}_K(\mathbf{z}) := \frac{1}{K+1} \left(q(\mathbf{z}|\psi) + \sum_{k=1}^{K} q(\mathbf{z}|\psi^{(k)}) \right)$$

Note that $B_K = 0 \Leftrightarrow K = 0$ or $q_\phi(\psi) = \delta(\psi - \mathbf{a})$.

Theorem

$$\lim_{K \to \infty} (\mathcal{L} + B_K) = \mathrm{ELBO} = \mathbb{E}_{\mathbf{z} \sim h_\phi(\mathbf{z})} \log \frac{p(\mathbf{x}, \mathbf{z})}{h_\phi(\mathbf{z})}.$$

Informal intuition: use the strong law of large numbers:

$$\lim_{K \to \infty} B_K = \mathbb{E}_{\psi \sim q_\phi(\psi)} \mathrm{KL}(q(\mathbf{z}|\psi) || h_\phi(\mathbf{z})).$$

$$\Rightarrow \mathcal{L} + B_\infty = \mathbb{E}_{\psi \sim q_\phi(\psi)} \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\psi)} \log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\psi)} +$$

$$\mathbb{E}_{\psi \sim q_\phi(\psi)} \mathrm{KL}(q(\mathbf{z}|\psi) || h_\phi(\mathbf{z})) =$$

$$\mathbb{E}_{\psi \sim q_\phi(\psi)} \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\psi)} \left(\log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\psi)} + \log \frac{q(\mathbf{z}|\psi)}{h_\phi(\mathbf{z})} \right) =$$

$$\mathbb{E}_{\mathbf{z} \sim h_\phi(\mathbf{z})} \log \frac{p(\mathbf{x}, \mathbf{z})}{h_\phi(\mathbf{z})} = \mathrm{ELBO}$$

Semi-Implicit Variational Inference: evaluation

Negative binomial model

$$x_i \sim \mathrm{NB}(r, p), \;\; r \sim \mathrm{Gamma}(a, 1/b),$$
$$p \sim \mathrm{Beta}(\alpha, \beta), \;\; a = b = \alpha = \beta = 0.01.$$

Therefore, the posterior $p(r, p | x_1, \dots, x_n)$ is intractable.

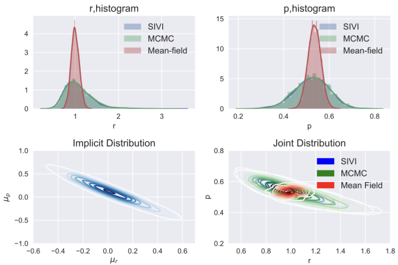
Mean-Field VI

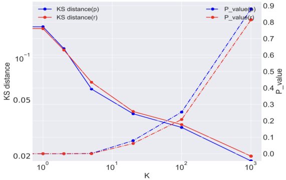
$$q(r, p) = \mathrm{Gamma}(r | \tilde{a}, 1/\tilde{b}) \mathrm{Beta}(p | \tilde{\alpha}, \tilde{\beta}).$$

SIVI:

$$q(r, p | \psi) = \mathrm{LogNorm}(r | \mu_r, \sigma_0^2) \mathrm{LogitNorm}(p | \mu_p, \sigma_0^2),$$
$\psi = (\mu_r, \mu_p) \sim q(\psi)$ is MLP-based.

The model is trained with $K = 1000$.





We see that $K = 20$ achieves a nice compromise between complexity and accuracy.

A Continuous relaxation of discrete random variables[4]

Challenge: discrete random variables lack useful reparameterizations due to the discontinuous nature of discrete states.
Solution: introduce Concrete random variables.
Background: Reparametrization trick:

$$\mathbb{E}_{x \sim p_\phi(x)} f(x) \to \min_\phi .$$

Assume that f is differentiable w.r.t x, $x \sim p_\phi(x) \Leftrightarrow z \sim p(z)$, $x = g_\phi(z)$, and $g_\phi(.)$ is differentiable w.r.t. ϕ.

$$\hat{\nabla}_\phi \mathbb{E}_{x \sim p_\phi(x)} f(x) = \frac{\partial f}{\partial g_\phi(z)} \frac{\partial g_\phi(z)}{\partial \phi}.$$

Gumbel-Max trick

$$d \sim \mathrm{Cat}(\alpha_1, \dots, \alpha_n) \Leftrightarrow$$
$$d = \arg\max_{k=\overline{1,n}} (\log \alpha_k \underbrace{- \log(- \log u_k)}_{g_k \sim \mathrm{Gumbel}(0,1)}),$$
$$u_k \overset{i.i.d.}{\sim} \mathcal{U}[0, 1].$$

Concrete random variable: given $\boldsymbol{\alpha} \in \mathbb{R}^n_{++}$

$$\mathbf{x} := \mathrm{softmax}((\log \boldsymbol{\alpha} + \mathbf{g})/\lambda) \sim \mathrm{Concrete}(\boldsymbol{\alpha}, \lambda),$$
$$\{g_i\} \overset{i.i.d.}{\sim} \mathrm{Gumbel}(0, 1),$$
$$\lambda \in \mathbb{R}_{++} \text{ temperature parameter.}$$

The $\mathrm{softmax}$ approaches $\arg\max$ as $\lambda \to 0$.

[4] Maddison C. et. al, The Concrete Distribution: A Continuous relaxation of discrete random variables, 2017

Properties of Concrete distribution

Theorem

The following is true for $\mathbf{x} \sim \mathrm{Concrete}(\boldsymbol{\alpha}, \lambda)$

- *(Rounding)* $\mathbb{P}(x_k > x_i, \; i \neq k) = \frac{\alpha_k}{\sum_{i=1}^n \alpha_i}$.
- *(Zero Temperature)* $\mathbb{P}(\lim_{\lambda \to 0} x_k = 1) = \frac{\alpha_k}{\sum_{i=1}^n \alpha_i}$.
- *(Convex eventually) if* $\lambda \leq (n-1)^{-1}$, *then* $p(\mathbf{x}|\boldsymbol{\alpha}, \lambda)$ *is log-convex in* $\mathbf{x}$.

Note: for any $\lambda > 0$ the gradient estimator is biased. The temperature sets a tradeoff between the bias and the variance of the estimator. The higher λ, the greater the bias.

VAE with a single discrete latent variable:

$$
q_\phi(d|\mathbf{x}) = \mathrm{Cat}(d|f_\theta(\mathbf{x})),
$$

$$
\mathbb{E}_{d \sim q_\phi(d|\mathbf{x})} \log \frac{p_\theta(\mathbf{x}, d)}{q_\phi(d)} \overset{relax}{\rightsquigarrow}
$$

$$
\mathbb{E}_{\mathbf{z} \sim q_{\boldsymbol{\alpha},\lambda}(\mathbf{z}|\mathbf{x},\phi)} \log \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_{\boldsymbol{\alpha},\lambda}(\mathbf{z}|\mathbf{x},\phi)}.
$$

Note that we assumed that $p(\mathbf{x}, \mathbf{z})$ is feasible, i.e. the decoder is able to condition on relaxed variable $\mathbf{z}$.

Continuous relaxation: evaluation

Setup: VAE with discrete latent variables. More specifically, the task is to predict the bottom half $\mathbf{x}_1$ of a MNIST image given the upper one $\mathbf{x}_2$. Consider IWAE objective with the prior $p_\theta(\mathbf{z}|\mathbf{x}_2)$ as the variational distribution.

$$\mathcal{L}_m(\mathbf{x}_1, \mathbf{x}_2) = \mathbb{E}_{\mathbf{z}_{1:m} \sim p_\theta(\mathbf{z}|\mathbf{x}_2)} \log \left(\frac{1}{m} \sum_{i=1}^{m} p_\theta(\mathbf{x}_1|\mathbf{z}_i) \right).$$

Comparison with a baseline

binary model	m	Test NLL Concrete	Test NLL VIMCO	Train NLL Concrete	Train NLL VIMCO
(392V–240H –240H–392V)	1	**58.5**	61.4	**54.2**	59.3
	5	**54.3**	54.5	**49.2**	52.7
	50	53.4	**51.8**	**48.2**	49.6
(392V–240H –240H–240H –392V)	1	**56.3**	59.7	**51.6**	58.4
	5	**52.7**	53.5	**46.9**	51.6
	50	52.0	**50.2**	**45.9**	47.9

It could be clearly seen that the proposed Concrete estimator outperforms the baseline.

Black-box gradient estimation[5]

Challenge: backpropagation w.r.t. encoder parameters could not be applied in case of discrete latent variables
Solution: introduce a learnable free-form control variate parameterized by a neural network.
Background: gradient estimators

$$\mathbb{E}_{p(b|\theta)}[f(b)] \to \min_{\theta} \Leftarrow \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z}),$$

$$\hat{g}_{\text{reinf}}[f] := f(b)\frac{\partial}{\partial\theta} \log p(b|\theta), \quad b \sim p(b|\theta),$$

$$\hat{g}_{\text{reparam}}[f] := \frac{\partial}{\partial\theta} f(b) = \frac{\partial f}{\partial T}\frac{\partial T(\theta, \epsilon)}{\partial\theta}, \; \epsilon \sim p(\epsilon).$$

Control variates: reduces the variance of a stochastic estimator.

$$\hat{g}_{\text{new}}(b) := \hat{g}(b) - c(b) + \mathbb{E}_{p(b|\theta)}[c(b)].$$

Constructing a differentiable surrogate: Assume that b - continuous and $b = T(\theta, \epsilon)$, $\epsilon \sim p(\epsilon)$; given c_ϕ, a differentiable surrogate of f, but f cannot be differentiated.

$$\hat{g}_{\text{LAX}} := \hat{g}_{\text{reinf}}[f] - \hat{g}_{\text{reinf}}[c_\phi] + \hat{g}_{\text{reparam}}[c_\phi] =$$
$$[f(b) - c_\phi(b)]\frac{\partial}{\partial\theta} \log p(b|\theta) + \frac{\partial}{\partial\theta} c_\phi(b).$$

Note that the estimator is unbiased for any c_ϕ.

[5] Grathwohl W. et. al, Backpropagation Through The Void: Optimizing Control Variates For Black-Box Gradient Estimation, 2018

Gradient-based optimization of the control variate:

$$\frac{\partial}{\partial \phi}\mathbb{V}[\hat{g}] = \frac{\partial}{\partial \phi}\mathbb{E}[\hat{g}^2] - \underbrace{\frac{\partial}{\partial \phi}\mathbb{E}[\hat{g}]^2}_{=0} = \mathbb{E}\left[\frac{\partial}{\partial \phi}\hat{g}^2\right].$$

So, we can directly minimize the variance of a gradient estimator. We alternate between θ and ϕ updates.

Discrete random variables and conditional reparametrization: let b be a discrete random variable. Introduce a "relaxed" continuous reparametrizable $z \sim p(z|\theta)$, $H(z) = b$, $b \sim p(b|\theta)$, where $H(.)$ is a deterministic mapping.

Theorem: The proposed $\hat{g}_{\text{relax}}$ is unbiased for any c_ϕ.

$$\underbrace{[f(b) - c_\phi(\tilde{z})]\frac{\partial}{\partial \theta}\log p(b|\theta) + \frac{\partial}{\partial \theta}c_\phi(z) - \frac{\partial}{\partial \theta}c_\phi(\tilde{z})}_{\hat{g}_{\text{relax}}},$$

where $b = H(z)$, $z \sim p(z|\theta)$, $\tilde{z} \sim p(z|b,\theta)$.

Example: when $p(b|\theta) = \mathrm{Be}(\theta)$, $H(z) = \mathbf{1}[z > 0]$.

$$z = \log\frac{\theta}{1-\theta} + \log\frac{u}{1-u} \sim p(z|\theta),\ u \sim \mathcal{U}[0,1],$$

$$\tilde{z} = \log\frac{\theta}{1-\theta} + \log\frac{v'}{1-v'} \sim p(z|b,\theta),$$

$$v' = v[(1-\theta)(1-b) + \theta b] + (1-\theta)b, v \sim \mathcal{U}[0,1].$$

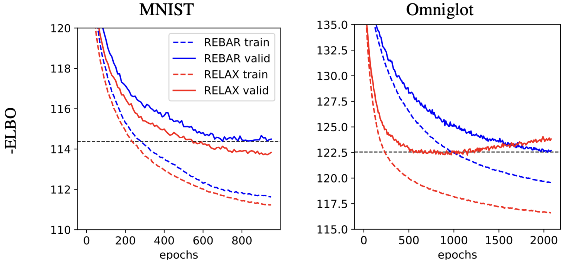
VAE with Bernoulli latent varibles

One-layer linear model

$$q(b_i|\mathbf{x}) = \mathrm{Be}(\sigma(\mathbf{W}_q\mathbf{x} + b_q)),$$
$$p(\mathbf{x}|\mathbf{b}) = \mathrm{Be}(\sigma(\mathbf{W}_p\mathbf{b} + \mathbf{b}_p)).$$

Dataset	Model	Concrete	NVIL	MuProp	REBAR	RELAX
MNIST	Nonlinear	−102.2	−101.5	-101.1	-81.01	**-78.13**
	linear one-layer	-111.3	−112.5	−111.7	-111.6	**-111.20**
	linear two-layer	-99.62	−99.6	−99.07	-98.22	**-98.00**
Omniglot	Nonlinear	−110.4	−109.58	-108.72	-56.76	**-56.12**
	linear one-layer	-117.23	−117.44	−117.09	-116.63	**-116.57**
	linear two-layer	-109.95	−109.98	−109.55	-108.71	**-108.54**

Training curves



The proposed approach improved validation performance as well increased convergence speed.

Vector Quantised - Variational AutoEncoder[6]

Challenge: the latent codes $\mathbf{z}$ are ignored when they are paired with a powerful decoder $p(\mathbf{x}|\mathbf{z})$ in VAE framework.

Solution: introduce a discrete latent model VQ-VAE.

Posterior collapse

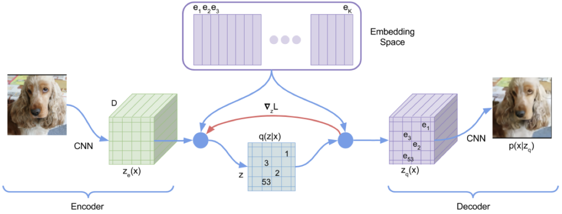
The posterior of $\mathbf{z}$ is collapses if $q_\phi(\mathbf{z}|\mathbf{x}) = p(\mathbf{z})$. So, when posterior collapse occurs, it prevents the latent variable from providing meaningful summary of the dataset.

The variational distribution Given a latent embeddings space $\mathbf{E} \in \mathbb{R}^{K \times D}$ and a deterministic encoder $\mathbf{z}_e : \mathbb{R}^{\dim \mathbf{x}} \to \mathbb{R}^D$.

Define the variational posterior by a nearest-neighbour look-up using $\mathbf{E}$:

$$q(z = k|\mathbf{x}) = \begin{cases} 1, & k = \arg\min_j \|\mathbf{z}_e(\mathbf{x}) - \mathbf{e}_j\|_2, \\ 0, & \text{otherwise.} \end{cases}$$

Define a latent variable $\mathbf{z}_q = \mathbf{e}_k$, $k = \arg\min_j \|\mathbf{z}_e(\mathbf{x}) - \mathbf{e}_j\|_2$.



[6] van den Oord A. et. al, Neural Discrete Representation Learning, 2018

Deriving the ELBO

$$\mathcal{L}_{\boldsymbol{\theta},\boldsymbol{\phi}} = \mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}[\log p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) - \log q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})]$$
$$= \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}_q)p(\mathbf{z}_q) \propto \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}_q) \rightarrow \max_{\boldsymbol{\phi},\boldsymbol{\theta},\mathbf{E}}.$$

Note that arg max is not differentiable, so copy gradients from decoder input $\mathbf{z}_q$ to encoder output $\mathbf{z}_e$.

Challenge: $\mathbf{E}$ receive no gradients due to the straight-through gradient.

Solution: Vector Quantization

$$\mathcal{L}_{\text{total}}(\mathbf{x}) = \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}_q) + \|\mathrm{sg}(\mathbf{z}_e(\mathbf{x})) - \mathbf{e}_k\|_2^2$$
$$+ \beta\|\mathbf{z}_e(\mathbf{x}) - \mathrm{sg}(\mathbf{e}_k)\|_2^2,$$

where $\mathrm{sg}(.)$ is the stop gradient operation. The last term is a *commitment loss*. The loss ensures that the outputs of the encoder do not grow.

The prior:

During training $p(\mathbf{z}_q)$ kept constant and uniform. Subsequently, learn an autoregressive prior $p(\mathbf{z})$ when there are more than one latent variable.

Summary

- Latent Variable Model
- An introduction to Variational Autoencoders
- Semi-Implicit Variational Inference
- Continuous relaxation and Concrete distribution
- Black-box gradient estimator and RELAX
- VQ-VAE