Deep Generative Models

Lecture 4

Roman Isachenko

Ozon Masters

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Recap of previous lecture

Variational lower Bound (ELBO)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) \geq \mathcal{L}(q, \boldsymbol{\theta}).$$

$$\mathcal{L}(q, \boldsymbol{\theta}) = \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z})||p(\mathbf{z}))$$

Log-likelihood decomposition

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z})||p(\mathbf{z})) + KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).$$

▶ Instead of maximizing incomplete likelihood, maximize ELBO

$$\max_{\boldsymbol{\theta}} p(\mathbf{x}|\boldsymbol{\theta}) \quad \rightarrow \quad \max_{q, \boldsymbol{\theta}} \mathcal{L}(q, \boldsymbol{\theta})$$

▶ Maximization of ELBO by variational distribution q is equivalent to minimization of KL

$$\max_q \mathcal{L}(q, \boldsymbol{\theta}) \equiv \min_q KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).$$

Recap of previous lecture

EM-algorithm

- E-step

$$q^*(\mathbf{z}) = \arg\max_q \mathcal{L}(q, \boldsymbol{\theta}^*) = \arg\min_q KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*));$$

- M-step

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \mathcal{L}(q^*, \boldsymbol{\theta});$$

Amortized variational inference

Restrict a family of all possible distributions $q(\mathbf{z})$ to a parametric class $q(\mathbf{z}|\mathbf{x}, \phi)$ conditioned on samples $\mathbf{x}$ with parameters ϕ.

Variational Bayes

- E-step

$$\phi_k = \phi_{k-1} + \eta \nabla_{\phi} \mathcal{L}(\phi, \boldsymbol{\theta}_{k-1})|_{\phi = \phi_{k-1}}$$

- M-step

$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} + \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}(\phi_k, \boldsymbol{\theta})|_{\boldsymbol{\theta} = \boldsymbol{\theta}_{k-1}}$$

Recap of previous lecture

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q(z|x,\phi)} \left[\log p(x|z, \theta) - \log \frac{q(z|x, \phi)}{p(z)} \right] \to \max_{\phi, \theta}.$$

M-step: $\nabla_\theta \mathcal{L}(\phi, \theta)$, Monte Carlo estimation

$$\nabla_\theta \mathcal{L}(\phi, \theta) = \int q(z|x, \phi) \nabla_\theta \log p(x|z, \theta) dz \approx$$
$$\approx \nabla_\theta \log p(x|z^*, \theta), \quad z^* \sim q(z|x, \phi).$$

E-step: $\nabla_\phi \mathcal{L}(\phi, \theta)$, reparametrization trick

$$\nabla_\phi \mathcal{L}(\phi, \theta) = \int r(\epsilon) \nabla_\phi \log p(x|g(x, \epsilon, \phi), \theta) d\epsilon - \nabla_\phi \text{KL}$$
$$\approx \nabla_\phi \log p(x|g(x, \epsilon^*, \phi), \theta) - \nabla_\phi \text{KL}$$

Variational assumption

$$r(\epsilon) = \mathcal{N}(0, I); \quad q(z|x, \phi) = \mathcal{N}(\mu_\phi(x), \sigma_\phi^2(x)).$$
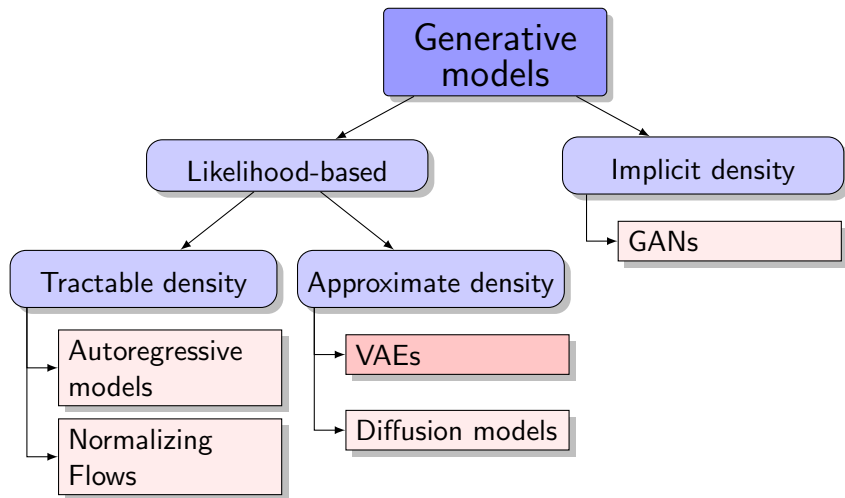$$z = g(x, \epsilon, \phi) = \sigma_\phi(x) \cdot \epsilon + \mu_\phi(x).$$

Outline

1. Variational autoencoder (VAE)

2. Posterior collapse and decoder weakening techniques

3. Tighter variational bound

Outline

Generative models zoo

Variational autoencoder (VAE)

Final algorithm

▶ pick random sample $\mathbf{x}_i$, $i \sim U[1, n]$.

▶ compute the objective:

$$\boldsymbol{\epsilon}^* \sim r(\boldsymbol{\epsilon}); \quad \mathbf{z}^* = g(\mathbf{x}, \boldsymbol{\epsilon}^*, \boldsymbol{\phi});$$

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) \approx \log p(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\theta}) - KL(q(\mathbf{z}^*|\mathbf{x}, \boldsymbol{\phi})||p(\mathbf{z}^*)).$$

▶ compute a stochastic gradients w.r.t. $\boldsymbol{\phi}$ and $\boldsymbol{\theta}$

$$\nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) \approx \nabla_{\boldsymbol{\phi}} \log p(\mathbf{x}|g(\mathbf{x}, \boldsymbol{\epsilon}^*, \boldsymbol{\phi}), \boldsymbol{\theta}) - \nabla_{\boldsymbol{\phi}} KL(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})||p(\mathbf{z}));$$
$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) \approx \nabla_{\boldsymbol{\theta}} \log p(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\theta}).$$

▶ update $\boldsymbol{\theta}, \boldsymbol{\phi}$ according to the selected optimization method (SGD, Adam, RMSProp):

$$\boldsymbol{\phi} := \boldsymbol{\phi} + \eta \nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}),$$
$$\boldsymbol{\theta} := \boldsymbol{\theta} + \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}).$$

Variational autoencoder (VAE)

- ▶ VAE learns stochastic mapping between **x**-space, from complicated distribution $\pi(\mathbf{x})$, and a latent **z**-space, with simple distribution.

- ▶ The generative model learns a joint distribution $p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$, with a prior distribution $p(\mathbf{z})$, and a stochastic decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$.

- ▶ The stochastic encoder $q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})$ (inference model), approximates the true but intractable posterior $p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})$ of the generative model.

Kingma D. P., Welling M. An introduction to variational autoencoders, 2019
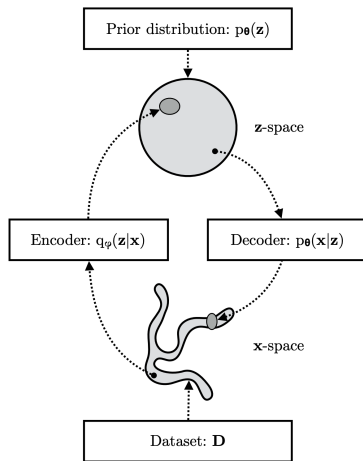
Variational Autoencoder
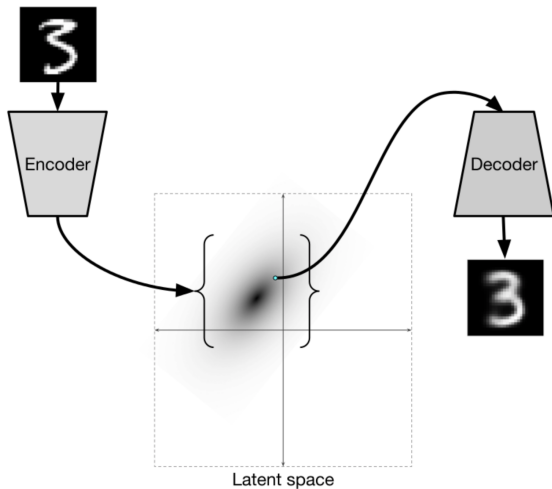
Variational autoencoder (VAE)

- ▶ Encoder $q(\mathbf{z}|\mathbf{x}, \phi) = \text{NN}_e(\mathbf{x}, \phi)$ outputs $\boldsymbol{\mu}_\phi(\mathbf{x})$ and $\boldsymbol{\sigma}_\phi(\mathbf{x})$.
- ▶ Decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \text{NN}_d(\mathbf{z}, \boldsymbol{\theta})$ outputs parameters of the sample distribution.
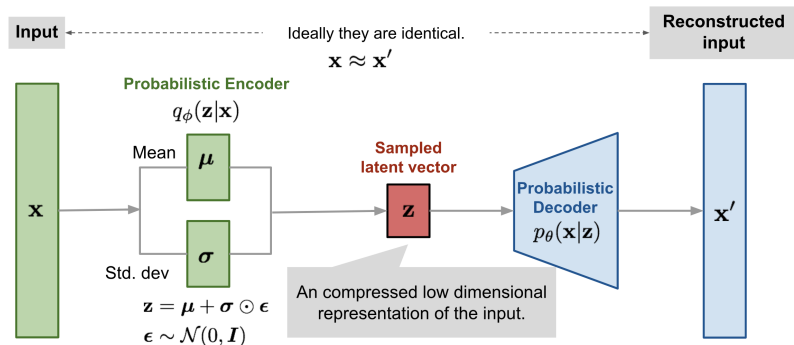

image credit:
https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

VAE limitations

▶ Poor generative distribution (decoder)

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\sigma}^2_{\boldsymbol{\theta}}(\mathbf{z})).$$

▶ Loose lower bound

$$\log p(\mathbf{x}|\boldsymbol{\theta}) - \mathcal{L}(q, \boldsymbol{\theta}) = (?).$$

▶ Poor prior distribution

$$p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I}).$$

▶ Poor variational posterior distribution (encoder)

$$q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_{\boldsymbol{\phi}}(\mathbf{x}), \boldsymbol{\sigma}^2_{\boldsymbol{\phi}}(\mathbf{x})).$$

VAE as Bayesian model

Posterior distribution

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{X})}$$

ELBO

$$
\begin{aligned}
\log p(\boldsymbol{\theta}|\mathbf{X}) &= \log p(\mathbf{X}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta}) - \log p(\mathbf{X}) \\
&= \mathcal{L}(q, \boldsymbol{\theta}) + KL(q||p) + \log p(\boldsymbol{\theta}) - \log p(\mathbf{X}) \\
&\geq [\mathcal{L}(q, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta})] - \log p(\mathbf{X}).
\end{aligned}
$$

EM-algorithm

▶ E-step

$$q(\mathbf{z}) = \arg\max_{q} \mathcal{L}(q, \boldsymbol{\theta}^*) = \arg\min_{q} KL(q||p) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*);$$

▶ M-step

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} [\mathcal{L}(q, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta})].$$

Outline

VAE limitations

▶ **Poor generative distribution (decoder)**

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu_\theta}(\mathbf{z}), \boldsymbol{\sigma_\theta^2}(\mathbf{z})).$$

▶ Loose lower bound

$$\log p(\mathbf{x}|\boldsymbol{\theta}) - \mathcal{L}(q, \boldsymbol{\theta}) = (?).$$

▶ Poor prior distribution

$$p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I}).$$

▶ Poor variational posterior distribution (encoder)

$$q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu_\phi}(\mathbf{x}), \boldsymbol{\sigma_\phi^2}(\mathbf{x})).$$

Posterior collapse

LVM

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

ELBO objective

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \left[\mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z})) \right].$$

- ▶ More powerful $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ leads to more powerful generative model $p(\mathbf{x}|\boldsymbol{\theta})$.
- ▶ If the decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ is too powerful (it could model $p(\mathbf{x}|\boldsymbol{\theta})$), then the latent variables $\mathbf{z}$ becomes irrelevant. ELBO avoids paying any cost $KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}))$ ($q(\mathbf{z}|\mathbf{x}, \phi) \approx p(\mathbf{z})$), the variational posterior $q(\mathbf{z}|\mathbf{x}, \phi)$ will not carry any information about $\mathbf{x}$.

How to make the generative model $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ more powerful?
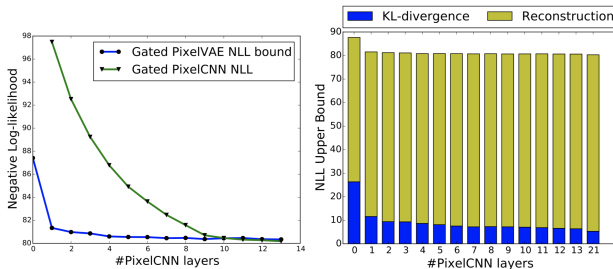
PixelVAE

Autoregressive decoder

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \prod_{j=1}^{m} p(x_j|\mathbf{x}_{1:j-1}, \mathbf{z}, \boldsymbol{\theta})$$

▶ Global structure is captured by latent variables.
▶ Local statistics are captured by limited receptive field autoregressive model.

MNIST results

Gulrajani I. et al. PixelVAE: A Latent Variable Model for Natural Images, 2016

Decoder weakening

- ▶ Powerful decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ makes the model expressive, but posterior collapse is possible.
- ▶ PixelVAE model uses the autoregressive PixelCNN model with small number of layers to limit receptive field.

How to force the model encode information about $\mathbf{x}$ into $\mathbf{z}$?

KL annealing

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \beta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \beta \cdot KL(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})||p(\mathbf{z}))$$

Start training with $\beta = 0$, increase it until $\beta = 1$ during training.

Free bits

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \lambda) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \max(\lambda, KL(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})||p(\mathbf{z}))).$$

It ensures the use of less than λ bits of information and results in $KL(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})||p(\mathbf{z})) \geq \lambda$.

Bowman S. R. et al. Generating Sentences from a Continuous Space, 2015
Kingma D. P. et al. Improving Variational Inference with Inverse Autoregressive Flow, 2016

Outline

VAE limitations

▶ Poor generative distribution (decoder)

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu_\theta}(\mathbf{z}), \boldsymbol{\sigma}_{\boldsymbol{\theta}}^2(\mathbf{z})).$$

▶ **Loose lower bound**

$$\log p(\mathbf{x}|\boldsymbol{\theta}) - \mathcal{L}(q, \boldsymbol{\theta}) = (?).$$

▶ Poor prior distribution

$$p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I}).$$

▶ Poor variational posterior distribution (encoder)

$$q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu_\phi}(\mathbf{x}), \boldsymbol{\sigma}_{\boldsymbol{\phi}}^2(\mathbf{x})).$$

Importance Sampling

LVM

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})d\mathbf{z} = \int \left[\frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})}\right] q(\mathbf{z}|\mathbf{x})d\mathbf{z}$$

$$= \int f(\mathbf{x}, \mathbf{z})q(\mathbf{z}|\mathbf{x})d\mathbf{z} = \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z})$$

Here $f(\mathbf{x}, \mathbf{z}) = \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})}$.

ELBO: derivation 1

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z}) \geq \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z}|\mathbf{x})} \log f(\mathbf{x}, \mathbf{z}) =$$

$$= \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z}|\mathbf{x})} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} = \mathcal{L}(q, \boldsymbol{\theta}).$$

Could we choose better $f(\mathbf{x}, \mathbf{z})$?

IWAE

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})d\mathbf{z} = \int \left[\frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} \right] q(\mathbf{z}|\mathbf{x})d\mathbf{z} = \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z})$$

Let define

$$f(\mathbf{x}, \mathbf{z}_1, \ldots, \mathbf{z}_K) = \frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})}$$

$$\mathbb{E}_{\mathbf{z}_1, \ldots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z}_1, \ldots, \mathbf{z}_K) = p(\mathbf{x}|\boldsymbol{\theta})$$

ELBO

$$
\begin{aligned}
\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \mathbb{E}_{\mathbf{z}_1, \ldots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z}, \ldots, \mathbf{z}_K) \geq \\
\geq \mathbb{E}_{\mathbf{z}_1, \ldots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log f(\mathbf{x}, \mathbf{z}, \ldots, \mathbf{z}_K) = \\
= \mathbb{E}_{\mathbf{z}_1, \ldots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log \left[\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right] = \mathcal{L}_K(q, \boldsymbol{\theta}).
\end{aligned}
$$

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

VAE objective

$$\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} \to \max_{q, \boldsymbol{\theta}}$$

$$\mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \left(\frac{1}{K} \sum_{k=1}^{K} \log \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right) \to \max_{q, \boldsymbol{\theta}}.$$

IWAE objective

$$\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right) \to \max_{q, \boldsymbol{\theta}}.$$

If $K = 1$, these objectives coincide.

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

Theorem

1. $\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}_K(q, \boldsymbol{\theta}) \geq \mathcal{L}_M(q, \boldsymbol{\theta}), \quad$ for $K \geq M$;
2. $\log p(\mathbf{x}|\boldsymbol{\theta}) = \lim_{K \to \infty} \mathcal{L}_K(q, \boldsymbol{\theta})$ if $\frac{p(\mathbf{x},\mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})}$ is bounded.

If $K > 1$ the bound could be tighter.

$$\mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})};$$

$$\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1,\ldots,\mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right).$$

- $\mathcal{L}_1(q, \boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta})$;
- $\mathcal{L}_\infty(q, \boldsymbol{\theta}) = \log p(\mathbf{x}|\boldsymbol{\theta})$.
- Which $q^*(\mathbf{z}|\mathbf{x})$ gives $\mathcal{L}(q^*, \boldsymbol{\theta}) = \log p(\mathbf{x}|\boldsymbol{\theta})$?
- Which $q^*(\mathbf{z}|\mathbf{x})$ gives $\mathcal{L}(q^*, \boldsymbol{\theta}) = \mathcal{L}_K(q, \boldsymbol{\theta})$?

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

Theorem
$\mathcal{L}(q^*, \boldsymbol{\theta}) = \mathcal{L}_K(q, \boldsymbol{\theta})$ for the following variational distribution
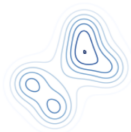
$$q^*(\mathbf{z}|\mathbf{x}) = \mathbb{E}_{\mathbf{z}_2,\ldots,\mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} q_{IW}(\mathbf{z}|\mathbf{x}, \mathbf{z}_{2:K}),$$
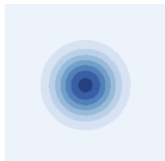
where

$$q_{IW}(\mathbf{z}|\mathbf{x}, \mathbf{z}_{2:K}) = \frac{\frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z}|\mathbf{x})}}{\frac{1}{K}\sum_{k=1}^{K}\frac{p(\mathbf{x},\mathbf{z}_k)}{q(\mathbf{z}_k|\mathbf{x})}} q(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x},\mathbf{z})}{\frac{1}{K}\left(\frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z}|\mathbf{x})} + \sum_{k=2}^{K}\frac{p(\mathbf{x},\mathbf{z}_k)}{q(\mathbf{z}_k|\mathbf{x})}\right)}.$$
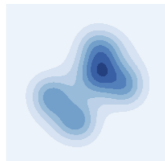
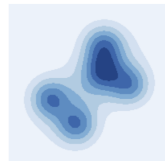### IWAE posterior

True posterior $k=1$ $k=10$ $k=100$

Cremer C., Morris Q., Duvenaud D. Reinterpreting Importance-Weighted Autoencoders, 2017

IWAE

Objective

$$\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1, \ldots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x}, \phi)} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x}, \phi)} \right) \to \max_{\phi, \boldsymbol{\theta}}.$$

Gradient

$$\Delta_K = \nabla_{\boldsymbol{\theta}, \phi} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x}, \phi)} \right), \quad \mathbf{z}_k \sim q(\mathbf{z}|\mathbf{x}, \phi).$$
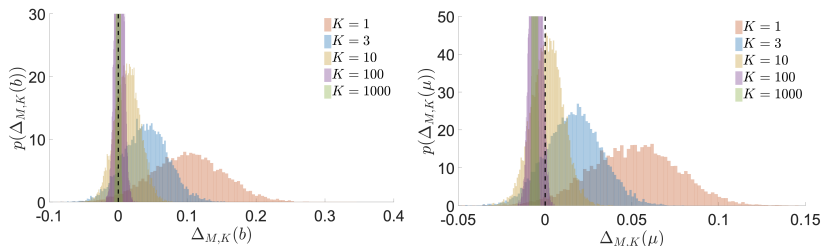
Theorem

$$\mathsf{SNR}_K = \frac{\mathbb{E}[\Delta_K]}{\sigma(\Delta_K)}; \quad \mathsf{SNR}_K(\boldsymbol{\theta}) = O(\sqrt{K}); \quad \mathsf{SNR}_K(\phi) = O\left(\sqrt{\frac{1}{K}} \right).$$

Hence, increasing K vanishes gradient signal of inference network
$q(\mathbf{z}|\mathbf{x}, \phi)$.

Rainforth T. et al. Tighter variational bounds are not necessarily better, 2018

IWAE

Theorem

$$\mathsf{SNR}_K = \frac{\mathbb{E}[\Delta_K]}{\sigma(\Delta_K)}; \quad \mathsf{SNR}_K(\boldsymbol{\theta}) = O(\sqrt{K}); \quad \mathsf{SNR}_K(\boldsymbol{\phi}) = O\left(\sqrt{\frac{1}{K}}\right).$$

- ▶ IWAE makes the variational bound tighter and extends the class of variational distributions.
- ▶ Gradient signal becomes really small, training is complicated.
- ▶ IWAE is very popular technique as a quality measure for VAE models.

Rainforth T. et al. Tighter variational bounds are not necessarily better, 2018

Summary

▶ The VAE model is an LVM with two neural network: stochastic encoder $q(z|x, \phi)$ and stochastic decoder $p(x|z, \theta)$.

▶ VAE is not a "true" bayesian model since parameters θ do not have a prior distribution.

▶ Standart VAE has several limitations that we will address later in the course.

▶ More powerful decoder in VAE leads to more expressive generative model. However, too expressive decoder could lead to the posterior collapse.

▶ The decoder weakening is a set of techniques to avoid the posterior collapse.

▶ The IWAE could get the tighter lower bound to the likelihood, but the training of such model becomes more difficult.