Deep Generative Models

Lecture 4

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Recap of previous lecture

EM-algorithm

► E-step

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

M-step

$$oldsymbol{ heta}^* = rg \max_{oldsymbol{ heta}} \mathcal{L}(q^*, oldsymbol{ heta});$$

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

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

Recap of previous lecture

$$\mathcal{L}(\phi, oldsymbol{ heta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[\log p(\mathbf{x}|\mathbf{z}, oldsymbol{ heta}) - \log rac{q(\mathbf{z}|\mathbf{x}, \phi)}{p(\mathbf{z})}
ight]
ightarrow \max_{\phi, heta}.$$

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

$$egin{aligned}
abla_{m{ heta}} \mathcal{L}(\phi, m{ heta}) &= \int q(\mathbf{z}|\mathbf{x}, \phi)
abla_{m{ heta}} \log p(\mathbf{x}|\mathbf{z}, m{ heta}) d\mathbf{z} pprox \\ &pprox
abla_{m{ heta}} \log p(\mathbf{x}|\mathbf{z}^*, m{ heta}), \quad \mathbf{z}^* \sim q(\mathbf{z}|\mathbf{x}, \phi). \end{aligned}$$

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

$$\nabla_{\phi} \mathcal{L}(\phi, \boldsymbol{\theta}) = \int r(\epsilon) \nabla_{\phi} \log p(\mathbf{x}|g(\mathbf{x}, \epsilon, \phi), \boldsymbol{\theta}) d\epsilon - \nabla_{\phi} \mathsf{KL}$$

$$pprox
abla_{m{\phi}} \log p(\mathbf{x}|g(\mathbf{x},m{\epsilon}^*,m{\phi}),m{ heta}) -
abla_{m{\phi}} \mathsf{KL}$$

Variational assumption

$$\begin{split} r(\epsilon) &= \mathcal{N}(\mathbf{0}, \mathbf{I}); \quad q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\boldsymbol{\mu}_{\phi}(\mathbf{x}), \boldsymbol{\sigma}_{\phi}^2(\mathbf{x})). \\ \mathbf{z} &= g(\mathbf{x}, \epsilon, \phi) = \boldsymbol{\sigma}_{\phi}(\mathbf{x}) \cdot \epsilon + \boldsymbol{\mu}_{\phi}(\mathbf{x}). \end{split}$$

Outline

1. Variational autoencoder (VAE)

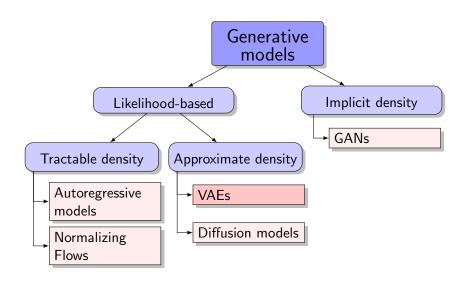
2. Posterior collapse and decoder weakening techniques

3. Tighter variational bound

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- 2. Posterior collapse and decoder weakening techniques
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Generative models zoo



Variational autoencoder (VAE)

Final EM-algorithm

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

$$egin{aligned} oldsymbol{\epsilon}^* &\sim r(oldsymbol{\epsilon}); \quad \mathbf{z}^* = g(\mathbf{x}, oldsymbol{\epsilon}^*, \phi); \ & \mathcal{L}(\phi, oldsymbol{\theta}) pprox \log p(\mathbf{x}|\mathbf{z}^*, oldsymbol{\theta}) - \mathit{KL}(q(\mathbf{z}^*|\mathbf{x}, \phi)||p(\mathbf{z}^*)). \end{aligned}$$

lacktriangle compute a stochastic gradients w.r.t. ϕ and heta

$$abla_{\phi} \mathcal{L}(\phi, \theta) pprox
abla_{\phi} \log p(\mathbf{x}|g(\mathbf{x}, \epsilon^*, \phi), \theta) -
abla_{\phi} \mathsf{KL}(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}));$$

$$abla_{\theta} \mathcal{L}(\phi, \theta) pprox
abla_{\theta} \log p(\mathbf{x}|\mathbf{z}^*, \theta).$$

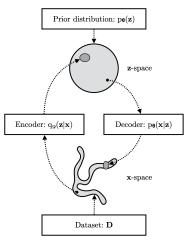
• update θ , ϕ according to the selected optimization method (SGD, Adam, RMSProp):

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

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

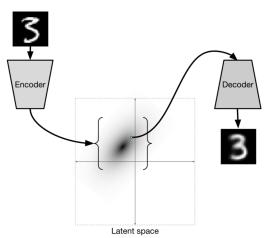
Variational autoencoder (VAE)

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



Variational Autoencoder

$$\mathcal{L}(\phi, oldsymbol{ heta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[\log p(\mathbf{x}|\mathbf{z}, oldsymbol{ heta}) - \log rac{q(\mathbf{z}|\mathbf{x}, \phi)}{p(\mathbf{z})}
ight]
ightarrow \max_{\phi, heta}.$$



Variational autoencoder (VAE)

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

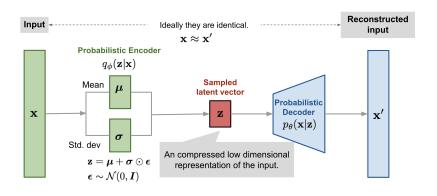


image credit:

VAE limitations

Poor generative distribution (decoder)

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\mu_{\boldsymbol{\theta}}(\mathbf{z}), \sigma_{\boldsymbol{\theta}}^2(\mathbf{z})) \quad \text{or } = \mathsf{Softmax}(\pi_{\boldsymbol{\theta}}(\mathbf{z})).$$

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)

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

VAE as Bayesian model

Posterior distribution

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

ELBO

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

EM-algorithm

► E-step

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

M-step

$$oldsymbol{ heta}^* = rg \max_{oldsymbol{q}} \left[\mathcal{L}(oldsymbol{q}, oldsymbol{ heta}) + \log p(oldsymbol{ heta})
ight].$$

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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

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

- 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 $\mathit{KL}(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})||p(\mathbf{z}))$ $(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) \approx p(\mathbf{z}))$, the variational posterior $q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})$ will not carry any information about \mathbf{x} .

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

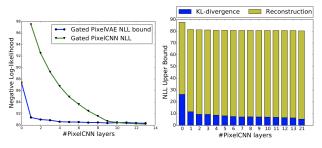
PixelVAF

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 techniques

- 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 x into z?

KL annealing

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

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

Free bits

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

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

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

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

Importance sampling

LVM

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

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

ELBO: derivation 1

$$\begin{split} \log p(\mathbf{x}|\boldsymbol{\theta}) &= \log \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} f(\mathbf{x}, \mathbf{z}) \geq \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \log f(\mathbf{x}, \mathbf{z}) = \\ &= \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} = \mathcal{L}(q, \boldsymbol{\theta}). \end{split}$$

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

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

Let define

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

$$\mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \cap g(\mathbf{z} | \mathbf{x}, \boldsymbol{\phi})} f(\mathbf{x}, \mathbf{z}_1, \dots, \mathbf{z}_K) = p(\mathbf{x} | \boldsymbol{\theta})$$

EL BO

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

VAE objective

$$\log p(\mathbf{x}|oldsymbol{ heta}) \geq \mathcal{L}(q,oldsymbol{ heta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},oldsymbol{\phi})} \log rac{p(\mathbf{x},\mathbf{z}|oldsymbol{ heta})}{q(\mathbf{z}|\mathbf{x},oldsymbol{\phi})}
ightarrow \max_{q,oldsymbol{ heta}}$$

$$\mathcal{L}(q, oldsymbol{ heta}) = \mathbb{E}_{\mathsf{z}_1, ..., \mathsf{z}_K \sim q(\mathsf{z}|\mathsf{x}, oldsymbol{\phi})} \left(rac{1}{K} \sum_{k=1}^K \log rac{p(\mathsf{x}, \mathsf{z}_k | oldsymbol{ heta})}{q(\mathsf{z}_k | \mathsf{x}, oldsymbol{\phi})}
ight)
ightarrow \max_{q, oldsymbol{ heta}}.$$

IWAE objective

$$\mathcal{L}_{K}(q, \theta) = \mathbb{E}_{\mathsf{z}_{1}, \dots, \mathsf{z}_{K} \sim q(\mathsf{z}|\mathsf{x}, \phi)} \log \left(\frac{1}{K} \sum_{l=1}^{K} \frac{p(\mathsf{x}, \mathsf{z}_{k}|\theta)}{q(\mathsf{z}_{k}|\mathsf{x}, \phi)} \right)
ightarrow \max_{q, \theta}.$$

If K = 1, these objectives coincide.

Theorem

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

If K > 1 the bound could be tighter.

$$egin{aligned} \mathcal{L}(q, oldsymbol{ heta}) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, oldsymbol{\phi})} \log rac{p(\mathbf{x}, \mathbf{z}|oldsymbol{ heta})}{q(\mathbf{z}|\mathbf{x}, oldsymbol{\phi})}; \ \mathcal{L}_{K}(q, oldsymbol{ heta}) &= \mathbb{E}_{\mathbf{z}_{1}, \dots, \mathbf{z}_{K} \sim q(\mathbf{z}|\mathbf{x}, oldsymbol{\phi})} \log \left(rac{1}{K} \sum_{k=1}^{K} rac{p(\mathbf{x}, \mathbf{z}_{k}|oldsymbol{ heta})}{q(\mathbf{z}_{k}|\mathbf{x}, oldsymbol{\phi})}
ight). \end{aligned}$$

- $ightharpoonup \mathcal{L}_1(q,\theta) = \mathcal{L}(q,\theta);$
- ▶ Which $q^*(\mathbf{z}|\mathbf{x}, \phi)$ gives $\mathcal{L}(q^*, \theta) = \log p(\mathbf{x}|\theta)$?

Objective

$$\mathcal{L}_{\mathcal{K}}(q, oldsymbol{ heta}) = \mathbb{E}_{\mathsf{z}_1, ..., \mathsf{z}_K \sim q(\mathsf{z}|\mathsf{x}, oldsymbol{\phi})} \log \left(rac{1}{K} \sum_{k=1}^K rac{p(\mathsf{x}, \mathsf{z}_k | oldsymbol{ heta})}{q(\mathsf{z}_k | \mathsf{x}, oldsymbol{\phi})}
ight)
ightarrow \max_{oldsymbol{\phi}, oldsymbol{ heta}}.$$

Gradient

$$\Delta_K =
abla_{ heta,\phi} \log \left(rac{1}{K} \sum_{k=1}^K rac{p(\mathbf{x}, \mathbf{z}_k | heta)}{q(\mathbf{z}_k | \mathbf{x}, \phi)}
ight), \quad \mathbf{z}_k \sim q(\mathbf{z} | \mathbf{x}, \phi).$$

Theorem

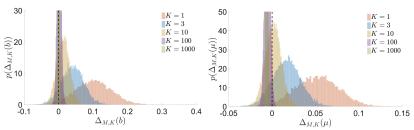
$$\mathsf{SNR}_{\mathcal{K}} = rac{\mathbb{E}[\Delta_{\mathcal{K}}]}{\sigma(\Delta_{\mathcal{K}})}; \quad \mathsf{SNR}_{\mathcal{K}}(oldsymbol{ heta}) = O(\sqrt{\mathcal{K}}); \quad \mathsf{SNR}_{\mathcal{K}}(\phi) = O\left(\sqrt{rac{1}{\mathcal{K}}}
ight).$$

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

Theorem

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



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

Summary

- The VAE model is an LVM with two neural network: stochastic encoder $q(\mathbf{z}|\mathbf{x}, \phi)$ and stochastic decoder $p(\mathbf{x}|\mathbf{z}, \theta)$.
- ightharpoonup VAE is not a "true" bayesian model since parameters heta 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.