

Deep Generative Models

Lecture 4

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AI 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

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

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

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

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

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

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

$$\begin{aligned} \nabla_{\theta} \mathcal{L}(\phi, \theta) &= \int q(\mathbf{z}|\mathbf{x}, \phi) \nabla_{\theta} \log p(\mathbf{x}|\mathbf{z}, \theta) d\mathbf{z} \approx \\ &\approx \nabla_{\theta} \log p(\mathbf{x}|\mathbf{z}^*, \theta), \quad \mathbf{z}^* \sim q(\mathbf{z}|\mathbf{x}, \phi). \end{aligned}$$

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

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

Variational assumption

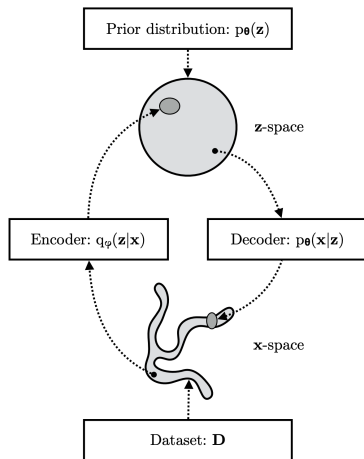
$$r(\epsilon) = \mathcal{N}(0, \mathbf{I}); \quad q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mu_{\phi}(\mathbf{x}), \sigma_{\phi}^2(\mathbf{x})).$$

$$\mathbf{z} = g(\mathbf{x}, \epsilon, \phi) = \sigma_{\phi}(\mathbf{x}) \cdot \epsilon + \mu_{\phi}(\mathbf{x}).$$

Recap of previous lecture

Variational autoencoder (VAE)

- ▶ VAE learns stochastic mapping between \mathbf{x} -space, from $\pi(\mathbf{x})$, and a latent \mathbf{z} -space, with simple distribution.
- ▶ The generative model learns distribution $p(\mathbf{x}, \mathbf{z} | \theta) = p(\mathbf{z})p(\mathbf{x} | \mathbf{z}, \theta)$, with a prior distribution $p(\mathbf{z})$, and a stochastic decoder $p(\mathbf{x} | \mathbf{z}, \theta)$.
- ▶ The stochastic encoder $q(\mathbf{z} | \mathbf{x}, \phi)$ (inference model), approximates the true but intractable posterior $p(\mathbf{z} | \mathbf{x}, \theta)$.



Outline

1. VAE limitations
2. Posterior collapse and decoder weakening techniques
3. Tighter variational bound
4. Normalizing flows prerequisites

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VAE limitations

- ▶ Poor generative distribution (decoder)

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

- ▶ 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)

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

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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

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

More powerful $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ leads to more powerful generative model $p(\mathbf{x}|\boldsymbol{\theta})$.

Extreme cast

$$p(\mathbf{x}|\boldsymbol{\theta}) \in \mathcal{P} = \{p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) | \forall \mathbf{z}, \boldsymbol{\theta}\}.$$

If the decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ is too powerful (it could model $p(\mathbf{x}|\boldsymbol{\theta})$), then 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} , the latent variables \mathbf{z} becomes irrelevant.

Autoregressive VAE decoder

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

PixelVAE/VLAE

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

- ▶ Global structure is captured by latent variables \mathbf{z} .
- ▶ Local statistics are captured by limited receptive field of autoregressive context $\mathbf{x}_{1:j-1}$.

PixelVAE/VLAE models use the autoregressive PixelCNN decoder model with small number of layers to limit receptive field.

<https://arxiv.org/abs/1611.05013> Gulrajani I. et al. *PixelVAE: A Latent Variable Model for Natural Images*, 2016,

<https://arxiv.org/abs/1611.02731> Chen X. et al. *Variational Lossy Autoencoder*, 2016

Decoder weakening techniques

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

KL annealing

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

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 $KL(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z})) \geq \lambda$.

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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VAE limitations

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- ▶ **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)

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

Importance sampling

LVM

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

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

ELBO: derivation 1

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

$f(\mathbf{x}, \mathbf{z})$ could be any function that satisfies $p(\mathbf{x}|\boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z} \sim q} f(\mathbf{x}, \mathbf{z})$.
Could we choose better $f(\mathbf{x}, \mathbf{z})$?

Importance Weighted Autoencoders (IWAE)

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

Let define

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

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

ELBO

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

Importance Weighted Autoencoders (IWAE)

VAE objective

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

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

IWAE objective

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

If $K = 1$, these objectives coincide.

Importance Weighted Autoencoders (IWAE)

Theorem

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

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

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

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

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

Importance Weighted Autoencoders (IWAE)

Objective

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

Theorem

Gradient signal of $q(\mathbf{z}|\mathbf{x}, \phi)$ vanishes as K increases:

$$\Delta_K = \nabla_{\theta, \phi} \mathcal{L}_K(q, \theta); \quad \text{SNR}_K = \frac{\mathbb{E}[\Delta_K]}{\sigma(\Delta_K)};$$

$$\text{SNR}_K(\theta) = O(\sqrt{K}); \quad \text{SNR}_K(\phi) = O\left(\sqrt{K^{-1}}\right).$$

- ▶ 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.

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Likelihood-based models so far...

Autoregressive models

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

- ▶ tractable likelihood,
- ▶ no inferred latent factors.

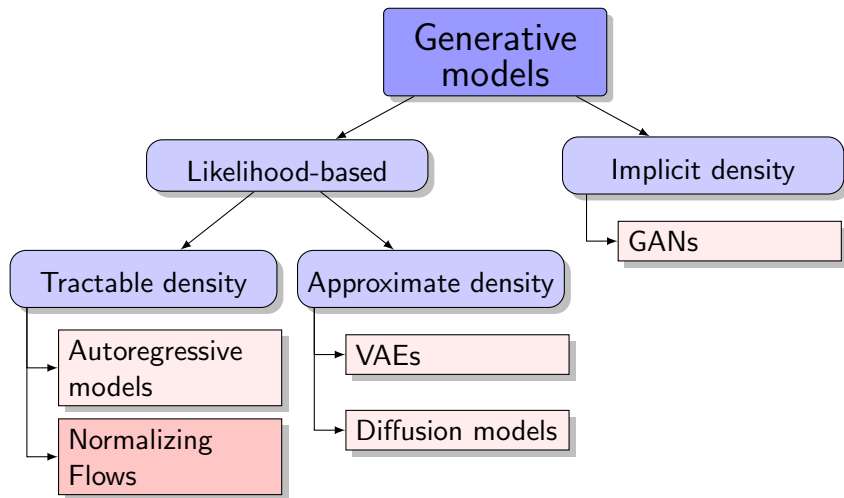
Latent variable models

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

- ▶ latent feature representation,
- ▶ intractable likelihood.

How to build model with latent variables and tractable likelihood?

Generative models zoo



Normalizing flows prerequisites

Jacobian matrix

Let $f : \mathbb{R}^m \rightarrow \mathbb{R}^m$ be a differentiable function.

$$\mathbf{z} = f(\mathbf{x}), \quad \mathbf{J} = \frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial z_m}{\partial x_1} & \cdots & \frac{\partial z_m}{\partial x_m} \end{pmatrix} \in \mathbb{R}^{m \times m}$$

Change of variable theorem (CoV)

Let \mathbf{x} be a random variable with density function $p(\mathbf{x})$ and $f : \mathbb{R}^m \rightarrow \mathbb{R}^m$ is a differentiable, **invertible** function (diffeomorphism). If $\mathbf{z} = f(\mathbf{x})$, $\mathbf{x} = f^{-1}(\mathbf{z}) = g(\mathbf{z})$, then

$$p(\mathbf{x}) = p(\mathbf{z}) |\det(\mathbf{J}_f)| = p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x})) \left| \det \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$
$$p(\mathbf{z}) = p(\mathbf{x}) |\det(\mathbf{J}_g)| = p(\mathbf{x}) \left| \det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right| = p(g(\mathbf{z})) \left| \det \left(\frac{\partial g(\mathbf{z})}{\partial \mathbf{z}} \right) \right|.$$

Summary

- ▶ Standard 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.
- ▶ Change of variable theorem allows to get the density function of the random variable under the invertible transformation.