# 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  $\phi$ .

#### 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

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

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

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

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

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

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

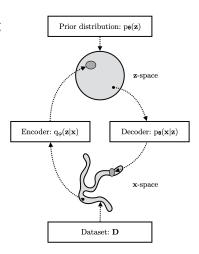
Variational assumption

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

# Recap of previous lecture

## Variational autoencoder (VAE)

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



## Outline

1. Posterior collapse and decoder weakening techniques

2. Tighter variational bound

3. Normalizing flows

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## VAE limitations

Poor generative distribution (decoder)

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

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)

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

# 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

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

- 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?

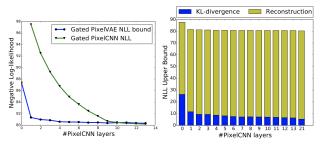
## **PixelVAF**

## 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

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

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  $\lambda$  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

## Outline

- 1. Posterior collapse and decoder weakening techniques
- 2. Tighter variational bound
- 3. Normalizing flows

## **VAE** limitations

Poor generative distribution (decoder)

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Loose lower bound

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Poor prior distribution

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

Poor variational posterior distribution (encoder)

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

# 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

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

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

#### 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

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

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

## **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.

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

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

## Objective

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

## 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

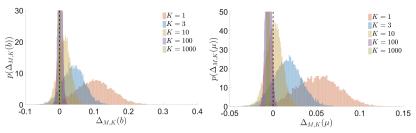
$$\mathsf{SNR}_{\mathcal{K}} = \frac{\mathbb{E}[\Delta_{\mathcal{K}}]}{\sigma(\Delta_{\mathcal{K}})}; \quad \mathsf{SNR}_{\mathcal{K}}(\boldsymbol{\theta}) = O(\sqrt{\mathcal{K}}); \quad \mathsf{SNR}_{\mathcal{K}}(\phi) = O\left(\sqrt{\frac{1}{\mathcal{K}}}\right).$$

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**

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



- ► 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.

## Outline

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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.

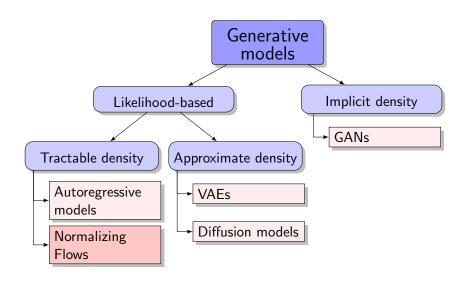
#### Latent variable models

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

- latent feature representation,
- intractable likelihood.

How to build model with latent variables and tractable likelihood?

## Generative models zoo



# Normalizing flows prerequisites

#### Jacobian matrix

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

## Change of variable theorem (CoV)

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

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

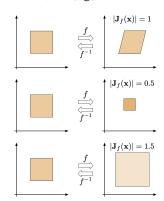
## Jacobian determinant

#### Inverse function theorem

If function f is invertible and Jacobian matrix is continuous and non-singular, then

$$\mathbf{J}_f = \mathbf{J}_{g^{-1}} = \mathbf{J}_g^{-1}, \quad |\det(\mathbf{J}_f)| = rac{1}{|\det(\mathbf{J}_g)|}$$

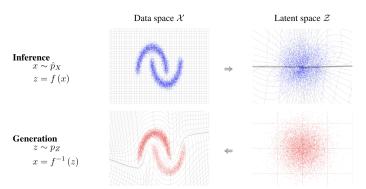
- **x** and **z** have the same dimensionality  $(\mathbb{R}^m)$ .
- $f(\mathbf{x}, \boldsymbol{\theta})$  could be parametric function.
- Determinant of Jacobian matrix  $\mathbf{J} = \frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}}$  shows how the volume changes under the transorfmation.



# Fitting flows

## MLE problem

$$p(\mathbf{x}|\boldsymbol{\theta}) = p(\mathbf{z}) \left| \det \left( \frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x}, \boldsymbol{\theta})) \left| \det \left( \frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}} \right) \right|$$
$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f(\mathbf{x}, \boldsymbol{\theta})) + \log |\det(\mathbf{J}_f)| \to \max_{\boldsymbol{\theta}}$$



# Summary

- 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.
- ► Flow models transform a simple base distribution to a complex one via a sequence of invertible transformations with tractable Jacobian.
- ► Flow models have a tractable likelihood that is given by the change of variable theorem.