# Deep Generative Models

Lecture 7

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# Recap of previous lecture

#### Gaussian AR NF

$$\mathbf{z} = g(\mathbf{z}, \boldsymbol{\theta}) \quad \Rightarrow \quad x_j = \sigma_j(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_j(\mathbf{x}_{1:j-1}).$$

$$\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta}) \quad \Rightarrow \quad z_j = (x_j - \mu_j(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_j(\mathbf{x}_{1:j-1})}.$$

- Sampling is sequential, density estimation is parallel.
- Forward KL is a natural loss.

#### Inverse gaussian AR NF

$$\mathbf{z} = g(\mathbf{z}, \boldsymbol{\theta}) \quad \Rightarrow \quad x_j = \tilde{\sigma}_j(\mathbf{z}_{1:j-1}) \cdot z_j + \tilde{\mu}_j(\mathbf{z}_{1:j-1})$$
$$\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta}) \quad \Rightarrow \quad z_j = (x_j - \tilde{\mu}_j(\mathbf{z}_{1:j-1})) \cdot \frac{1}{\tilde{\sigma}_j(\mathbf{z}_{1:j-1})}.$$

- ▶ Sampling is parallel, density estimation is sequential.
- Reverse KL is a natural loss.

# Recap of previous lecture

Let split **x** and **z** in two parts:

$$\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2] = [\mathbf{x}_{1:d}, \mathbf{x}_{d+1:m}]; \quad \mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2] = [\mathbf{z}_{1:d}, \mathbf{z}_{d+1:m}].$$

#### Coupling layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \boldsymbol{\sigma}(\mathbf{z}_1, \boldsymbol{\theta}) + \boldsymbol{\mu}(\mathbf{z}_1, \boldsymbol{\theta}). \end{cases} \begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = (\mathbf{x}_2 - \boldsymbol{\mu}(\mathbf{x}_1, \boldsymbol{\theta})) \odot \frac{1}{\boldsymbol{\sigma}(\mathbf{x}_1, \boldsymbol{\theta})}. \end{cases}$$

Estimating the density takes 1 pass, sampling takes 1 pass!

#### Jacobian

$$\det\left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}\right) = \det\left(\frac{\mathbf{I}_d}{\frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_1}} \quad \frac{0_{d \times m - d}}{\frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_2}}\right) = \prod_{i = 1}^{m - d} \frac{1}{\sigma_j(\mathbf{x}_1, \boldsymbol{\theta})}.$$

Coupling layer is a special case of autoregressive flow.

# Recap of previous lecture

	VAE	NF
Objective	ELBO $\mathcal L$	Forward KL/MLE
Encoder	stochastic $\mathbf{z} \sim q(\mathbf{z} \mathbf{x}, oldsymbol{\phi})$	
Decoder Parameters	$egin{aligned} stochastic \ \mathbf{x} \sim p(\mathbf{x} \mathbf{z}, oldsymbol{ heta}) \ \phi, oldsymbol{ heta} \end{aligned}$	$\begin{aligned} & \text{deterministic} \\ & \mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta}) \\ & p(\mathbf{x} \mathbf{z}, \boldsymbol{\theta}) = \delta(\mathbf{x} - g(\mathbf{z}, \boldsymbol{\theta})) \\ & \boldsymbol{\theta} \equiv \boldsymbol{\phi} \end{aligned}$

#### **Theorem**

MLE for normalizing flow is equivalent to maximization of ELBO for VAE model with deterministic encoder and decoder:

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \delta(\mathbf{x} - f^{-1}(\mathbf{z}, \boldsymbol{\theta})) = \delta(\mathbf{x} - g(\mathbf{z}, \boldsymbol{\theta}));$$
$$q(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) = \delta(\mathbf{z} - f(\mathbf{x}, \boldsymbol{\theta})).$$

Nielsen D., et al. SurVAE Flows: Surjections to Bridge the Gap between VAEs and Flows. 2020

Discrete data vs continuous model
 Discretization of continuous distribution
 Dequantization of discrete data

### 2. ELBO surgery

VAE limitations
 VAE prior
 VAE posterior

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#### Discrete data vs continuous model

Let our data  $\mathbf{y}$  comes from discrete distribution  $\Pi(\mathbf{y})$  and we have continuous model  $p(\mathbf{x}|\theta) = \mathsf{NN}(\mathbf{x},\theta)$ .

- ▶ Images (and not only images) are discrete data, pixels lie in the integer domain ({0, 255}).
- By fitting a continuous density model  $p(\mathbf{x}|\theta)$  to discrete data  $\Pi(\mathbf{y})$ , one can produce a degenerate solution with all probability mass on discrete values.

#### Discrete model

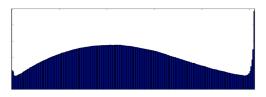
- Use **discrete** model (e.x.  $P(\mathbf{y}|\theta) = \mathsf{Cat}(\pi(\theta))$ ).
- ▶ Minimize any suitable divergence measure  $D(\Pi, P)$ .
- ► NF works only with continuous data **x** (there are discrete NF, see papers below).
- ▶ If pixel value is not presented in the train data, it won't be predicted.

#### Discrete data vs continuous model

#### Continuous model

- Use **continuous** model (e.x.  $p(\mathbf{x}|\theta) = \mathcal{N}(\mu_{\theta}(\mathbf{x}), \sigma_{\theta}^2(\mathbf{x}))$ ), but
  - **discretize** model (make the model outputs discrete): transform  $p(\mathbf{x}|\theta)$  to  $P(\mathbf{y}|\theta)$ ;
  - **dequantize** data (make the data continuous): transform  $\Pi(y)$  to  $\pi(x)$ .
- Continuous distribution know numerical relationships.

#### CIFAR-10 pixel values distribution



1. Discrete data vs continuous model Discretization of continuous distribution

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# Discretization of continuous distribution

#### Model discretization through CDF

$$F(\mathbf{x}|\boldsymbol{\theta}) = \int_{-\infty}^{\mathbf{x}} p(\mathbf{x}'|\boldsymbol{\theta}) d\mathbf{x}'; \quad P(\mathbf{y}|\boldsymbol{\theta}) = F(\mathbf{y} + 0.5|\boldsymbol{\theta}) - F(\mathbf{y} - 0.5|\boldsymbol{\theta})$$

Mixture of logistic distributions

$$p(x|\mu,s) = \frac{\exp^{-(x-\mu)/s}}{s(1+\exp^{-(x-\mu)/s})^2}; \quad p(x|\pi,\mu,s) = \sum_{k=1}^K \pi_k p(x|\mu_k,s_k).$$

#### PixelCNN++

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{m} p(x_j|\mathbf{x}_{1:j-1},\boldsymbol{\theta}); \quad p(x_j|\mathbf{x}_{1:j-1},\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k p(x|\mu_k,s_k).$$

Here,  $\pi_k = \pi_{k,\theta}(\mathbf{x}_{1:j-1}), \ \mu_k = \mu_{k,\theta}(\mathbf{x}_{1:j-1}), \ s_k = s_{k,\theta}(\mathbf{x}_{1:j-1}).$ 

For the pixel edge cases of 0, replace x-0.5 by  $-\infty$ , and for 255 replace x+0.5 by  $+\infty$ .

Salimans T. et al. PixelCNN++: Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications, 2017

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# Uniform discretization

Let dequantize discrete distribution  $\Pi(\mathbf{y})$  to continuous distribution  $\pi(\mathbf{x})$  in the following way:  $\mathbf{x} = \mathbf{y} + \mathbf{u}$ , where  $\mathbf{u} \sim U[0,1]$ .

#### **Theorem**

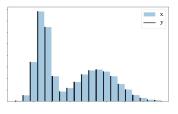
Fitting continuous model  $p(\mathbf{x}|\boldsymbol{\theta})$  on uniformly dequantized data is equivalent to maximization of a lower bound on log-likelihood for a discrete model:

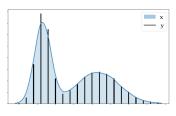
$$P(\mathbf{y}|\boldsymbol{\theta}) = \int_{U[0,1]} p(\mathbf{y} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u}$$

#### Proof

$$\begin{split} \mathbb{E}_{\pi} \log p(\mathbf{x}|\boldsymbol{\theta}) &= \int \pi(\mathbf{x}) \log p(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{x} = \sum \Pi(\mathbf{y}) \int_{U[0,1]} \log p(\mathbf{y} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} \leq \\ &\leq \sum \Pi(\mathbf{y}) \log \int_{U[0,1]} p(\mathbf{y} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} = \\ &= \sum \Pi(\mathbf{y}) \log P(\mathbf{y}|\boldsymbol{\theta}) = \mathbb{E}_{\Pi} \log P(\mathbf{y}|\boldsymbol{\theta}). \end{split}$$

# Variational dequantization





- ▶  $p(\mathbf{x}|\boldsymbol{\theta})$  assign uniform density to unit hypercubes  $\mathbf{y} + U[0,1]$  (left fig).
- Smooth dequantization is more natural (right fig).
- Neural network density models are smooth function approximators.

Introduce variational dequantization noise distribution  $q(\mathbf{u}|\mathbf{y})$ , which tells what kind of noise we have to add to our discrete data. Treat it as an approximate posterior as in VAE model.

# Variational dequantization

#### Variational lower bound

$$egin{aligned} \log P(\mathbf{y}|oldsymbol{ heta}) &= \left[\log \int q(\mathbf{u}|\mathbf{y}) rac{p(\mathbf{y}+\mathbf{u}|oldsymbol{ heta})}{q(\mathbf{u}|\mathbf{y})} d\mathbf{u}
ight] \geq \ &\geq \int q(\mathbf{u}|\mathbf{y}) \log rac{p(\mathbf{y}+\mathbf{u}|oldsymbol{ heta})}{q(\mathbf{u}|\mathbf{y})} d\mathbf{u} = \mathcal{L}(q,oldsymbol{ heta}). \end{aligned}$$

Uniform dequantization is a special case of variational dequantization  $(q(\mathbf{u}|\mathbf{y}) = U[0,1])$ .

#### Flow++: flow-based variational dequantization

Let  $\mathbf{u} = g(\epsilon, \mathbf{y}, \lambda)$  is a flow model with base distribution  $\epsilon \sim p(\epsilon)$ :

$$q(\mathbf{u}|\mathbf{y}) = p(f(\mathbf{u},\mathbf{y},\lambda)) \cdot \left| \det \frac{\partial f(\mathbf{u},\mathbf{y},\lambda)}{\partial \mathbf{u}} \right|.$$

$$\log P(\mathbf{y}|oldsymbol{ heta}) \geq \mathcal{L}(oldsymbol{\lambda},oldsymbol{ heta}) = \int p(oldsymbol{\epsilon}) \log \left(rac{p(\mathbf{y}+g(oldsymbol{\epsilon},\mathbf{y},oldsymbol{\lambda})|oldsymbol{ heta})}{p(oldsymbol{\epsilon})\cdot \left|\det \mathbf{J}_{oldsymbol{\epsilon}}
ight|^{-1}}
ight) doldsymbol{\epsilon}.$$

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

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# **ELBO** surgery

$$\frac{1}{n}\sum_{i=1}^{n}\mathcal{L}_{i}(q,\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \left[\mathbb{E}_{q(\mathbf{z}|\mathbf{x}_{i})}\log p(\mathbf{x}_{i}|\mathbf{z},\boldsymbol{\theta}) - KL(q(\mathbf{z}|\mathbf{x}_{i})||p(\mathbf{z}))\right].$$

#### **Theorem**

$$\frac{1}{n} \sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_{i})||p(\mathbf{z})) = KL(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z})) + \mathbb{I}_{q}[\mathbf{x}, \mathbf{z}];$$

- ▶  $\mathbb{I}_q[\mathbf{x}, \mathbf{z}]$  mutual information between  $\mathbf{x}$  and  $\mathbf{z}$  under empirical data distribution and distribution  $q(\mathbf{z}|\mathbf{x})$ .
- First term pushes  $q_{agg}(z)$  towards the prior p(z).
- Second term reduces the amount of information about x stored in z.

# **ELBO** surgery

#### **Theorem**

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_i)||p(\mathbf{z})) = KL(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x},\mathbf{z}].$$

#### Proof

$$\begin{split} &\frac{1}{n}\sum_{i=1}^{n} \textit{KL}(q(\mathbf{z}|\mathbf{x}_{i})||p(\mathbf{z})) = \frac{1}{n}\sum_{i=1}^{n}\int q(\mathbf{z}|\mathbf{x}_{i})\log\frac{q(\mathbf{z}|\mathbf{x}_{i})}{p(\mathbf{z})}d\mathbf{z} = \\ &= \frac{1}{n}\sum_{i=1}^{n}\int q(\mathbf{z}|\mathbf{x}_{i})\log\frac{q_{\text{agg}}(\mathbf{z})q(\mathbf{z}|\mathbf{x}_{i})}{p(\mathbf{z})q_{\text{agg}}(\mathbf{z})}d\mathbf{z} = \int \frac{1}{n}\sum_{i=1}^{n}q(\mathbf{z}|\mathbf{x}_{i})\log\frac{q_{\text{agg}}(\mathbf{z})}{p(\mathbf{z})}d\mathbf{z} + \\ &+ \frac{1}{n}\sum_{i=1}^{n}\int q(\mathbf{z}|\mathbf{x}_{i})\log\frac{q(\mathbf{z}|\mathbf{x}_{i})}{q_{\text{agg}}(\mathbf{z})}d\mathbf{z} = \textit{KL}(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z})) + \frac{1}{n}\sum_{i=1}^{n}\textit{KL}(q(\mathbf{z}|\mathbf{x}_{i})||q_{\text{agg}}(\mathbf{z})) \end{split}$$

Without proof:

$$\mathbb{I}_q[\mathbf{x},\mathbf{z}] = \frac{1}{n} \sum_{i=1}^n KL(q(\mathbf{z}|\mathbf{x}_i)||q_{\text{agg}}(\mathbf{z})) \in [0,\log n].$$

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound. 2016

# **ELBO** surgery

# **ELBO** revisiting

$$\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}_{i}(q, \theta) = \frac{1}{n} \sum_{i=1}^{n} \left[ \mathbb{E}_{q(\mathbf{z}|\mathbf{x}_{i})} \log p(\mathbf{x}_{i}|\mathbf{z}, \theta) - KL(q(\mathbf{z}|\mathbf{x}_{i})||p(\mathbf{z})) \right] =$$

$$= \underbrace{\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}|\mathbf{x}_{i})} \log p(\mathbf{x}_{i}|\mathbf{z}, \theta) - \mathbb{I}_{q}[\mathbf{x}, \mathbf{z}] - KL(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

Prior distribution  $p(\mathbf{z})$  is only in the last term.

### Optimal VAE prior

$$KL(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z})) = 0 \quad \Leftrightarrow \quad p(\mathbf{z}) = q_{\text{agg}}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i).$$

The optimal prior  $p(\mathbf{z})$  is the aggregated posterior  $q_{agg}(\mathbf{z})$ !

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound. 2016

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#### **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

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

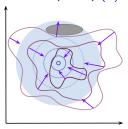
Poor variational posterior distribution (encoder)

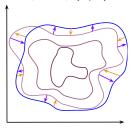
$$q(\mathsf{z}|\mathsf{x},\phi) = \mathcal{N}(\mathsf{z}|\pmb{\mu}_{\phi}(\mathsf{x}),\pmb{\sigma}_{\phi}^2(\mathsf{x})).$$

# Optimal VAE prior

- ▶ Standard Gaussian  $p(\mathbf{z}) = \mathcal{N}(0, I) \Rightarrow$  over-regularization;
- $p(z) = q_{agg}(z) = \frac{1}{n} \sum_{i=1}^{n} q(z|x_i) \Rightarrow \text{overfitting and highly}$ expensive.

# Non learnable prior p(z) Learnable prior $p(z|\lambda)$





# ELBO revisiting

$$\frac{1}{n}\sum_{i=1}^{n}\mathcal{L}_{i}(q,\boldsymbol{\theta}) = \mathsf{RL} - \mathsf{MI} - \mathcal{KL}(q_{\mathsf{agg}}(\mathbf{z})||p(\mathbf{z}|\boldsymbol{\lambda}))$$

It is Forward KL with respect to  $p(\mathbf{z}|\lambda)$ .

# Flow-based VAE prior

#### Flow model in latent space

$$\log p(\mathbf{z}|\boldsymbol{\lambda}) = \log p(\mathbf{z}^*) + \log \left| \det \left( \frac{d\mathbf{z}^*}{d\mathbf{z}} \right) \right| = \log p(f(\mathbf{z}, \boldsymbol{\lambda})) + \log \left| \det(\mathbf{J}_f) \right|$$

 $z = g(z^*, \lambda) = f^{-1}(z^*, \lambda)$ 

- RealNVP with coupling layers.
- ▶ Autoregressive flow (fast  $f(\mathbf{z}, \lambda)$ , slow  $g(\mathbf{z}^*, \lambda)$ ).
- ▶ Is it OK to use IAF for VAE prior?

#### ELBO with flow-based VAE prior

$$\begin{split} \mathcal{L}(\phi, \theta) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[ \log p(\mathbf{x}|\mathbf{z}, \theta) + \log p(\mathbf{z}|\lambda) - \log q(\mathbf{z}|\mathbf{x}, \phi) \right] \\ &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[ \log p(\mathbf{x}|\mathbf{z}, \theta) + \underbrace{\left( \log p(f(\mathbf{z}, \lambda)) + \log \left| \det(\mathbf{J}_f) \right| \right)}_{\text{flow-based prior}} - \log q(\mathbf{z}|\mathbf{x}, \phi) \right] \end{split}$$

Is it possible to use non-invertible model in VAE prior?

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#### **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)

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

# Variational posterior

#### ELBO decomposition

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

- ► E-step of EM-algorithm:  $KL(q(\mathbf{z}|\mathbf{x},\phi)||p(\mathbf{z}|\mathbf{x},\theta)) = 0$ . (In this case the lower bound is tight  $\log p(\mathbf{x}|\theta) = \mathcal{L}(q,\theta)$ ).
- $q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_{\phi}(\mathbf{x}), \boldsymbol{\sigma}_{\phi}^{2}(\mathbf{x}))$  is a unimodal distribution (not expressive enough).
- NF convert a simple distribution to a complex one. Let use NF in VAE posterior.

Apply a sequence of transformations to the random variable

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

Let  $q(\mathbf{z}|\mathbf{x}, \phi)$  (VAE encoder) be a base distribution for a flow model.

# Summary

- Lots of data are discrete. We able to discretize the model or to dequantize our data to use continuous model.
- Uniform dequantization is the simplest form of dequantization. Variational dequantization is a more natural type that uses variational inference.
- ► The ELBO surgery reveals insights about a prior distribution in VAE. The optimal prior is the aggregated posterior.
- We could use flow-based prior in VAE (even autoregressive).
- We could use flows to make variational posterior more expressive.