

Deep Generative Models

Lecture 7

Roman Isachenko

Moscow Institute of Physics and Technology

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Recap of previous lecture

Gaussian AR NF

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

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

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

Inverse gaussian AR NF

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

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

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

Recap of previous lecture

Let split \mathbf{x} and \mathbf{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

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

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

Jacobian

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

Coupling layer is a special case of autoregressive flow.

Recap of previous lecture

	VAE	NF
Objective	ELBO \mathcal{L}	Forward KL/MLE
Encoder	stochastic $\mathbf{z} \sim q(\mathbf{z} \mathbf{x}, \phi)$	deterministic $\mathbf{z} = f(\mathbf{x}, \theta)$ $q(\mathbf{z} \mathbf{x}, \theta) = \delta(\mathbf{z} - f(\mathbf{x}, \theta))$
Decoder	stochastic $\mathbf{x} \sim p(\mathbf{x} \mathbf{z}, \theta)$	deterministic $\mathbf{x} = g(\mathbf{z}, \theta)$ $p(\mathbf{x} \mathbf{z}, \theta) = \delta(\mathbf{x} - g(\mathbf{z}, \theta))$
Parameters	ϕ, θ	$\theta \equiv \phi$

Theorem

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

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

$$q(\mathbf{z}|\mathbf{x}, \theta) = p(\mathbf{z}|\mathbf{x}, \theta) = \delta(\mathbf{z} - f(\mathbf{x}, \theta)).$$

Outline

1. Discrete data vs continuous model

- Discretization of continuous distribution
- Dequantization of discrete data

2. ELBO surgery

3. 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 $p(\mathbf{x}|\theta) = \text{NN}(\mathbf{x}, \theta)$.

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

Hoogeboom E. et al. Integer discrete flows and lossless compression, 2019

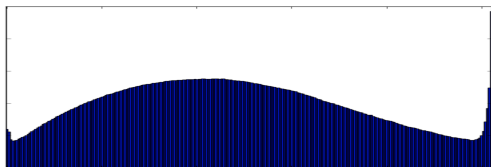
Tran D. et al. Discrete flows: Invertible generative models of discrete data, 2019

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 $\Pi(\mathbf{y})$ to $\pi(\mathbf{x})$.
- ▶ Continuous distribution knows numerical relationships.

CIFAR-10 pixel values distribution



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Discretization of continuous distribution

Model discretization through CDF

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

Mixture of logistic distributions

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

PixelCNN++

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

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 $y - 0.5$ by $-\infty$, and for 255 replace $y + 0.5$ by $+\infty$.

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

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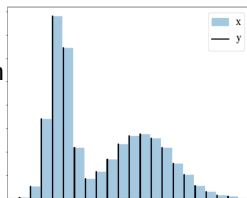
Uniform dequantization

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

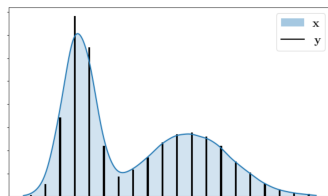
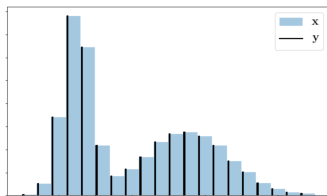
$$P(\mathbf{y}|\theta) = \int_{U[0,1]} p(\mathbf{y} + \mathbf{u}|\theta) d\mathbf{u}$$



Proof

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

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

$$\begin{aligned}\log P(\mathbf{y}|\boldsymbol{\theta}) &= \left[\log \int q(\mathbf{u}|\mathbf{y}) \frac{p(\mathbf{y} + \mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{y})} d\mathbf{u} \right] \geq \\ &\geq \int q(\mathbf{u}|\mathbf{y}) \log \frac{p(\mathbf{y} + \mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{y})} d\mathbf{u} = \mathcal{L}(q, \boldsymbol{\theta}).\end{aligned}$$

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

Flow++: flow-based variational dequantization

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

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

$$\log P(\mathbf{y}|\boldsymbol{\theta}) \geq \mathcal{L}(\boldsymbol{\lambda}, \boldsymbol{\theta}) = \int p(\boldsymbol{\epsilon}) \log \left(\frac{p(\mathbf{y} + g(\boldsymbol{\epsilon}, \mathbf{y}, \boldsymbol{\lambda})|\boldsymbol{\theta})}{p(\boldsymbol{\epsilon}) \cdot |\det \mathbf{J}_g|^{-1}} \right) d\boldsymbol{\epsilon}.$$

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

Theorem

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

- ▶ $q_{\text{agg}}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q(\mathbf{z}|\mathbf{x}_i)$ – **aggregated** posterior distribution.
- ▶ $\mathbb{I}_q[\mathbf{x}, \mathbf{z}]$ – mutual information between \mathbf{x} and \mathbf{z} under empirical data distribution and distribution $q(\mathbf{z}|\mathbf{x})$.
- ▶ **First term** pushes $q_{\text{agg}}(\mathbf{z})$ towards the prior $p(\mathbf{z})$.
- ▶ **Second term** reduces the amount of information about \mathbf{x} stored in \mathbf{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

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

Without proof:

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

ELBO surgery

ELBO revisiting

$$\begin{aligned}\frac{1}{n} \sum_{i=1}^n \mathcal{L}_i(q, \theta) &= \frac{1}{n} \sum_{i=1}^n [\mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}, \theta) - KL(q(\mathbf{z}|\mathbf{x}_i)||p(\mathbf{z}))] = \\ &= \underbrace{\frac{1}{n} \sum_{i=1}^n \mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}, \theta)}_{\text{Reconstruction loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{MI}} - \underbrace{KL(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}\end{aligned}$$

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 $q_{\text{agg}}(\mathbf{z})$!

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)

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

- ▶ Loose lower bound

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

- ▶ **Poor prior distribution**

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

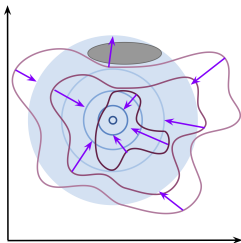
- ▶ Poor variational posterior distribution (encoder)

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

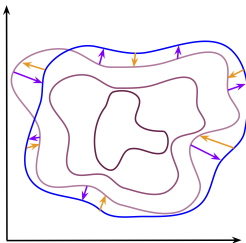
Optimal VAE prior

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

Non learnable prior $p(\mathbf{z})$



Learnable prior $p(\mathbf{z}|\lambda)$



ELBO revisiting

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

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

Flow-based VAE prior

Flow model in latent space

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

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

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

ELBO with flow-based VAE prior

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

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

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- ▶ 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)**

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

Variational posterior

ELBO decomposition

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

- ▶ E-step of EM-algorithm: $KL(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) = 0$.
(In this case the lower bound is tight $\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta})$).
- ▶ $q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}_\phi^2(\mathbf{x}))$ 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

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

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.