

Deep Generative Models

Lecture 4

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Autumn, 2021

Recap of previous lecture

Latent variable models (LVM)

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

MLE problem for LVM

$$\begin{aligned}\boldsymbol{\theta}^* &= \arg \max_{\boldsymbol{\theta}} \log p(\mathbf{X}|\boldsymbol{\theta}) = \arg \max_{\boldsymbol{\theta}} \sum_{i=1}^n \log p(\mathbf{x}_i|\boldsymbol{\theta}) = \\ &= \arg \max_{\boldsymbol{\theta}} \log \sum_{i=1}^n \int p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta})p(\mathbf{z}_i)d\mathbf{z}_i.\end{aligned}$$

Naive Monte-Carlo estimation

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z})d\mathbf{z} = \mathbb{E}_{p(\mathbf{z})}p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) \approx \frac{1}{K} \sum_{k=1}^K p(\mathbf{x}|\mathbf{z}_k, \boldsymbol{\theta}),$$

where $\mathbf{z}_k \sim p(\mathbf{z})$.

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

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

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

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

ELBO gradients

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

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

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

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

Difference from M-step: density function $q(\mathbf{z}|\mathbf{x}, \phi)$ depends on the parameters ϕ , it is impossible to use the Monte-Carlo estimation:

$$\begin{aligned} \nabla_{\phi} \mathcal{L}(\phi, \theta) &= \nabla_{\phi} \int q(\mathbf{z}|\mathbf{x}, \phi) \left[\log p(\mathbf{x}|\mathbf{z}, \theta) + \log \frac{p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x}, \phi)} \right] d\mathbf{z} \\ &\neq \int q(\mathbf{z}|\mathbf{x}, \phi) \nabla_{\phi} \left[\log p(\mathbf{x}|\mathbf{z}, \theta) + \log \frac{p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x}, \phi)} \right] d\mathbf{z} \end{aligned}$$

Reparametrization trick

Law of the unconscious statistician (LOTUS)

Let X be a random variable and let $Y = g(X)$. Then

$$\mathbb{E}_{p_Y} Y = \mathbb{E}_{p_X} g(X) = \int g(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}.$$

Examples

- ▶ $r(x) = \mathcal{N}(x|0, 1)$, $y = \sigma \cdot x + \mu$, $p_Y(y|\theta) = \mathcal{N}(y|\mu, \sigma^2)$, $\theta = [\mu, \sigma]$.
- ▶ $\epsilon^* \sim r(\epsilon)$, $\mathbf{z} = g(\mathbf{x}, \epsilon, \phi)$, $\mathbf{z} \sim q(\mathbf{z}|\mathbf{x}, \phi)$

$$\begin{aligned} \nabla_{\phi} \int q(\mathbf{z}|\mathbf{x}, \phi) f(\mathbf{z}) d\mathbf{z} &= \nabla_{\phi} \int r(\epsilon) f(\mathbf{z}) d\epsilon \\ &= \int r(\epsilon) \nabla_{\phi} f(g(\mathbf{x}, \epsilon, \phi)) d\epsilon \approx \nabla_{\phi} f(g(\mathbf{x}, \epsilon^*, \phi)) \end{aligned}$$

ELBO gradient (E-step, $\nabla_{\phi} \mathcal{L}(\phi, \theta)$)

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

Variational assumption

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

$$\mathbf{z} = g(\mathbf{x}, \epsilon, \phi) = \boldsymbol{\sigma}_{\phi}(\mathbf{x}) \cdot \epsilon + \boldsymbol{\mu}_{\phi}(\mathbf{x}).$$

Here $\boldsymbol{\mu}_{\phi}(\cdot)$, $\boldsymbol{\sigma}_{\phi}(\cdot)$ are parameterized functions (outputs of neural network).

- ▶ $p(\mathbf{z})$ – prior distribution on latent variables \mathbf{z} . We could specify any distribution that we want. Let say $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$.
- ▶ $p(\mathbf{x}|\mathbf{z}, \theta)$ - generative distribution. Since it is a parameterized function let it be neural network with parameters θ .

Variational autoencoder (VAE)

Final algorithm

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

$$\epsilon^* \sim r(\epsilon); \quad \mathbf{z}^* = g(\mathbf{x}, \epsilon^*, \phi);$$

$$\mathcal{L}(\phi, \theta) \approx \log p(\mathbf{x}|\mathbf{z}^*, \theta) - KL(q(\mathbf{z}^*|\mathbf{x}, \phi)||p(\mathbf{z}^*)).$$

- ▶ compute a stochastic gradients w.r.t. ϕ and θ

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

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

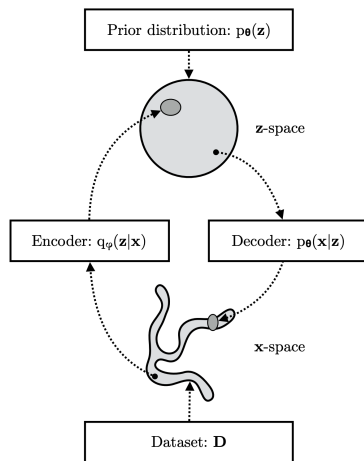
- ▶ update θ, ϕ according to the selected optimization method (SGD, Adam, RMSProp):

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

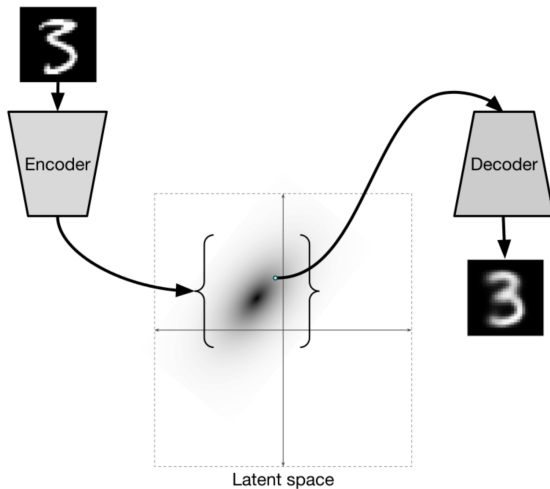
$$\theta := \theta + \eta \nabla_{\theta} \mathcal{L}(\phi, \theta).$$

Variational autoencoder (VAE)

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



Variational Autoencoder



Variational autoencoder (VAE)

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

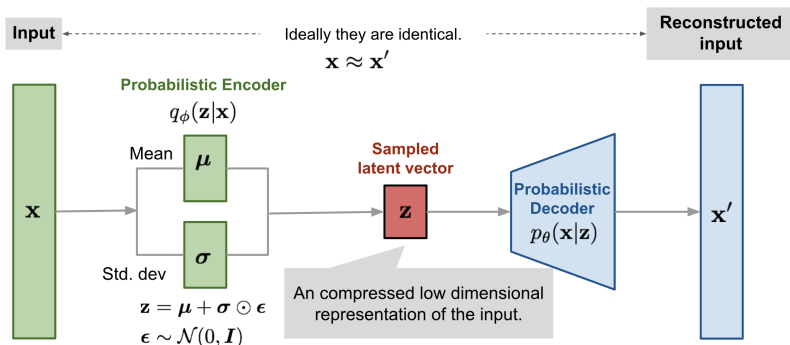


image credit:

<https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html>

Bayesian framework

Posterior distribution

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

Bayesian inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\theta)p(\theta|\mathbf{X})d\theta$$

Maximum a posteriori (MAP) estimation

$$\theta^* = \arg \max_{\theta} \log p(\theta|\mathbf{X}) = \arg \max_{\theta} (\log p(\mathbf{X}|\theta) + \log p(\theta))$$

MAP inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\theta)p(\theta|\mathbf{X})d\theta = \int p(\mathbf{x}|\theta)\delta(\theta - \theta^*)d\theta \approx p(\mathbf{x}|\theta^*).$$

VAE as Bayesian model

Posterior distribution

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

ELBO

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

EM-algorithm

► E-step

$$q(\mathbf{z}) = \arg \max_q \mathcal{L}(q, \theta^*) = \arg \min_q KL(q||p) = p(\mathbf{z}|\mathbf{x}, \theta^*);$$

► M-step

$$\theta^* = \arg \max_{\theta} [\mathcal{L}(q, \theta) + \log p(\theta)].$$

VAE limitations

- ▶ Poor variational posterior distribution (inference model encoder)

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

- ▶ Poor prior distribution

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

- ▶ Poor probabilistic model (generative model, decoder)

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

- ▶ Loose lower bound

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

Likelihood-based models so far...

Autoregressive models

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

- ▶ 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?

Change of variables

Theorem

- ▶ \mathbf{x} is a random variable with density function $p(\mathbf{x})$;
- ▶ $f : \mathbb{R}^m \rightarrow \mathbb{R}^m$ is a differentiable, invertible function (diffeomorphism);
- ▶ $\mathbf{z} = f(\mathbf{x})$, $\mathbf{x} = f^{-1}(\mathbf{z}) = g(\mathbf{z})$ (here $g = f^{-1}$).

Then

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

- ▶ \mathbf{x} and \mathbf{z} have the same dimensionality (lies in \mathbb{R}^m);
- ▶ $\left| \det \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \left| \det \left(\frac{\partial g^{-1}(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \left| \det \left(\frac{\partial g(\mathbf{z})}{\partial \mathbf{z}} \right) \right|^{-1}$;
- ▶ $f(\mathbf{x}, \boldsymbol{\theta})$ could be parametric function.

Fitting flows

MLE problem

$$\theta^* = \arg \max_{\theta} p(\mathbf{X}|\theta) = \arg \max_{\theta} \prod_{i=1}^n p(\mathbf{x}_i|\theta) = \arg \max_{\theta} \sum_{i=1}^n \log p(\mathbf{x}_i|\theta).$$

Challenge

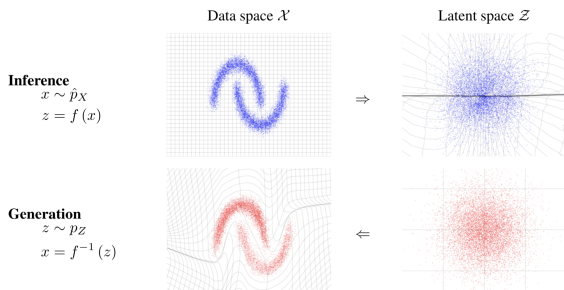
$p(\mathbf{x}|\theta)$ can be intractable.

Fitting flow to solve MLE

$$p(\mathbf{x}|\theta) = p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x}, \theta)) \left| \det \left(\frac{\partial f(\mathbf{x}, \theta)}{\partial \mathbf{x}} \right) \right|$$

$$\log p(\mathbf{x}|\theta) = \log p(f(\mathbf{x}, \theta)) + \log \left| \det \left(\frac{\partial f(\mathbf{x}, \theta)}{\partial \mathbf{x}} \right) \right|$$

Flows



Computational requirement

- ▶ Evaluating model density $p(\mathbf{x}|\boldsymbol{\theta})$ requires computing the transformation $\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta})$ and its Jacobian determinant $\left| \det \left(\frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}} \right) \right|$, and evaluating the density $p(\mathbf{z})$.
- ▶ Sampling \mathbf{x} from the model requires the ability to sample from $p(\mathbf{z})$ and to compute the transformation $\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta}) = f^{-1}(\mathbf{z}, \boldsymbol{\theta})$.

Forward KL vs Reverse KL

Forward KL

$$\begin{aligned} KL(\pi||p) &= \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\boldsymbol{\theta})} d\mathbf{x} \\ &= -\mathbb{E}_{\pi(\mathbf{x})} \log p(\mathbf{x}|\boldsymbol{\theta}) + \text{const} \rightarrow \min_{\boldsymbol{\theta}} \end{aligned}$$

Maximum likelihood estimation is equivalent to minimization of the Monte-Carlo estimation of forward KL.

Forward KL for flow model

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

- ▶ We need to be able to compute $f(\mathbf{x}, \boldsymbol{\theta})$ and its Jacobian.
- ▶ We need to be able to compute the density $p(\mathbf{z})$.
- ▶ We don't need to think about computing the function $g(\mathbf{z}, \boldsymbol{\theta}) = f^{-1}(\mathbf{z}, \boldsymbol{\theta})$ until we want to sample from the flow.

Forward KL vs Reverse KL

Reverse KL

$$\begin{aligned} KL(p||\pi) &= \int p(\mathbf{x}|\boldsymbol{\theta}) \log \frac{p(\mathbf{x}|\boldsymbol{\theta})}{\pi(\mathbf{x})} d\mathbf{x} \\ &= \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} [\log p(\mathbf{x}|\boldsymbol{\theta}) - \log \pi(\mathbf{x})] \rightarrow \min_{\boldsymbol{\theta}} \end{aligned}$$

Reverse KL for flow model

$$\log p(\mathbf{z}) = \log p(\mathbf{x}|\boldsymbol{\theta}) + \log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right|$$

$$KL(p||\pi) = \mathbb{E}_{p(\mathbf{z})} \left[\log p(\mathbf{z}) - \log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right| - \log \pi(g(\mathbf{z}, \boldsymbol{\theta})) \right]$$

- ▶ We need to be able to compute $g(\mathbf{z}, \boldsymbol{\theta})$ and its Jacobian.
- ▶ We need to be able to sample from the density $p(\mathbf{z})$ (do not need to evaluate it).
- ▶ We don't need to think about computing the function $f(\mathbf{x}, \boldsymbol{\theta})$.

Composition of flows

Theorem

Diffeomorphisms are **composable** (If f_1, f_2 satisfy conditions of the change of variable theorem (differentiable and invertible), then $\mathbf{z} = f(\mathbf{x}) = f_2 \circ f_1(\mathbf{x})$ also satisfies it).

$$\begin{aligned} p(\mathbf{x}) &= p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x})) \left| \det \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \\ &= p(f(\mathbf{x})) \left| \det \left(\frac{\partial f_2 \circ f_1(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}_2}{\partial \mathbf{f}_1} \cdot \frac{\partial \mathbf{f}_1}{\partial \mathbf{x}} \right) \right| = \\ &= p(f(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}_2}{\partial \mathbf{f}_1} \right) \right| \cdot \left| \det \left(\frac{\partial \mathbf{f}_1}{\partial \mathbf{x}} \right) \right| \end{aligned}$$

What will we get in the case $\mathbf{z} = f(\mathbf{x}) = f_n \circ \dots \circ f_1(\mathbf{x})$?

Flows

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

Definition

Normalizing flow is a *differentiable, invertible* mapping from data \mathbf{x} to the noise \mathbf{z} .

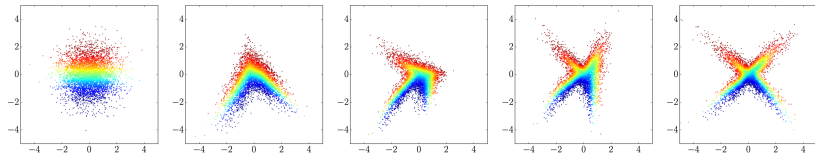
- ▶ "Normalizing" means that the inverse flow takes samples from $p(\mathbf{x})$ and normalizes them into samples from density $p(\mathbf{z})$.
- ▶ "Flow" refers to the trajectory followed by samples from $p(\mathbf{z})$ as they are transformed by the sequence of transformations

$$\mathbf{z} = f_K \circ \dots \circ f_1(\mathbf{x}); \quad \mathbf{x} = f_1^{-1} \circ \dots \circ f_K^{-1}(\mathbf{z}) = g_1 \circ \dots \circ g_K(\mathbf{z})$$

$$\begin{aligned} p(\mathbf{x}) &= p(f_K \circ \dots \circ f_1(\mathbf{x})) \left| \det \left(\frac{\partial f_K \circ \dots \circ f_1(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \\ &= p(f_K \circ \dots \circ f_1(\mathbf{x})) \prod_{k=1}^K \left| \det \left(\frac{\partial \mathbf{f}_k}{\partial \mathbf{f}_{k-1}} \right) \right|. \end{aligned}$$

Flows

Example of a 4-step flow



Flow likelihood

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

What is the complexity of the determinant computation?

What we want

- ▶ Efficient computation of Jacobian $\frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}}$;
- ▶ Efficient sampling from the base distribution $p(\mathbf{z})$;
- ▶ Efficient inversion of $f(\mathbf{x}, \boldsymbol{\theta})$.

Papamakarios G. et al. *Normalizing flows for probabilistic modeling and inference*, 2019

Summary

- ▶ The reparametrization trick gets unbiased gradients w.r.t to a variational posterior distribution.
- ▶ The VAE model is an LVM with two neural network: for stochastic encoder $q(\mathbf{z}|\mathbf{x}, \phi)$ and for stochastic decoder $p(\mathbf{x}|\mathbf{z}, \theta)$.
- ▶ VAE is not a "true" bayesian model since parameters θ do not have a prior distribution.
- ▶ Standart VAE has several limitations that we will address later in the course.
- ▶ Forward KL minimization is equivalent to MLE. Reverse KL is used in variational inference.
- ▶ Flow models transform a simple base distribution to a complex one via a sequence of invertible transformations.
- ▶ Flow models have a tractable likelihood that is given by the change of variable theorem.