

Deep Generative Models

Lecture 3

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Recap of previous lecture

Posterior distribution

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

Bayesian inference

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

Maximum a posteriori (MAP) estimation

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

MAP inference

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

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

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

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

ELBO derivation 1 (inequality)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} \geq \mathbb{E}_q \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} = \mathcal{L}(q, \boldsymbol{\theta})$$

ELBO derivation 2 (equality)

$$\begin{aligned} \mathcal{L}(q, \boldsymbol{\theta}) &= \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \int q(\mathbf{z}) \log \frac{p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})p(\mathbf{x}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \\ &= \log p(\mathbf{x}|\boldsymbol{\theta}) - KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) \end{aligned}$$

Variational decomposition

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

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

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

Outline

1. ELBO gradients, reparametrization trick
2. Variational autoencoder (VAE)
3. Tighter variational bound (IWAE)

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

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

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

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

Naive Monte-Carlo estimation

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

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

The variational posterior $q(\mathbf{z}|\mathbf{x}, \phi)$ assigns typically more probability mass in a smaller region than the prior $p(\mathbf{z})$.

image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

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

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:

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

Reparametrization trick (LOTUS trick)

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

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

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

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

Variational assumption

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

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

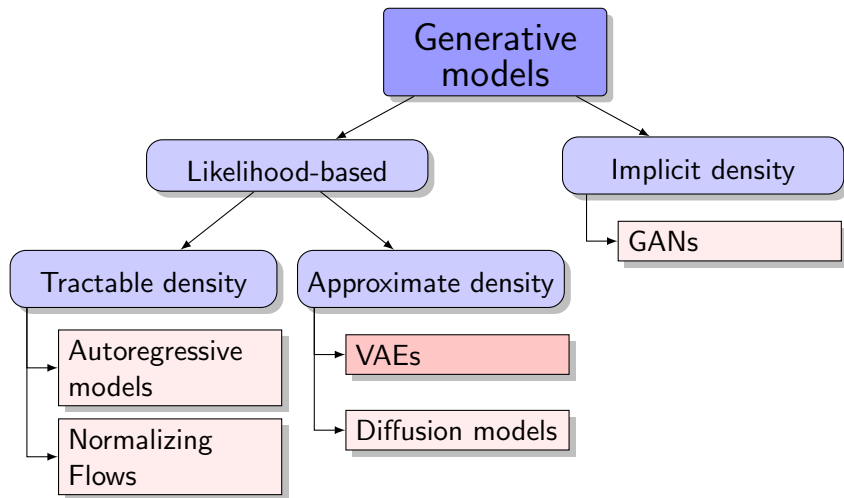
Here $\mu_{\phi}(\cdot), \sigma_{\phi}(\cdot)$ are parameterized functions (outputs of neural network).

- ▶ $p(\mathbf{z})$ – 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 .

Outline

1. ELBO gradients, reparametrization trick
2. Variational autoencoder (VAE)
3. Tighter variational bound (IWAE)

Generative models zoo



Variational autoencoder (VAE)

Final EM-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

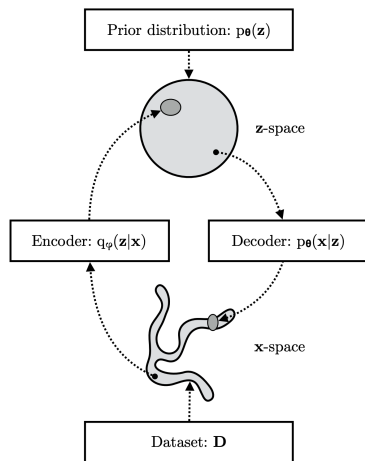
$$\begin{aligned}\nabla_{\phi} \mathcal{L}(\phi, \theta) &\approx \nabla_{\phi} \log p(\mathbf{x}|g_{\phi}(\mathbf{x}, \epsilon^*), \theta) - \nabla_{\phi} KL(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z})); \\ \nabla_{\theta} \mathcal{L}(\phi, \theta) &\approx \nabla_{\theta} \log p(\mathbf{x}|\mathbf{z}^*, \theta).\end{aligned}$$

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

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

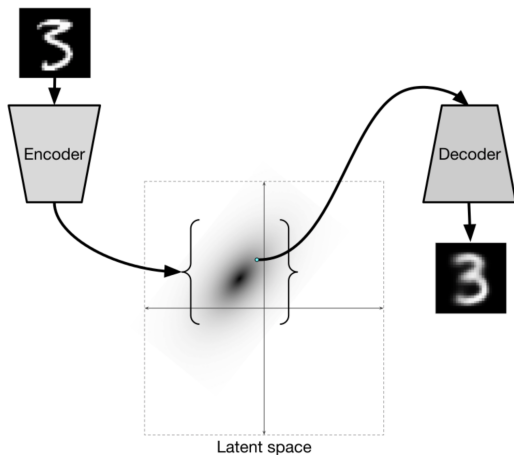
Variational autoencoder (VAE)

- ▶ 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

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



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.

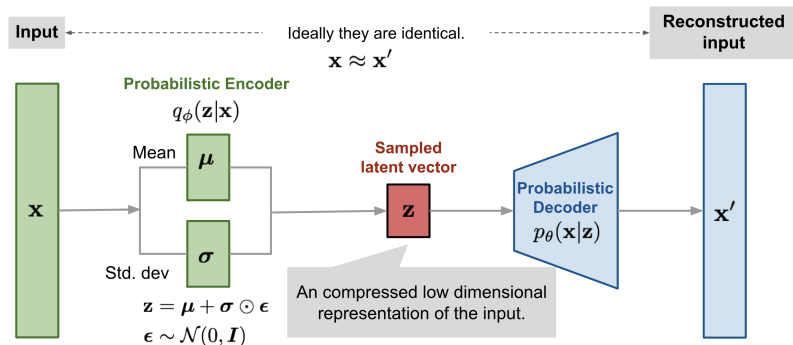


image credit:

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

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

- ▶ **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)

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

Importance sampling

LVM

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

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

ELBO: derivation 1

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

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

Summary

- ▶ Amortized variational inference allows to efficiently compute the stochastic gradients for ELBO using Monte-Carlo estimation.
- ▶ The reparametrization trick gets unbiased gradients w.r.t to the variational posterior distribution $q(\mathbf{z}|\mathbf{x}, \phi)$.
- ▶ The VAE model is an LVM with two neural network: stochastic encoder $q(\mathbf{z}|\mathbf{x}, \phi)$ and stochastic decoder $p(\mathbf{x}|\mathbf{z}, \theta)$.
- ▶ Standart VAE has several limitations that we will address later in the course.
- ▶ The IWAE could get the tighter lower bound to the likelihood, but the training of such model becomes more difficult.