Lec 10

Re-cap:

① AE → minimize reconstruction loss (deterministic)

↓

hidden space is not aligned well
(since we never impose such structure)

② VAE → latent variable model

mimic $p(z|x)$

$z \sim q_\phi(z|x)$

$x' \sim p(x|z)$

$\boxed{x} \rightarrow \boxed{\text{Encoder}} \rightarrow \boxed{z} \rightarrow \boxed{\text{Decoder}} \rightarrow \boxed{x'}$

$\left\{ \begin{array}{l} P_\theta(z) \\ P_\theta(x|z) \end{array} \right. \Rightarrow$ model $\Rightarrow$ inference on $P_\theta(z|x)$

Model Setting

intractable

⇓

Variational Inference

→ use $q_\phi(z|x)$ to approximate $p_\theta(z|x)$

via $\max_{\theta,\phi}$ ELBO

Today's lecture

① Introduction

a) $D_{KL}(p \| q) := \int_{\mathcal{X}} p(x) \log \frac{p(x)}{q(x)} \, dx$

b) Monte-Carlo Approximation

$$\mathbb{E}_{x \sim p(\cdot)} [f(X)] \approx \frac{1}{N} \sum_{i=1}^{N} f(x^{(i)}) \qquad x^{(i)} \sim p \text{ (i.i.d)}$$

c) ELBO (Decomposition)

$$\log p_\theta(x) = \underbrace{\boxed{\mathbb{E}_{z \sim q(\cdot)} \left[\log \left(\frac{p_\theta(x, z)}{q(z)} \right) \right]}}_{\text{ELBO}}$$

$$+ D_{KL}(q(z) \| p_\theta(z|x))$$

$$\Rightarrow \log p_\theta(x) \geq \text{ELBO} := \mathbb{E}_{z \sim q(\cdot)} \left[\log \left(\frac{p_\theta(x, z)}{q(z)} \right) \right]$$

② Optimize in ELBO

$$\max_{\theta} \log p_\theta(x)$$

$$\Big\downarrow \text{surrogate}$$

$$\max_{\theta, \varphi} \text{ELBO} := \mathcal{L}(\mathcal{D}; \theta, \varphi)$$

$$= \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_{z \sim q_\varphi(\cdot | x^{(i)})} \left[\log \left(\frac{p_\theta(x^{(i)}, z)}{q_\varphi(z | x^{(i)})} \right) \right]$$

For simplicity, we conside 1-sample $\mathcal{L} = \mathbb{E}_{z \sim q_\varphi(\cdot | x)} \left[\log \left(\frac{p_\theta(x, z)}{q_\varphi(z | x)} \right) \right]$

③ <u>Issue</u>: without compute the explicit form of "L"

consider the gradient $\nabla_\theta L$ & $\nabla_\varphi L$

a) $\nabla_\theta L = \mathbb{E}_{z \sim q_\varphi(\cdot|x)} [\nabla_\theta \log P_\theta(x, z)]$

(easy task)

b) $\nabla_\varphi L \neq \mathbb{E}_{z \sim q_\varphi(\cdot|x)} [\nabla_\varphi \log (\frac{P_\theta(x, z)}{q_\varphi(z|x)})]$

$\Downarrow$ <u>Reparameterization Trick</u>

<u>idea</u>:

we want to write $z \sim q_\phi(\cdot|x)$ as

the <u>equivalent form</u> $z = \mu + x + C^{\frac{1}{2}} u$

$\Rightarrow z \sim N(\mu + x, C)$

④ Reparameterization Trick

$\boxed{\text{Setting}}$

$\mu, \sigma^2 = \phi(x)$

$z|x \sim N(\mu, \sigma^2 I) \Leftrightarrow z|x = \mu(x) + \sigma^2(x) u$

$= q_\phi(\cdot|x)$ where $u \sim N(0, I)$

$\boxed{\text{Idea}} \Rightarrow$ use Gaussian with <u>trainable mean & variance</u>

to <u>approximate posterior $P_\theta(z|x)$</u>

$$q_\phi(\cdot|x) = N(\mu(x), \sigma^2(x) I) \approx P_\theta(z|x)$$

Then $\nabla_\varphi L = \nabla_\varphi \mathbb{E}_{z \sim q_\phi(\cdot|x)} [L(x, z)]$

$$= \mathbb{E}_{u \sim N(0,I)} \left[\nabla_\varphi \tilde{L}(x, \mu(x) + \sigma(x) u) \right]$$

via Monte-Carlo Approximation

⑤ Model of $p_\theta(x|z)$ $p_\theta(z)$ $q_\varphi(z|x)$

a) Consider Classification Scenario $\Rightarrow$ $p_\theta(x|z)$: Bernoulli

$$\Rightarrow \begin{cases} s_\theta = \text{DecodingNN}(z; \theta) \\ p_\theta(x|z) = s_\theta^{\,x} (1-s_\theta)^{1-x} \end{cases} \Leftrightarrow \log p(x|z) = x \log s_\theta + (1-x) \log(1-s_\theta)$$

$$\log p_\theta(z) = \sum_j -\frac{1}{2} \log(2\pi) - \frac{1}{2} z_j^2$$

b) $p_\theta(z) \longrightarrow N(0, I)$

$\boxed{\text{vector}}$

$\boxed{\log \sigma_\varphi}$ for technique consideration

c) $$\begin{cases} (\mu_\varphi, \boxed{\sigma_\varphi^2}) = \text{EncodingNN}(x; \varphi) \\ q_\varphi(z|x) = \text{Gaussian}(z; \mu_\varphi, \sigma_\varphi^2 I) \end{cases}$$

$\Downarrow$ Reparameterization Trick

$$\boxed{z \sim q_\varphi(\cdot|x)}$$

$\Updownarrow$

$$\boxed{\begin{array}{l} u \sim \text{Gaussian}(0, I) \\ z := \mu_\varphi + \sigma_\varphi \circ u \end{array}}$$

$$\Rightarrow \log q_\varphi(z|x) = \sum_j -\frac{1}{2} \log(2\pi \sigma_j^2) - \frac{1}{2} \left(\frac{z_j - \mu_j}{\sigma_j} \right)^2$$

$$= \boxed{\sum_j -\frac{1}{2}\log(2\pi\sigma_j^2) - \frac{1}{2}u_j^2}$$

⑥ Summary:

$\boxed{x \in \mathbb{R}^d} \rightarrow$ input dimension

a) $\log p_\theta(x|z) = \sum_i x_i \log s_{\theta,i} + (1-x_i)\log(1-s_{\theta,i})$

b) $\log p_\theta(z) = \sum_j -\frac{1}{2}\log 2\pi - \frac{1}{2} z_j^2$

$$= \sum_j -\frac{1}{2}\log 2\pi - \frac{1}{2}(\sigma_j u_j + \mu_j)^2$$

c) $\log q_\phi(z|x) = \sum_j -\frac{1}{2}\log(2\pi\sigma_j^2) - \frac{1}{2}u_j^2$

$\Rightarrow$

a) $\mathbb{E}_{z\sim q_\phi(\cdot|x)}[\log p_\theta(x|z)]$

b) $\mathbb{E}_{z\sim q_\phi(\cdot|x)}[\log p_\theta(z)] = \mathbb{E}_u[\sum_j \text{const} - \frac{1}{2}(\sigma_j u_j + \mu_j)^2]$

$$= -\frac{1}{2}\sum_j(\mu_j^2 + \sigma_j^2)$$

c) $\mathbb{E}_{z\sim q_\phi(\cdot|x)}[\log q_\phi(z|x)]$

$$= \mathbb{E}_u[\sum_j -\frac{1}{2}\log\sigma_j^2 - \frac{1}{2}u_j^2]$$

$$= \sum_j -\frac{1}{2}\log\sigma_j^2 = -\sum_j \log\sigma_j$$

$$\boxed{\hat{\theta}, \hat{\phi} = \arg\max \text{ ELBO}}$$

Recap: $\text{ELBO} = \mathbb{E}_{z\sim q_\phi(\cdot|x)}\left[\log\left(\frac{p_\theta(x,z)}{q_\phi(z|x)}\right)\right]$

$\Downarrow$

$$L = -\text{ELBO} = -\mathbb{E}_z\left[\log\left(\frac{p_\theta(x,z)}{q_\phi(z|x)}\right)\right]$$

$$= \boxed{- \mathbb{E}_{z \sim q_\phi(\cdot|x)} \left[\log p_\theta(x|z) \right]}$$

$$+ \boxed{D_{KL}\left(q_\phi(z|x) \,\|\, p_\theta(z) \right)}$$

reconstruction loss

Normalization (Regularization)

$$= \underline{\frac{1}{2} \| \mu_\phi \|_2^2 + \frac{1}{2} \| \sigma_\phi \|_2^2 - \sum_j \log \sigma_{\phi, j}}$$