LEC07

Variational inference

$$p(z|x) = \frac{p(x|z)\,p(z)}{p(x)}$$

$$= \frac{p(x,z)}{p(x)}$$

$$= \frac{p(x,z)}{\int p(x,z')\,dz'}$$

easy

hard :-c

I. Variational inference

Approximate $p(z|x)$ with some variational distribution $q_\phi(z)$.

see end of file

Renew KL

$$KL\left(q_\phi(z)\,\|\,p(z|x)\right)$$

$$= \mathbb{E}_{q_\phi(z)}\left[\log \frac{q_\phi(z)}{p(z|x)}\right]$$

Can't evaluate since we don't know $p(z|x)$!

$$= \mathbb{E}_{q_\phi(z)}\left[\log q_\phi(z)\right] - \mathbb{E}_{q_\phi(z)}\left[\log p(z|x)\right]$$

Bayes

$$= \mathbb{E}_{q_\phi(z)}[\log q_\phi(z)] - \mathbb{E}_{q_\phi(z)}[\log p(x,z) - \log p(x)]$$

$$= \mathbb{E}_{q_\phi(z)}[\log q_\phi(z) - \log p(x,z)] + \log p(x)$$

$$= -\underbrace{\mathbb{E}_{q_\phi(z)}\left[\log \frac{p(x,z)}{q_\phi(z)}\right]}_{\text{ELBO}(\phi)} + \log p(x)$$

$\Rightarrow \min_\phi \; KL(q_\phi(z) \,\|\, p(z|x))$ is equivalent to $\max_\phi \; \text{ELBO}(\phi)$

$$\boxed{\begin{aligned} \text{ELBO}(\phi) &= \mathbb{E}_{q_\phi(z)}\left[\log \frac{p(x,z)}{q_\phi(z)}\right] \\ &= \mathbb{E}_{q_\phi(z)}[\log p(x,z)] + \mathbb{H}[q_\phi(z)] \end{aligned}}$$

II. ADVI

automatic differentiation variational inf.

How to choose q ?

1) Transform the support of the latent variables z such that they live in $\mathbb{R}^K$.

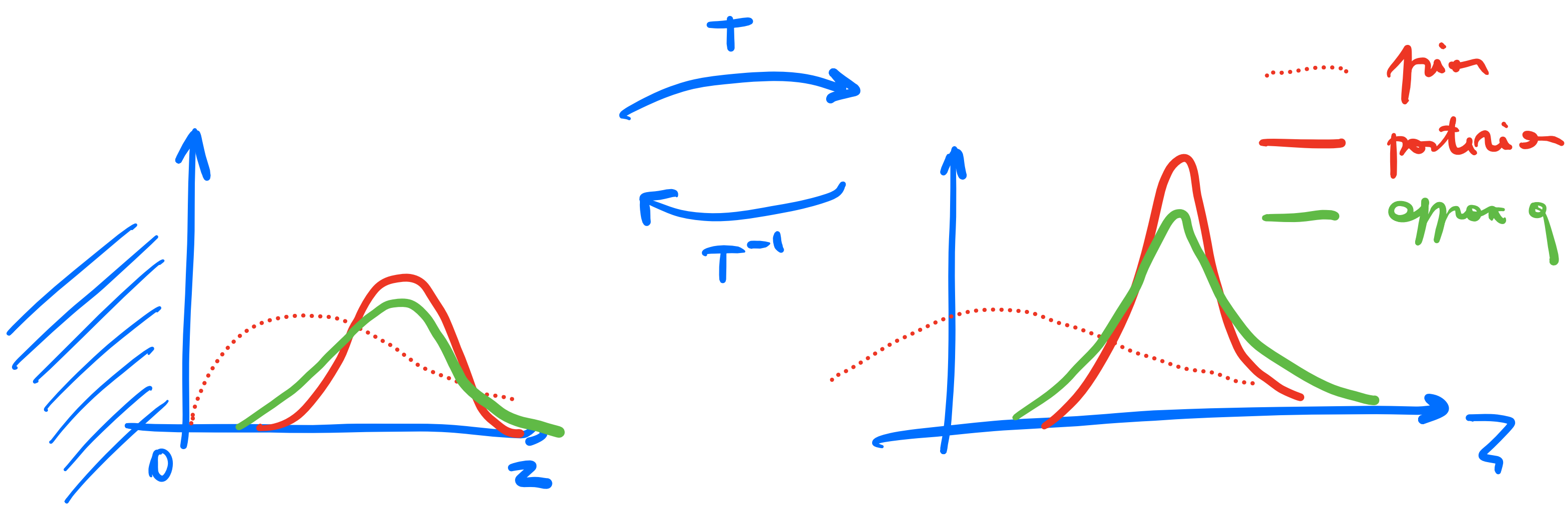
$$T : \text{support}(p(z)) \longmapsto \mathbb{R}^K$$

will be easier to define q over $\mathbb{R}^K$ (e.g. $q := \mathcal{N}$)

$$\zeta = T(z)$$

$$\Rightarrow \quad p(x, \zeta) = p(x, T^{-1}(\zeta)) \left| \det J_{T^{-1}}(\zeta) \right|$$

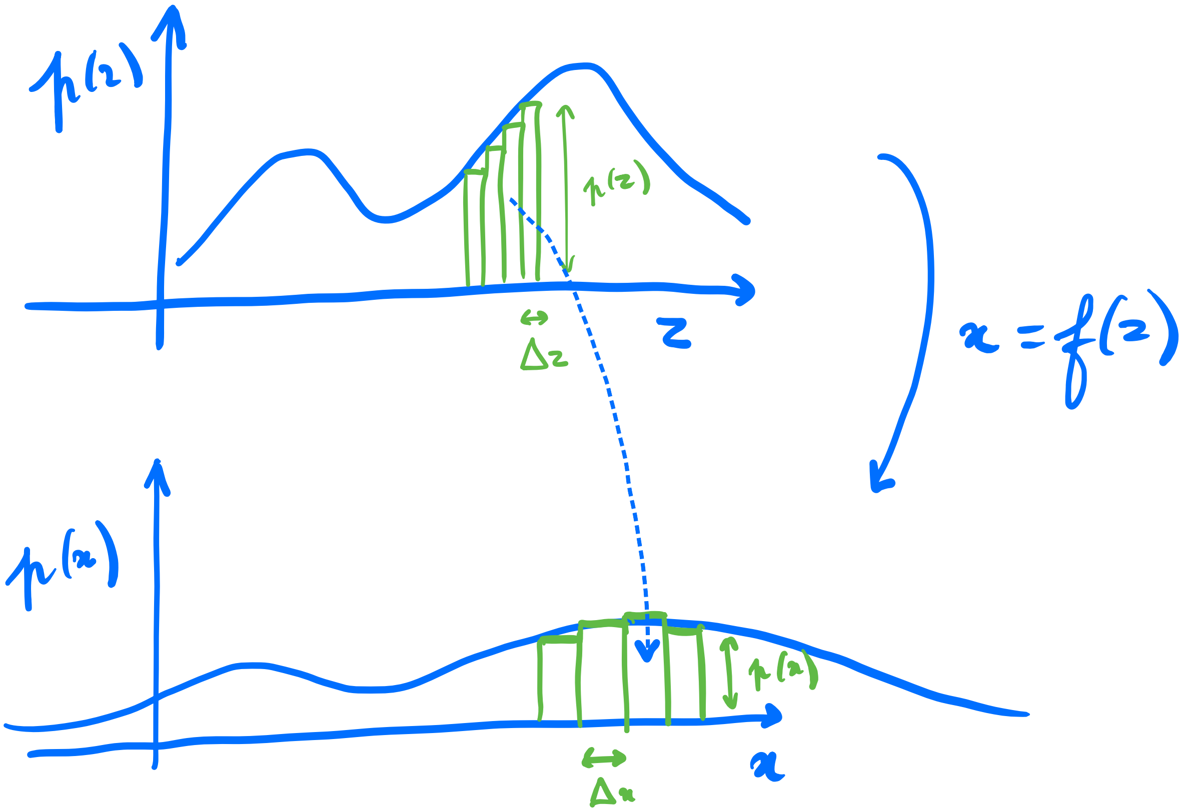
change of variable thm



latent variable space (e.g. $[0;+\infty[$)

real coordinate space $\mathbb{R}$

Change of variable theorem:



Conservation de la densité

$$p(z)\,\Delta z = p(x)\,\Delta x$$

Change of volume

→ stretching z to x must be compensated by reducing p(x)

① → $p(x) = p(z)\,\dfrac{\Delta z}{\Delta x}$

$z = f^{-1}(x)$

$$= p(f^{-1}(x))\,\frac{\Delta f^{-1}}{\Delta x}$$

$\Delta x \to 0$

$$= p(f^{-1}(x))\left|\frac{\partial f^{-1}}{\partial x}\right|$$

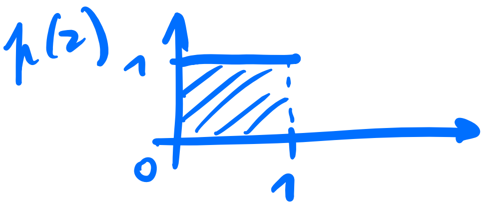
→ |.| because of ratio of two areas

② → $p(x) = p(z)\,\dfrac{\Delta z}{\Delta x}$

$$p(f(z)) = p(z)\,\frac{\Delta z}{\Delta f} = \left(\frac{\Delta f}{\Delta z}\right)^{-1} \qquad x = f(z)$$

$$\overset{\Delta z \to 0}{=} p(z)\left|\frac{\partial f}{\partial z}\right|^{-1}$$

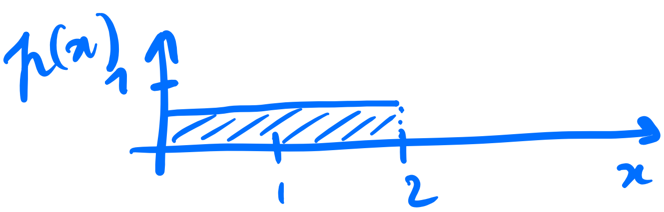
Example:



$$p(z) = \begin{cases} 1 & \text{if } z \in [0;1] \\ 0 & \text{else} \end{cases}$$

$$x = f(z) = 2z \longrightarrow z = f^{-1}(x) = \frac{1}{2}x$$

$$p(x) = p(f^{-1}(x))\left|\frac{\partial f^{-1}}{\partial x}\right| = p(f^{-1}(x))\,\frac{1}{2}$$



$$\begin{array}{cc} & j \\ i & \begin{bmatrix} \cdots & \frac{\partial f_i}{\partial x_j} & \end{bmatrix} \end{array}$$

Multivariate case:

$$p(x) = p(f^{-1}(x))\left|\det \frac{\partial f^{-1}}{\partial x}\right| \longrightarrow \text{Jacobian of } f^{-1}$$

$$p(x = f(z)) = p(z)\left|\det \frac{\partial f}{\partial x}\right|^{-1} \longrightarrow \text{Jacobian of } f$$

2) Posit a mean-field Gaussian variational approximation:

$$q_{\phi}(\underline{z}) = \mathcal{N}(\underline{z} \mid \underline{\mu}, \underline{\sigma}^2)$$

$$= \prod_{k=1}^{K} \mathcal{N}(z_k \mid \underbrace{\mu_k, \sigma_k^2}) \qquad \phi = \{\mu_1, \sigma_1, \dots, \mu_k, \sigma_k\}$$

⚠ Strong assumption
⇒ no posterior covariance

(1) + (2):

$$\mathcal{L}(\underline{\mu}, \underline{\sigma}^2) = \mathbb{E}_{q(z)}\left[\log p(x, T^{-1}(z)) \left|\det J_{T^{-1}}(z)\right|\right] + \underbrace{\mathbb{H}[q(z)]}_{= \frac{K}{2}(1 + \log 2\pi) + \sum_{k=1}^{K} \log \sigma_k^2}$$

3) Optimization:

$$\underline{\mu}^*, \underline{\sigma}^{2*} = \arg\max_{\underline{\mu}, \underline{\sigma}^2} \mathcal{L}(\underline{\mu}, \underline{\sigma}^2)$$

$$\text{s.t} \quad \underline{\sigma}^2 > 0$$

$\Rightarrow$ Stochastic gradient ascent on $\mathcal{L}$.

⚠ - How to enforce $\underline{\sigma}^2 > 0$?

$\Rightarrow$ Reparametrize $\underline{\omega} = \log \underline{\sigma}^2 \in \mathbb{R}^K$

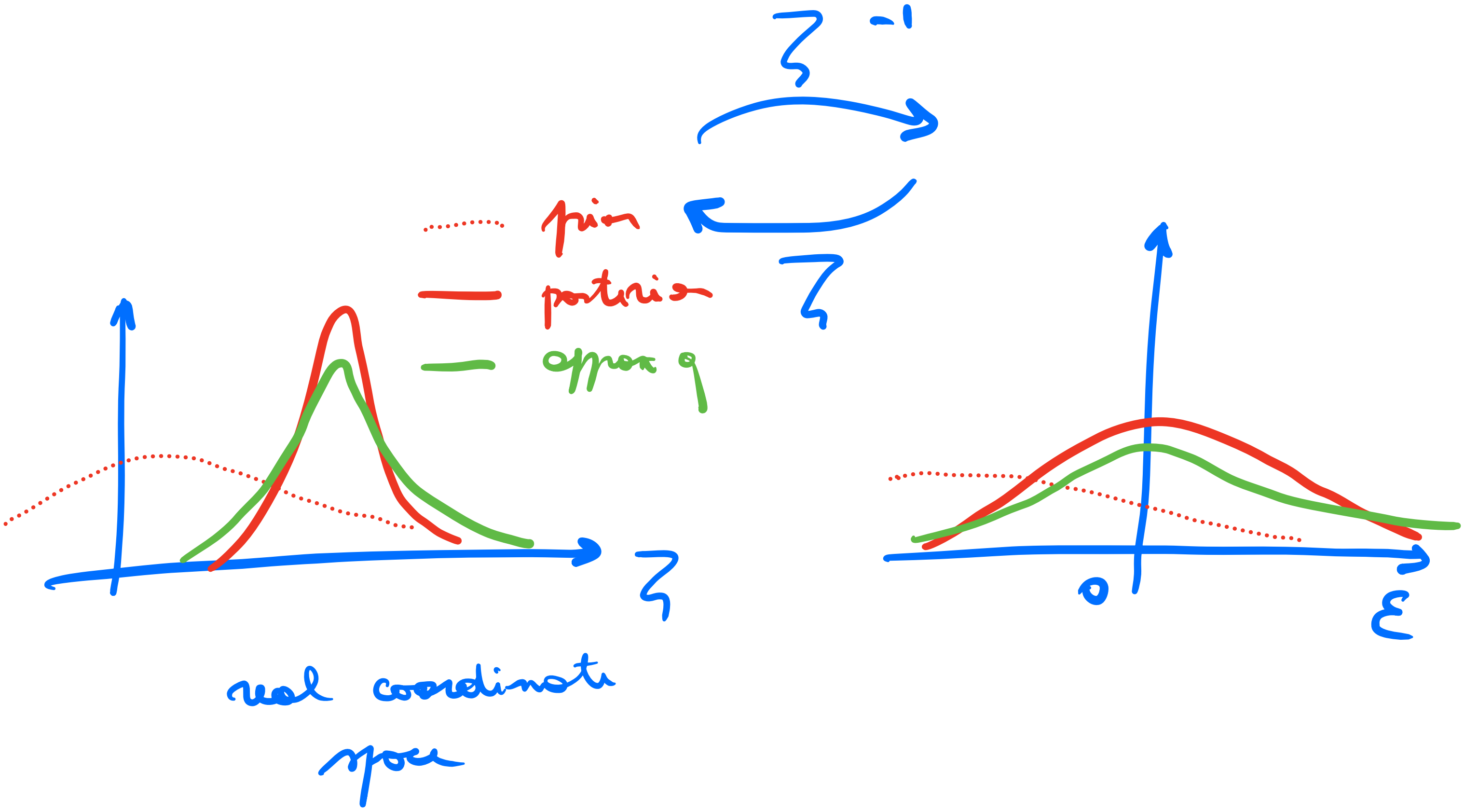
- $\mathbb{E}_q$ depends on ϕ, here

$$\nabla_\phi \mathbb{E}_{q_\phi} \neq \mathbb{E}_{q_\phi} \nabla_\phi$$

3b) Reparametrization trick:

$$\underline{\varepsilon} \sim \mathcal{N}(0, I)$$

$$\underline{z} = \underline{\mu} + \operatorname{diag}\left(\sqrt{\exp(\underline{\omega})}\right) \underline{\varepsilon}$$



$= p(x|z)\, p(z)$

$$\underline{\mu}^*, \underline{\omega}^* = \arg\max_{\mu,\omega} \mathcal{L}(\underline{\mu}, \underline{\omega})$$

$$= \arg\max_{\underline{\mu}, \underline{\omega}} \mathbb{E}_{\mathcal{N}(\varepsilon; 0, I)} \Big[\log p(x, T^{-1}(\zeta(\varepsilon))) + \log \left| \det J_{T^{-1}}(\zeta(\varepsilon)) \right| \Big] + \sum_{k=1}^{K} \omega_k$$

$$\nabla_\mu \mathcal{L} = \mathbb{E}_{\mathcal{N}(\varepsilon)}[\underbrace{\nabla_\mu (\ldots)}]$$

$$\nabla_{w_k} \mathcal{L} = \mathbb{E}_{\mathcal{N}(\varepsilon)}[\underbrace{\nabla_{w_k} (\ldots)}] + 1$$

with auto-diff

approximate the expectation using M samples

Start with the forward KL → better choice if q has high capacity

II. Neural posterior approximation

amortize over all x

$$\min_\phi \mathbb{E}_{p(x)}\Big[\underbrace{KL}_{\text{forward KL}}\big(p(z|x)\,\|\,\underbrace{q_\phi(z|x)}_{\text{neural density estimator}}\big)\Big]$$

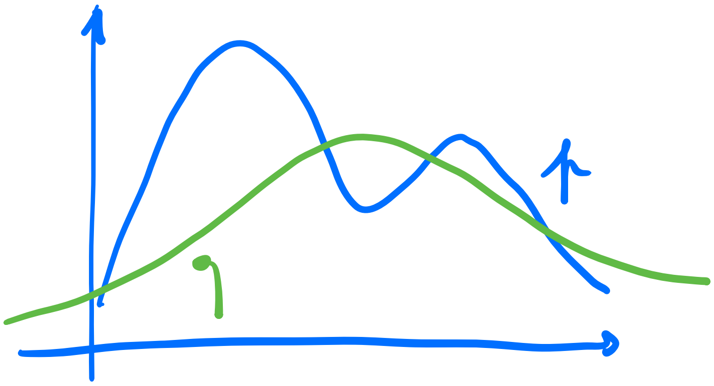
$$= \min_\phi \mathbb{E}_{p(x)\,p(z|x)}\left[\log \frac{p(z|x)}{q_\phi(z|x)}\right]$$

$$= \max_\phi \mathbb{E}_{p(x,z)}\left[\log q_\phi(z|x)\right]$$

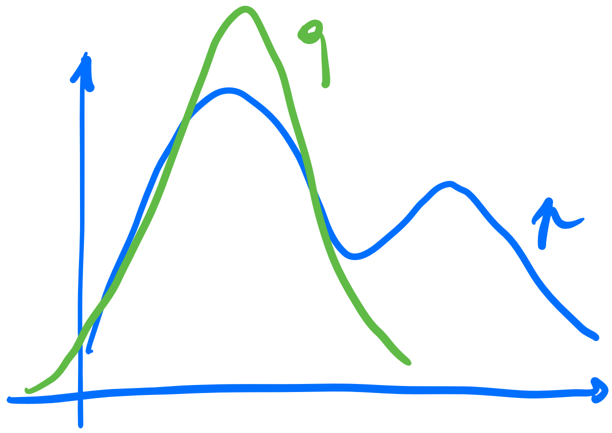
Forward KL vs. Reverse KL

$$KL(p \,\|\, q) = \mathbb{E}_p\left[\log \frac{p}{q}\right]$$

$$KL(q \,\|\, p) = \mathbb{E}_q\left[\log \frac{q}{p}\right]$$



mean-seeking



mode-seeking