





$$\mathbb{E}_z \log p(x; \theta) = \mathbb{E}_z \log \left[\sum_z p(x; z; \theta) \right]$$

when z is high-dim eg. $\{0, 1\}^D$, the summation/integral is intractable

Need approximation

• Naïve Monte Carlo

$$\begin{aligned} p_\theta(x) &= \sum_{z \in \mathcal{U}(z)} p_\theta(x; z) = |\mathcal{U}(z)| \sum_{z \in \mathcal{U}(z)} \frac{1}{|\mathcal{U}(z)|} p_\theta(x; z) \\ &= |\mathcal{U}(z)| \cdot \mathbb{E}_{z \sim \text{uniform}(\mathcal{U}(z))} [p_\theta(x; z)] \\ &\approx |\mathcal{U}(z)| \cdot \frac{1}{K} \sum_{z^i} p_\theta(x; z^i) \end{aligned}$$

randomly sample $z^1, \dots, z^K \sim \text{uniform}(\mathcal{U}(z))$

$$\text{approximate } \sum_{z \in \mathcal{U}(z)} p_\theta(x; z) \approx |\mathcal{U}(z)| \cdot \frac{1}{K} \sum_{z^i} p_\theta(x; z^i)$$

problems: most $p_\theta(x; z)$ will be very low (most image completion does not make sense)

some $p_\theta(x; z)$ is very high, but is rarely sampled by uniform sampling

Need a clever way to select z^i to reduce the variance of the estimator

• Importance Sampling

$$\begin{aligned} p_\theta(x) &= \sum_{z \in \mathcal{U}(z)} p_\theta(x; z) = \sum_{z \in \mathcal{U}(z)} \frac{q(z)}{q(z)} \cdot p_\theta(x; z) \\ &= \mathbb{E}_{z \sim q} \left[\frac{p_\theta(x; z)}{q(z)} \right] \\ &\approx \frac{1}{K} \sum_{z^i} \frac{p_\theta(x; z^i)}{q(z^i)} \end{aligned}$$

randomly sample $z^1, \dots, z^K \sim q(z)$

$$\text{approximate } p_\theta(x) \approx \frac{1}{K} \sum_{z^i} \frac{p_\theta(x; z^i)}{q(z^i)}$$

$$\begin{aligned} \log(p_\theta(x)) &\approx \log \left(\frac{1}{K} \sum_{z^i} \frac{p_\theta(x; z^i)}{q(z^i)} \right) \\ &\approx \log \left(\frac{p_\theta(x; z^k)}{q(z^k)} \right) \end{aligned}$$

$$\log \left[\mathbb{E}_{z \sim q} \left[\frac{p_\theta(x; z)}{q(z)} \right] \right] \neq \mathbb{E}_{z \sim q} \left[\log \left(\frac{p_\theta(x; z)}{q(z)} \right) \right]$$

$$\begin{aligned} \mathbb{E}_{z \sim q} \left[\frac{1}{K} \sum_{i=1}^K \frac{p_\theta(x; z^i)}{q(z^i)} \right] &= \mathbb{E}_{z \sim q} \left[\frac{p_\theta(x; z)}{q(z)} \right] \\ &= \sum_z q(z) \frac{p_\theta(x; z)}{q(z)} \\ &= p_\theta(x) \quad \text{unbiased estimator} \end{aligned}$$

$$\begin{aligned} \text{Var}_{z \sim q} \left[\frac{1}{K} \sum_{i=1}^K \frac{p_\theta(x; z^i)}{q(z^i)} \right] &= \frac{1}{K} \text{Var}_{z \sim q} \left(\frac{p_\theta(x; z)}{q(z)} \right) \\ &= \frac{1}{K} \left(\mathbb{E}_{z \sim q} \left[\left(\frac{p_\theta(x; z)}{q(z)} \right)^2 \right] - \mathbb{E}_{z \sim q} \left[\frac{p_\theta(x; z)}{q(z)} \right]^2 \right) \\ &= \frac{1}{K} \left(\mathbb{E}_{z \sim q} \left[\left(\frac{p_\theta(x; z)}{q(z)} \right)^2 \right] - p_\theta(x)^2 \right) \end{aligned}$$

when $\frac{p_\theta(x; z)}{q(z)} \approx p_\theta(x)$, the var is small

$$q(z) = p_\theta(z|x)$$

unless $\frac{p_\theta(x; z)}{q(z)}$ is constant $\forall z$

• Variational Inference

suppose $q(z)$ is any distribution over z

$$\begin{aligned} \log p(x; \theta) &= \log \left[\sum_z q(z) \cdot \frac{p(x; z; \theta)}{q(z)} \right] \\ &\geq \sum_z q(z) \cdot \log \frac{p(x; z; \theta)}{q(z)} \end{aligned}$$

equality holds if $q(z) = p_\theta(z|x)$

$$\begin{aligned}
 &= \sum_z q(z) \cdot \log p(x, z; \theta) - \sum_z q(z) \cdot \log q(z) \\
 &= \underbrace{\sum_z q(z) \cdot \log p(x, z; \theta)}_{\text{lower bound}} + H(q)
 \end{aligned}$$

$$\begin{aligned}
 \log p(x; \theta) &= \sum_z q(z) \log p(x, z; \theta) \\
 &= \sum_z q(z) \left[\log p(x, z; \theta) + \log q(z) - \log q(z) \right] \\
 &= \sum_z q(z) \left[\log \frac{p(x, z; \theta)}{q(z; \theta)} + \log q(z) - \log q(z) \right] \\
 &= \sum_z q(z) \left[\log \frac{q(z)}{p(z; \theta)} + \log p(x, z; \theta) - \log q(z) \right] \\
 &= \text{KL}(q(z) \| p(z; \theta)) + \text{lower bound}
 \end{aligned}$$

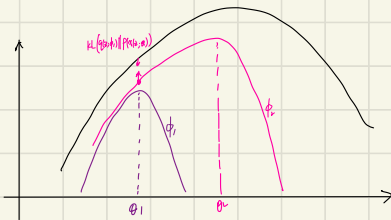
the closer $q(z)$ is to $p(z; \theta)$, the closer the lower bound is to $\log p(x; \theta)$

variational Inference: choose a parametric form $q(z; \phi)$, and make $q(z; \phi)$ as close as possible to $p(z; \theta)$

eg

Assume $p(x_{train}, z; \theta)$ has high prob if (x, z) looks like real digits

suppose we choose a binomial distribution
 $q(z; \phi) = \prod (\phi_i)^{z_i} (1 - \phi_i)^{1 - z_i}$



— lower bound $\sum_z q(z; \phi) \log p(x, z; \theta) + H(q; \phi)$ $\phi = \phi_1$

— lower bound $\sum_z q(z; \phi) \log p(x, z; \theta) + H(q; \phi)$ $\phi = \phi_2$

• Lower Bound for entire dataset

$$\begin{aligned}
 \ell(\theta) &= \sum_i \log p(x_i; \theta) = \sum_i \log \sum_z p(x_i, z; \theta) \\
 &= \sum_i \left(\log \sum_z q(z; \phi_i) \frac{p(x_i, z; \theta)}{q(z; \phi_i)} \right) \\
 &\geq \sum_i \sum_z q(z; \phi_i) \cdot \log \frac{p(x_i, z; \theta)}{q(z; \phi_i)} \\
 &= \sum_i \left[\sum_z q(z; \phi_i) \cdot \log p(x_i, z; \theta) + H(q_i) + \text{KL}(q_i(z; \phi_i) \| p(z; \theta_i)) \right]
 \end{aligned}$$

let $\theta^* = \arg\max_{\theta} \ell(\theta)$ $\ell(\theta, \hat{\phi}) = \arg\max_{\theta, \hat{\phi}} \sum_i \sum_{z_i} q_i(z_i; \phi_i) \cdot \log \frac{p(x_i, z_i; \theta)}{q_i(z_i; \phi_i)}$

$$\sum_i \sum_{z_i} q_i(z_i; \hat{\phi}_i) \cdot \log \frac{p(x_i, z_i; \hat{\theta})}{q_i(z_i; \hat{\phi}_i)} \leq \sum_i \log \sum_{z_i} p(x_i, z_i; \hat{\theta}) = \ell(\hat{\theta}) \leq \ell(\theta^*)$$

for each x_i , need to find a ϕ_i such that $KL(q_i(z_i; \phi_i) \| p(z_i | x_i, \theta))$ is small
(can be expensive)

Learning via Stochastic Variational Inference

the lower bound $\mathcal{L}(x_i; \theta, \phi_i) = \sum_{z_i} q_i(z_i; \phi_i) \cdot \log \frac{p(x_i, z_i; \theta)}{q_i(z_i; \phi_i)} = \mathbb{E}_{z_i \sim q_i} \left[\log \frac{p(x_i, z_i; \theta)}{q_i(z_i; \phi_i)} \right]$

optimize $\sum_i \mathcal{L}(x_i; \theta, \phi_i)$ with stochastic gradient descent

initialize $\theta, \phi_i \leftarrow \phi^*$
 randomly sample x_i from D
 optimize $\mathcal{L}(x_i; \theta, \phi_i)$ w.r.t ϕ_i
 compute $\nabla_{\phi_i} \mathcal{L}(x_i; \theta, \phi_i)$
 apply gradient ascent until $\phi_i \approx \arg\max_{\phi_i} \mathcal{L}(x_i; \theta, \phi_i)$
 compute $\nabla_{\theta} \mathcal{L}(x_i; \theta, \phi_i)$
 update θ with gradient ascent, go to 2

$$\begin{aligned} & \max_{\phi_i} \sum_{z_i} q_i(z_i; \phi_i) \cdot \log \frac{p(x_i, z_i; \theta)}{q_i(z_i; \phi_i)} \\ &= \max_{\phi_i} \sum_{z_i} \left[q_i(z_i; \phi_i) \cdot \log \frac{p(x_i, z_i; \theta) \cdot p(z_i; \phi_i)}{q_i(z_i; \phi_i)} \right] \\ &= \max_{\phi_i} \sum_{z_i} q_i(z_i; \phi_i) \log \frac{p(x_i, z_i; \theta)}{q_i(z_i; \phi_i)} - \sum_{z_i} q_i(z_i; \phi_i) \cdot p(x_i; \theta) \\ &= \max_{\phi_i} \sum_{z_i} q_i(z_i; \phi_i) \log \frac{p(x_i, z_i; \theta)}{q_i(z_i; \phi_i)} \\ &= \min_{\phi_i} KL(q_i(z_i; \phi_i) \| p(z_i | x_i, \theta)) \end{aligned}$$

to evaluate the bound. sample $z_i^{(k)} \sim q_i(z_i; \phi_i)$

approximate $\mathcal{L}(x_i; \theta, \phi_i) = \mathbb{E}_{z_i \sim q_i} \left[\log \frac{p(x_i, z_i; \theta)}{q_i(z_i; \phi_i)} \right] \approx \frac{1}{K} \sum_k \log \frac{p(x_i, z_i^{(k)}; \theta)}{q_i(z_i^{(k)}; \phi_i)}$

(Assume $q_i(\cdot)$ is easy to evaluate and sample from)

so $\mathbb{E}_{z_i \sim q_i} \left[\log p(x_i, z_i; \theta) - \log q_i(z_i; \phi_i) \right] = \mathbb{E}_{z_i \sim q_i} \left[\nabla_{\theta} \log p(x_i, z_i; \theta) \right] \approx \frac{1}{K} \sum_k \nabla_{\theta} \log p(x_i, z_i; \theta)$

evaluating ∇_{ϕ_i} is hard

Computing $\nabla_{\phi_i} \mathbb{E}_{z_i \sim q_i} [-\log q_i(z_i; \phi_i)]$ when z_i is continuous

$$\mathbb{E}_{z_i \sim q_i} [-\log q_i(z_i; \phi_i)] = - \int_{z_i} q_i(z_i; \phi_i) \log q_i(z_i; \phi_i) dz_i$$

suppose q_i is $\mathcal{N}(u_i, b_i^2 I)$, to sample from q_i , there are 2 equivalent ways

1 sample $z_i \sim \mathcal{N}(u_i, b_i^2 I)$

2 sample $t_i \sim \mathcal{N}(0, I)$, $z_i = u_i + t_i \cdot b_i$, $b_i = g(t_i, u_i, b_i)$