SGVI(Stochastic Gradient Variational Inference)

> https://www.bilibili.com/video/av32047507?p=5

Black Box Variational Inference

> https://arxiv.org/pdf/1401.0118.pdf

Let $\mathcal{L}(\phi) \triangleq \mathrm{ELBO} = \mathbb{E}_{q(z|\phi)}[\log p(x,z) - \log q(z|\phi)]$

NOTE: 这个属于EM 算法的E步, 固定 $p(x,z)$, $argmax\ q(z|\phi)$

对 $\mathcal{L}$ 的参数 ϕ 求导得:

$$\begin{aligned}
\nabla_\phi \mathcal{L} &= \nabla_\phi \mathbb{E}_{q(z|\phi)}[\log p(x,z) - \log q(z|\phi)] && (0)\\
&= \nabla_\phi \int (\log p(x,z) - \log q(z|\phi)) q(z|\phi) dz && (1)\\
&= \int \nabla_\phi [(\log p(x,z) - \log q(z|\phi)) q(z|\phi)] dz && (2)\\
&= \int \nabla_\phi [\log p(x,z) - \log q(z|\phi)] q(z|\phi) dz + \int \nabla_\phi q(z|\phi)(\log p(x,z) - \log q(z|\phi)) dz && (3)\\
&= -\mathbb{E}_{q(z|\phi)}[\log q(z|\phi)] + \int \nabla_\phi q(z|\phi)(\log p(x,z) - \log q(z|\phi)) dz && (4)
\end{aligned}$$

- (1) 将期望展开
- (2) 交换了积分和求导的位置
- (3) 用了分步求导：前导后不导 + 前不导后导
- (4) 注意到 $\nabla_\phi \log p(x,z) = 0$

Let $\mathrm{a} = -\mathbb{E}_{q(z|\phi)}[\log q(z|\phi)], \quad \mathrm{b} = \int \nabla_\phi q(z|\phi)(\log p(x,z) - \log q(z|\phi)) dz$

So $\nabla_\phi \mathcal{L} = \mathrm{a} + \mathrm{b}$

首先求 a

$$\begin{aligned}
&= -\mathbb{E}_{q(z|\phi)}\left[\nabla_\phi \log q(z|\phi)\right]\\
&= -\mathbb{E}_{q(z|\phi)}\left[\frac{\nabla_\phi q(z|\phi)}{q(z|\phi)}\right]\\
&= -\int \frac{\nabla_\phi q(z|\phi)}{q(z|\phi)} q(z|\phi) dz\\
&= -\int \nabla_\phi q(z|\phi) dz\\
&= -\nabla_\phi \int q(z|\phi) dz = -\nabla_\phi 1 = 0
\end{aligned}$$

接着求 b

$$\begin{aligned}
&= \int \nabla_\phi [q(z|\phi)] (\log p(x,z) - \log q(z|\phi)) dz\\
&= \int \left[\nabla_\phi [\log q(z|\phi)] (\log p(x,z) - \log q(z|\phi))\right] q(z|\phi) dz && (5)\\
&= \mathbb{E}_{q(z|\phi)}\left[\nabla_\phi [\log q(z|\phi)] (\log p(x,z) - \log q(z|\phi))\right]
\end{aligned}$$

- (5) 用到了 $\nabla_\phi [q(z|\phi)] = \nabla_\phi [\log q(z|\phi)] q(z|\phi)$

$$\text{So,} \quad \nabla_\phi \mathcal{L} = \mathrm{a} + \mathrm{b} = \mathbb{E}_{q(z|\phi)}\left[\nabla_\phi \log q(z|\phi)(\log p(x,z) - \log q(z|\phi))\right] \qquad (6)$$

所以我们可以使用蒙特卡洛方法，Draw S samples from $q(z|\phi)$

$$\nabla_\phi \mathcal{L} \approx \frac{1}{S}\sum_{s=1}^{S} \nabla_\phi \log q(z[s]|\phi)(\log p(x, z[s]) - \log q(z[s]|\phi))$$

然后梯度上升更新参数

$$\phi = \phi + \rho \nabla_\phi \mathcal{L}$$

但是这里存在一个问题，定性的分析是 $\nabla_\phi[\log q(z[s]|\phi)]$ 在 $q(z[s]|\phi)$ 趋近于0附近变化很剧烈，这就造成使用蒙特卡洛方法得到的 ∇_ϕ 方差会很大，从而使得采样数量要求非常巨大，所以我们要想办法减小方差。

The reparameterization trick

> https://arxiv.org/pdf/1312.6114.pdf

1. random variable $\mathbf{Z} \sim q_\phi(\mathbf{z}|\mathbf{x})$
2. noise variable $\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$, 分布 $p(\boldsymbol{\epsilon})$ 是我们挑选的，所以已知
3. using a differentiable transformation $\mathbf{Z} = g_\phi(\boldsymbol{\epsilon}, \mathbf{x})$
4. $\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}^{(i)})}[f(\mathbf{z})] = \mathbb{E}_{p(\epsilon)}\left[f\left(g_\phi\left(\boldsymbol{\epsilon}, \mathbf{x}^{(i)}\right)\right)\right] \simeq \frac{1}{L}\sum_{l=1}^{L} f\left(g_\phi\left(\epsilon^{(l)}, \mathbf{x}^{(i)}\right)\right) \quad \text{where} \quad \epsilon^{(l)} \sim p(\epsilon)$

$$\begin{aligned}
\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}^{(i)})}[f(\mathbf{z})] &= \int q_\phi\left(\mathbf{z}|\mathbf{x}^{(i)}\right) f(\mathbf{z}) dz &(7)\\
&= \int q_\phi\left(g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})\right) f\left(g_\phi\left(\boldsymbol{\epsilon}, \mathbf{x}^{(i)}\right)\right) d(g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})) &(8)\\
&= \int q_\phi\left(g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})\right) f\left(g_\phi\left(\boldsymbol{\epsilon}, \mathbf{x}^{(i)}\right)\right) \nabla_\epsilon[g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})] d\boldsymbol{\epsilon} &(9)\\
&= \int p(\epsilon)\left[f\left(g_\phi\left(\boldsymbol{\epsilon}, \mathbf{x}^{(i)}\right)\right)\right] d\epsilon &(10)\\
&= \mathbb{E}_{p(\epsilon)}\left[f\left(g_\phi\left(\boldsymbol{\epsilon}, \mathbf{x}^{(i)}\right)\right)\right] &(11)\\
&= \mathbb{E}_{p(\epsilon)}[f(\mathbf{z})] &(12)
\end{aligned}$$

- (7) 将期望展开成积分形式
- (8) 采用定积分里面的换元法 $\mathbf{Z} = g_\phi(\boldsymbol{\epsilon}, \mathbf{x})$
- (9) 对换元后的结果进一步计算，对 ϵ 求梯度，即

$$\frac{d(g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)}))}{d\boldsymbol{\epsilon}} = \nabla_\epsilon[g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})]$$
$$d(g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})) = \nabla_\epsilon[g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})] d\boldsymbol{\epsilon}$$

- (10) 用到了

$$\begin{aligned}
\int p(\boldsymbol{\epsilon}) d\boldsymbol{\epsilon} = 1 \\
&= \int q_\phi(\mathbf{z}|\mathbf{x}) dz \\
&= \int q_\phi\left(g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})\right) d(g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})) \\
&= \int q_\phi\left(g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})\right) \nabla_\epsilon[g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})] d\boldsymbol{\epsilon}
\end{aligned}$$

So, $p(\boldsymbol{\epsilon}) = q_\phi\left(g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})\right) \nabla_\phi[g_\phi(\boldsymbol{\epsilon}, \mathbf{x}^{(i)})]$

- (11) 将定积分转为期望形式
- (12) 使用 $\mathbf{Z} = g_\phi(\boldsymbol{\epsilon}, \mathbf{x})$

所以我们可以得出

$$\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}^{(i)})}[f(\mathbf{z})] = \mathbb{E}_{p(\epsilon)}[f(\mathbf{z})] \tag{13}$$

将 (13) 应用到 (0) 中

$$\begin{aligned}
\nabla_\phi \mathcal{L} &= \nabla_\phi \mathbb{E}_{q(z|\phi)}[\log p(x^{(i)}, z) - \log q(z|\phi)] \\
&= \nabla_\phi \mathbb{E}_{p(\epsilon)}[\log p(x^{(i)}, z) - \log q(z|\phi)] \qquad (14) \\
&= \mathbb{E}_{p(\epsilon)}[\nabla_\phi (\log p(x^{(i)}, z) - \log q(z|\phi))] \qquad (15) \\
&= \mathbb{E}_{p(\epsilon)}[\frac{d}{dz}(\log p(x^{(i)}, z) - \log q(z|\phi))\frac{dz}{d\phi}] \qquad (16) \\
&= \mathbb{E}_{p(\epsilon)}[(\frac{d}{dz}(\log p(x^{(i)}, z) - \log q(z|\phi)))(\frac{d}{d\phi} g_\phi(\boldsymbol{\epsilon}, \mathbf{x^{(i)}}))] \qquad (17)
\end{aligned}$$

- (14) 相当于令 (13) 中的 $f(\mathbf{z}) = \log p(x^{(i)}, z) - \log q(z|\phi)$
- (15) 交换梯度与期望的顺序，因为 $p(\epsilon)$ 与 ϕ 无关
- (16) 采用了链式求导 $\frac{dx}{d\phi} = \frac{dx}{dz}\frac{dz}{d\phi}$
- (17) $\mathbf{Z} = g_\phi(\boldsymbol{\epsilon}, \mathbf{x})$

这样就可以使用蒙特卡洛方法计算 (17)

采样 $\boldsymbol{\epsilon}^{(l)} \sim p(\boldsymbol{\epsilon})$， $l = 1, 2, \ldots, L$

$$\nabla_\phi \mathcal{L} \approx \frac{1}{L}\sum_{l=1}^{L}[(\frac{d}{dz}(\log p(x^{(i)}, z) - \log q(z|\phi)))(\frac{d}{d\phi} g_\phi(\boldsymbol{\epsilon}, \mathbf{x^{(i)}}))]$$
$$\text{where} \quad \mathbf{Z} = g_\phi(\boldsymbol{\epsilon}, \mathbf{x})$$

然后梯度上升更新参数:

$$\phi = \phi + \rho \nabla_\phi \mathcal{L}$$