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

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 $\nabla_\phi \log p(x,z) = 0$

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

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

首先求 a

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

接着求 b

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

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

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

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. $\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}^{(i)})}[f(\mathbf{z})] = \mathbb{E}_{p(\epsilon)}\left[f\left(g_\phi\left(\boldsymbol{\epsilon}, \mathbf{x}^{(i)}\right)\right)\right] \simeq \frac{1}{L}\sum_{l=1}^{L} f\left(g_\phi\left(\epsilon^{(l)}, \mathbf{x}^{(i)}\right)\right) \quad \text{where} \quad \epsilon^{(l)} \sim p(\epsilon)$

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

- (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
- (10) 用到了

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

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

- (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

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

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

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

然后梯度上升更新参数：

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