12. 变分推断 Variational Inference

P1 背景　频率角度 $\rightarrow$ 优化问题

线性回归:

①模型: $f(w)=w^T x$

②策略: loss function: $\begin{cases} L(w)=\sum_{i=1}^{N}\|w^T x_i - y_i\|^2 \\ \hat{w}=\arg\min L(w). \end{cases}$　无约束.

③算法: $\begin{cases} \text{解析解}: \frac{\partial L(w)}{\partial w} \triangleq 0 \Rightarrow w^* = (X^T X)^{-1} X^T Y. \\ \text{数值解}: GD \rightarrow \text{Gradient Descent}. \end{cases}$

支持向量机(SVM)

①模型: $f(w)=\text{sign}(w^T x+b).$

②策略: Loss function: $\begin{cases} \min \frac{1}{2} w^T w \\ s.t.\ \ y_i(w^T x_i + b) \geq 1,\ i=1,\cdots,N \end{cases}$　有约束, SGD优化

③算法: QP.

贝叶斯角度 $\longrightarrow$ 积分问题

$$P(\theta|X)=\frac{P(X|\theta)\cdot P(\theta)}{P(X)}.$$

贝叶斯 Inference.

贝叶斯决策　X: N个样本

$\tilde{x}$ 新的样本, 求 $P(\tilde{x}|X)$.

$$P(\tilde{x}|X)=\int_\theta P(\tilde{x},\theta|X)d\theta=\int_\theta P(\tilde{x}|\theta,X)\cdot P(\theta|X)\,d\theta.$$

$$=\int_\theta P(\tilde{x}|\theta)\cdot \underbrace{P(\theta|X)}_{\text{后验}}d\theta.\quad (\tilde{x}\perp X|\theta)$$

$$=E_{\theta|X}[P(\tilde{x}|\theta)]$$

Inference: $\begin{cases} \text{精确推断}. \\ \text{近似推断}: \begin{cases} \text{确定性近似} — \text{VI} \\ \text{随机近似} — \text{MCMC}. \end{cases} \end{cases}$

P2 变分推断

X: Observed data. Z: Latent variable + parameter.

(X, Z): complete data.

$$\log P(X) = \log P(X,Z) - \log P(Z|X)$$
$$= \log \frac{P(X,Z)}{q(Z)} - \log \frac{P(Z|X)}{q(Z)}$$

$$\text{左边} = \int_z \log P(X)\, q(z)\, dz = \log P(X) \underbrace{\int_z q(z)\, dz}_{=1} = \log P(X)$$

$$\text{右边} = \underbrace{\int_z q(z) \log \frac{P(X,Z)}{q(Z)}\, dz}_{\text{ELBO(evidence lower bound)}} \underbrace{- \int_z q(z) \log \frac{P(Z|X)}{q(Z)}\, dz}_{KL(q\|p)}$$

$$= \underbrace{L(q)}_{\text{变分}} + \underbrace{KL(q\|p)}_{\geq 0}$$

$$\tilde{q}(z) = \arg\max_{q(z)} L(q) \Rightarrow \tilde{q}(z) \approx p(z|X)$$

$$q(z) = \prod_{i=1}^{M} q_i(z_i) \rightarrow \text{mean theory} \rightarrow q_j(z_j)$$ $q_j(z_j) = \hat{P}(X, z_j)$

$$L(q) = \underbrace{\int_z q(z) \log P(X,z)\, dz}_{①} - \underbrace{\int_z q(z) \log q(z)\, dz}_{②}$$

$$① = \int_z \prod_{i=1}^{M} q_i(z_i) \log P(X,z)\, dz_1 \cdots dz_M$$
$$= \int_{z_j} q_j(z_j) \left[\int_{\substack{z_1 \cdots z_m \\ (i \neq j)}} \prod_{i=1}^{M} q_i(z_i) \cdot \log P(X,z) \cdot \underset{(i\neq j)}{dz_1 \cdots dz_M} \right] dz_j$$
$$= \int_{z_j} q_j(z_j) \left[\int_{\substack{z_1 \cdots z_m \\ (i \neq j)}} \log P(X,z) \prod_{i=1}^{M} q_i(z_i)\, dz_i \right] dz_j$$
$$= \int_{z_j} q_j(z_j) \cdot E_{\prod_{i=1 (i\neq j)}^{M} q_i(z_i)} \left[\log P(x|z) \right] dz_j$$

$\hookrightarrow \log \hat{P}(x, z_j)$

$$② = \int_z q(z) \log q(z)\, dz = \int_z \prod_{i=1}^{M} q_i(z_i) \cdot \sum_{i=1}^{M} \log p_i(z_i)\, dz$$
$$= \int_z \prod_{i=1}^{M} q_i(z_i) \left[\log q_1(z_1) + \cdots + \log q_M(z_M) \right] dz$$
$$= \sum_{i=1}^{M} \int_{z_i} q_i(z_i) \log q_i(z_i)\, dz_i = \int_{z_j} q_j(z_j) \log q_j(z_j)\, dz_j + C$$

$$\int_Z \prod_{i=1}^{M} q_i(z_i) \cdot \log q_1(z_1)\, dz = \int_Z q_1 q_2 \cdots q_M \cdot \log q_1\, dz_1 \cdots dz_M$$

$$= \int_{z_1} q_1 \log q_1\, dz_1 \cdot \underbrace{\int_{z_2} q_2\, dz_2}_{=1} \cdots \underbrace{\int_{z_M} q_M\, dz_M}_{=1}$$

$$= \int_{z_1} q_1 \log q_1\, dz_1$$

$$① - ② = \int_{z_j} q_j(z_j) \cdot \log \frac{\hat{p}(x, z_j)}{q_j(z_j)}\, dz_j = -KL(q_j \| \hat{p}(x, z_j)) \le 0$$