2 Gradient of energy-based models

$$p(x;\theta) = e^{-V(x;\theta)}/Z_\theta$$

$$Z_\theta = \int e^{-V(x;\theta)}dx$$

$$L(\theta) = -\frac{1}{n}\sum_{i=1}^{n}\log p(x_i;\theta)$$

$$\hat{p}_n = \frac{1}{n}\delta(\cdot - x_i)$$

Prove $\nabla L(\theta) = \mathbb{E}_{x\sim\hat{p}_n}[\nabla V(x_i;\theta)] - \mathbb{E}_{x\sim p_\theta}[\nabla V(x;\theta)]$

Proof.

$$\nabla L(\theta) = -\frac{1}{n}\sum_{i=1}^{n}\frac{\nabla p(x_i;\theta)}{p(x_i;\theta)}$$

$$= -\frac{1}{n}\sum_{i=1}^{n}\frac{-e^{-V(x_i;\theta)}\nabla V(x_i;\theta)Z_\theta + e^{-V(x_i;\theta)}\int e^{-V(x;\theta)}\nabla V(x;\theta)\,dx}{e^{-V(x_i;\theta)}Z_\theta}$$

(derivative rule)

$$= \frac{1}{n}\sum_{i=1}^{n}\nabla V(x_i;\theta) - \frac{1}{n}\sum_{i=1}^{n}\frac{\int e^{-V(x;\theta)}\nabla V(x;\theta)\,dx}{\int e^{-V(x;\theta)}dx}$$

$$= \frac{1}{n}\sum_{i=1}^{n}\nabla V(x_i;\theta) - \frac{\int \nabla V(x;\theta)e^{-V(x;\theta)}dx}{\int e^{-V(x;\theta)}dx}$$

$$= \mathbb{E}_{x\sim\hat{p}_n}[\nabla V(x_i;\theta)] - \mathbb{E}_{x\sim p_\theta}[\nabla V(x;\theta)] \quad \#$$

(definition)

3 Universal Approximation of energy-based model

$K = [0,1]^d \quad P = \mathrm{Unif}\,[0,1]^d$

$\mathcal{V} \subseteq C(K)$ dense in $C(K)$

$$\mathcal{Q} := \left\{ Q(x) = \frac{e^{-V(x)}}{\mathbb{E}_P[e^{-V}]} : V \in \mathcal{V} \right\}$$

(a) $V_1, V_2 \in C(K)$

$$KL(Q_1 \| Q_2) \leq 2 \|V_1 - V_2\|_{C(K)}$$

Proof.

$$KL(Q_1 \| Q_2) = \mathbb{E}_{X\sim Q_1} \log \frac{e^{-V_1(x)}}{\mathbb{E}_P e^{-V_1}} \frac{\mathbb{E}_P e^{-V_2}}{e^{-V_2(x)}}$$

$$= \mathbb{E}_{X\sim Q_1} V_2(x) - V_1(x) + \mathbb{E}_{X\sim Q_1} \log \mathbb{E}_P e^{-V_2} - \log \mathbb{E}_P e^{-V_1}$$

$$\leq \|V_1 - V_2\|_{C(K)} + \mathbb{E}_{X\sim Q_1} \log \mathbb{E}_P e^{-V_{min}} - \log \mathbb{E}_P e^{-V_{max}} \quad \text{(Lemma)}$$

$$\leq \|V_1 - V_2\|_{C(K)} + \mathbb{E}_{X\sim Q_1} \log \mathbb{E}_P e^{-V_{max}} e^{\|V_1 - V_2\|} - \log \mathbb{E}_P e^{-V_{max}}$$

$$= 2\|V_1 - V_2\|_{C(K)} \ . \ \#$$

Lemma. $\log \mathbb{E}_P e^{-V_2} - \log \mathbb{E}_P e^{-V_1} \leq \log \mathbb{E}_P e^{-V_{min}} - \log \mathbb{E}_P e^{-V_{max}}$

Proof. This is equivalent to

$$\mathbb{E}_P e^{-V_2} \cdot \mathbb{E}_P e^{-V_{max}} \leq \mathbb{E}_P e^{-V_1} \cdot \mathbb{E}_P e^{-V_{min}}$$

i.e.

$$\int e^{-V_2} dx \int e^{-V_{max}} dx \leq \int e^{-V_1} dx \int e^{-V_{min}} dx$$

This holds since

$$\int e^{-V_2} dx \leq \int e^{-V_{min}} dx \ ;$$

$$\int e^{-V_{max}} dx \leq \int e^{-V_1} dx \quad \#$$

(b) $Q_* \in \mathcal{P}_{ac}(K) \cap C(K)$ $p|_K > 0$, $p = \frac{dQ_*}{dL}$, L is Lebesgue measure on $\mathbb{R}^d$.

$\exists Q_m \in \mathcal{Q}$, $\lim_{m \to \infty} KL(Q_* | Q_m) = 0$

Proof.

Let $Q_*(x)$ be density of Q_*, $Q_*(x) \in C(K)$. $\inf_x Q_*(x) = C_0 > 0$

$$Q_*(x) = \frac{e^{-\ln Q_*(x)}}{E_p e^{-\ln Q_*(x)}} \qquad V_*(x) := \ln Q_*(x) \in C(K).$$

Acording to definition of $\mathcal{V}$, for any $n > 0$

$\exists V_n \in \mathcal{V}$, $\|V_n - V_*\| \le \frac{1}{n}$ in K.

$\Rightarrow KL(Q_* | Q_n) \le 2 \|V_* - V_n\|_{C(K)} \le \frac{2}{n}$

We are done. #

(c) Generalize to general Q_*

Proof Let $Q_*^n = (1 - \frac{1}{n}) Q_* + \frac{1}{n} P$ Q_*^n is strictly positive.

Let $R_n \in \mathcal{Q}$ be that $KL(Q_*^n | R_n) \le \frac{1}{n}$.

We have

$$\begin{aligned}
& KL(Q_* | R_n) \\
& \le KL(Q_* | Q_*^n) + KL(Q_*^n | R_n) \\
& \le (1 - \tfrac{1}{n}) KL(Q_* | Q_*) + \tfrac{1}{n} KL(Q_* | P) + \tfrac{1}{n} \\
& = \tfrac{1}{n} (1 + KL(Q_* | P))
\end{aligned}$$

$\lim_{n \to \infty} KL(Q_* | R_n) = 0$. #