DDPM Training Objective Proof 2023

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Problem 1.

Please provide a detailed mathematical proof for the training objective of the Denoising Diffusion Probabilistic Model (DDPM), which aims to maximize the log-likelihood of data $\log p(x_0;\theta)$ where θ represents the model parameters. Your proof should demonstrate the derivation started from

$$\mathbb{E}_q\left[-\frac{\log p_\theta(x_{0:T})}{q(x_{1:T}|x_0)}\right]$$

to the training objective as following

$$\mathbb{E}_q\left[-\log p_\theta(x_0|x_1) + \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_t,x_0)||p_\theta(x_{t-1}|x_t)) + D_{KL}(q(x_T|x_0)||p(x_T))\right].$$

Hint: Given $x_0, x_1, \ldots, x_T$, which form a first-order Markov chain. Then we have

$$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1}) = \prod_{t=1}^{T} q(x_t|x_{t-1},x_0).$$

Proof. For simplicity, we will first omit the expected value.

$$\begin{aligned}
-\log\left(\frac{p_\theta(x_{0:T})}{q(x_{1:T}|x_0)}\right) &= -\log p(x_T) - \sum_{t=1}^{T}\log\left(\frac{p_\theta(x_{t-1}|x_t)}{q(x_t|x_{t-1})}\right) \\
&\qquad \text{since } q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1}), \text{ and } p_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t). \\
&= -\log p(x_T) - \sum_{t=2}^{T}\log\left(\frac{p_\theta(x_{t-1}|x_t)}{q(x_t|x_{t-1})}\right) - \log\left(\frac{p_\theta(x_0|x_1)}{q(x_1|x_0)}\right) \\
&= -\log p(x_T) - \sum_{t=2}^{T}\log\left(\frac{p_\theta(x_{t-1}|x_t)}{q(x_{t-1}|x_t,x_0)}\frac{q(x_{t-1}|x_0)}{q(x_t|x_0)}\right) - \log\left(\frac{p_\theta(x_0|x_1)}{q(x_1|x_0)}\right) \\
&= -\log\left(\frac{p(x_T)}{q(x_T|x_0)}\right) - \sum_{t=2}^{T}\log\left(\frac{p_\theta(x_{t-1}|x_t)}{q(x_{t-1}|x_t,x_0)}\right) - \log p_\theta(x_0|x_1) \\
&= D_{KL}(q(x_T|x_0)||p(x_T)) + \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_t,x_0)||p_\theta(x_{t-1}|x_t)) - \log p_\theta(x_0|x_1).
\end{aligned}$$

$$\begin{aligned}
\mathbb{E}_q\left[-\log\left(\frac{p_\theta(x_{0:T})}{q(x_{1:T}|x_0)}\right)\right] &= \mathbb{E}_q\Bigg[-\log p_\theta(x_0|x_1) \\
&\qquad + \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_t,x_0)||p_\theta(x_{t-1}|x_t)) + D_{KL}(q(x_T|x_0)||p(x_T))\Bigg]
\end{aligned}$$