Prove DDPM Q1

problem:

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

Show $q(x_{1-T}|x_0) = q(x_T|x_0) \prod_{t=T}^{2} q(x_{t-1}|x_t, x_0)$

Because $x_1, x_2, \cdots x_T$ form a Markov chain when conditioned on x_0, we can rewrite $q(x_t|x_{t-1}) = q(x_t|x_{t-1}, x_0)$, where x_0 term is superfluous due to the Markov property.

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

$$= q(x_1|x_0) \prod_{t=2}^{T} q(x_t|x_{t-1}, x_0) \longrightarrow 1$$

Then, according to Bayes rule, we have the following derivation.

$$q(x_t \mid x_{t-1}, x_0) = \frac{q(x_t, x_{t-1}, x_0)}{q(x_{t-1}, x_0)}$$

$$= \frac{q(x_{t-1}, x_t, x_0)}{q(x_{t-1}, x_0)}$$

$$= \frac{q(x_{t-1} \mid x_t, x_0)\, q(x_t, x_0)}{q(x_{t-1}, x_0)}$$

$$= \frac{q(x_{t-1} \mid x_t, x_0)\, q(x_t \mid x_0)\, \cancel{q(x_0)}}{q(x_{t-1} \mid x_0)\, \cancel{q(x_0)}}$$

$$= \frac{q(x_{t-1} \mid x_t, x_0)\, q(x_t \mid x_0)}{q(x_{t-1} \mid x_0)} \longrightarrow 2$$

Now we can substitude 2 into 1.

$$q(x_{1-T} \mid x_0) = q(x_1 \mid x_0) \prod_{t=2}^{T} q(x_t \mid x_{t-1}, x_0)$$

$$= q(x_1 \mid x_0) \prod_{t=2}^{T} \frac{q(x_{t-1} \mid x_t, x_0)\, q(x_t \mid x_0)}{q(x_{t-1} \mid x_0)}$$

$$= q(x_1|x_0) \frac{q(x_1|x_2, x_0)\,\cancel{q(x_2|0)}}{q(x_1|x_0)} \frac{q(x_2|x_3, x_0)\,\cancel{q(x_3|0)}}{\cancel{q(x_2|x_0)}}$$

$$\cdots\cdots \frac{q(x_{T-1}|x_T, x_0)\,q(x_T|0)}{\cancel{q(x_{T-1}|x_0)}}$$

$$= \cancel{q(x_1|x_0)} \frac{q(x_T|x_0)}{\cancel{q(x_1|x_0)}} \prod_{t=2}^{T} q(x_{t-1}|x_t, x_0)$$

$$= q(x_T|x_0) \prod_{t=2}^{T} q(x_{t-1}|x_t, x_0) \quad \#$$

DDPM Q2

1. Proof of Eq(4) in DDPM paper

Given $q(x_t|x_{t-1}) = N(x_t; \sqrt{1-\beta_t}\, x_{t-1}, \beta_t I)$

let $\alpha_t = 1-\beta_t$

$$q(x_t|x_{t-1}) = N(x_t; \sqrt{\alpha_t}\, x_{t-1}, (1-\alpha_t) I)$$

With the reparameterization trick, $x_t \sim q(x_t|x_{t-1})$ can be rewritten as:

$$x_t = \sqrt{\alpha_t}\, x_{t-1} + \sqrt{1-\alpha_t}\, \epsilon \quad \text{with } \epsilon \sim N(\epsilon; 0, I)$$

Then, we can do the following derivation:

$$\begin{aligned}
x_t &= \sqrt{\alpha_t}\, x_{t-1} + \sqrt{1-\alpha_t}\, \epsilon^*_{t-1} \\
&= \sqrt{\alpha_t}\left(\sqrt{\alpha_{t-1}}\, x_{t-2} + \sqrt{1-\alpha_{t-1}}\, \epsilon^*_{t-2}\right) + \sqrt{1-\alpha_t}\, \epsilon^*_{t-1} \\
&= \sqrt{\alpha_t \alpha_{t-1}}\, x_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1}}\, \epsilon^*_{t-2} + \sqrt{1-\alpha_t}\, \epsilon^*_{t-1} \\
&= \sqrt{\alpha_t \alpha_{t-1}}\, x_{t-2} + \sqrt{\sqrt{\alpha_t - \alpha_t \alpha_{t-1}}^2 + \sqrt{1-\alpha_t}^2}\, \epsilon_{t-2} \\
&= \sqrt{\alpha_t \alpha_{t-1}}\, x_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1} + 1 - \alpha_t}\, \epsilon_{t-2} \\
&= \sqrt{\alpha_t \alpha_{t-1}}\, x_{t-2} + \sqrt{1 - \alpha_t \alpha_{t-1}}\, \epsilon_{t-2} \\
&= \cdots \\
&= \sqrt{\prod_{i=1}^{t} \alpha_i}\, x_0 + \sqrt{1 - \prod_{i=1}^{t} \alpha_i}\, \epsilon_0
\end{aligned}$$

let $\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$, we have

$$x_t = \sqrt{\bar{\alpha}_t}\, x_0 + \sqrt{1-\bar{\alpha}_t}\, \epsilon_0 \sim N(x_t; \sqrt{\bar{\alpha}_t}\, x_0, (1-\bar{\alpha}_t) I)$$

$$q(x_t|x_0) = N(x_t; \sqrt{\bar{\alpha}_t}\, x_0, (1-\bar{\alpha}_t) I)$$ #

2. Proof of Eq(6) in DDPM paper

In 1., we have derived the Gaussian form of $q(x_t|x_0)$, this also means that with some modification we are able to obtain the Gaussian form of $q(x_{t-1}|x_0)$. With these prerequisites, we can start calculate the form of $q(x_{t-1}|x_t, x_0)$ by substituting into the Bayes rule expansion:

$$q(x_{t-1}|x_t, x_0) = \frac{q(x_t|x_{t-1}, x_0)\, q(x_{t-1}|x_0)}{q(x_t|x_0)}$$

$$= \frac{\mathcal{N}(x_t; \sqrt{\alpha_t}\, x_{t-1}, (1-\alpha_t)I)\, \mathcal{N}(x_{t-1}; \sqrt{\bar{\alpha}_{t-1}}\, x_0, (1-\bar{\alpha}_{t-1})I)}{\mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}\, x_0, (1-\bar{\alpha}_t)I)}$$

$$\propto \exp\left\{-\left[\frac{(x_t-\sqrt{\alpha_t}\, x_{t-1})^2}{2(1-\alpha_t)} + \frac{(x_{t-1}-\sqrt{\bar{\alpha}_{t-1}}\, x_0)^2}{2(1-\bar{\alpha}_{t-1})} - \frac{(x_t-\sqrt{\bar{\alpha}_t}\, x_0)^2}{2(1-\bar{\alpha}_t)}\right]\right\}$$

$$= \exp\left\{-\frac{1}{2}\left[\frac{(x_t-\sqrt{\alpha_t}\, x_{t-1})^2}{1-\alpha_t} + \frac{(x_{t-1}-\sqrt{\bar{\alpha}_{t-1}}\, x_0)^2}{1-\bar{\alpha}_{t-1}} - \frac{(x_t-\sqrt{\bar{\alpha}_t}\, x_0)^2}{1-\bar{\alpha}_t}\right]\right\}$$

$$= \exp\left\{-\frac{1}{2}\left[\frac{(-2\sqrt{\alpha_t}\, x_t x_{t-1} + \alpha_t x_{t-1}^2)}{1-\alpha_t} + \frac{(x_{t-1}^2 - 2\sqrt{\bar{\alpha}_{t-1}}\, x_{t-1} x_0)}{1-\bar{\alpha}_{t-1}} + C(x_t, x_0)\right]\right\}$$

$$= \exp\left\{-\frac{1}{2}\left[-\frac{2\sqrt{\alpha_t}\, x_t x_{t-1}}{1-\alpha_t} + \frac{\alpha_t x_{t-1}^2}{1-\alpha_t} + \frac{x_{t-1}^2}{1-\bar{\alpha}_{t-1}} - \frac{2\sqrt{\bar{\alpha}_{t-1}}\, x_{t-1} x_0}{1-\bar{\alpha}_{t-1}} + C(x_t, x_0)\right]\right\}$$

$$= \exp\left\{-\frac{1}{2}\left[\left(\frac{\alpha_t}{1-\alpha_t}+\frac{1}{1-\bar{\alpha}_{t-1}}\right)x_{t-1}^2-2\left(\frac{\sqrt{\alpha_t}\,x_t}{1-\alpha_t}+\frac{\sqrt{\bar{\alpha}_{t-1}}\,x_0}{1-\bar{\alpha}_{t-1}}\right)x_{t-1}+C(x_t,x_0)\right]\right\}$$

$$= \exp\left\{-\frac{1}{2}\left[\frac{\alpha_t(1-\bar{\alpha}_{t-1})+1-\alpha_t}{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}x_{t-1}^2-2\left(\frac{\sqrt{\alpha_t}\,x_t}{1-\alpha_t}+\frac{\sqrt{\bar{\alpha}_{t-1}}\,x_0}{1-\bar{\alpha}_{t-1}}\right)x_{t-1}+C(x_t,x_0)\right]\right\}$$

$$= \exp\left\{-\frac{1}{2}\left[\frac{\alpha_t-\bar{\alpha}_t+1-\alpha_t}{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}x_{t-1}^2-2\left(\frac{\sqrt{\alpha_t}\,x_t}{1-\alpha_t}+\frac{\sqrt{\bar{\alpha}_{t-1}}\,x_0}{1-\bar{\alpha}_{t-1}}\right)x_{t-1}+C(x_t,x_0)\right]\right\}$$

$$= \exp\left\{-\frac{1}{2}\left[\frac{1-\bar{\alpha}_t}{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}x_{t-1}^2-2\left(\frac{\sqrt{\alpha_t}\,x_t}{1-\alpha_t}+\frac{\sqrt{\bar{\alpha}_{t-1}}\,x_0}{1-\bar{\alpha}_{t-1}}\right)x_{t-1}+C(x_t,x_0)\right]\right\}$$

$$= \exp\left\{-\frac{1}{2}\left(\frac{1-\bar{\alpha}_t}{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}\right)\left[x_{t-1}^2-2\,\frac{\left(\frac{\sqrt{\alpha_t}\,x_t}{1-\alpha_t}+\frac{\sqrt{\bar{\alpha}_{t-1}}\,x_0}{1-\bar{\alpha}_{t-1}}\right)}{\frac{1-\bar{\alpha}_t}{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}}\,x_{t-1}+C'(x_t,x_0)\right]\right\}$$

$$= \exp\left\{-\frac{1}{2}\left(\frac{1-\bar{\alpha}_t}{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}\right)\left[x_{t-1}^2-2\,\frac{\left(\frac{\sqrt{\alpha_t}\,x_t}{1-\alpha_t}+\frac{\sqrt{\bar{\alpha}_{t-1}}\,x_0}{1-\bar{\alpha}_{t-1}}\right)(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\,x_{t-1}+C'(x_t,x_0)\right]\right\}$$

$$= \exp\left\{-\frac{1}{2}\left(\frac{1}{\frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}}\right)\left[x_{t-1}^2-2\,\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t+\sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)x_0}{1-\bar{\alpha}_t}\,x_{t-1}+C'(x_t,x_0)\right]\right\}$$

$$\propto \mathcal{N}\left(x_{t-1};\ \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t+\sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)x_0}{1-\bar{\alpha}_t},\ \frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{I}\right)$$

Where $C(x_t, x_0)$ and $C'(x_t, x_0)$ are functions that composed only of x_t, x_0 and α, in which $C'(x_t, x_0)$ can be shown to complete the square.

$$x_{t-1}^2 - 2\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)x_0}{1-\bar{\alpha}_t} x_{t-1} + C'(x_t, x_0) = \left(x_{t-1} - \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)x_0}{1-\bar{\alpha}_t} \right)^2$$

Using the notations $\tilde{\mu}_t(x_t, x_0) = \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t} x_0 + \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t} x_t$ and

$\tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\alpha_t}\beta_t$, we have

$$q(x_{t-1} \mid x_t, x_0) = \mathcal{N}(x_{t-1}; \tilde{\mu}_t(x_t, x_0), \tilde{\beta}_t I) \quad \#$$

3. Proof of Eq(8) in DDPM paper

Given the denoising matching term

$$L_{t-1} = \mathbb{E}_{q(x_t|x_0)}\left[D_{KL}(q(x_{t-1}|x_t, x_0) \| p_\theta(x_{t-1}|x_t))\right]$$

We already know the gaussian form of $q(x_{t-1}|x_t, x_0)$, thus we can set the variance of $p_\theta(x_{t-1}|x_t)$ to match exactly, optimizing the KL term reduces to minimizing the difference between the means of the two distributions.

let $\sigma_t^2 = \tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$, $\Sigma(t) = \sigma_t^2 I$

$$L_{t-1} = \mathbb{E}_{q(x_t|x_0)}\left[D_{KL}(\mathcal{N}(x_{t-1}; \tilde{\mu}_t, \Sigma(t)) \| \mathcal{N}(x_{t-1}; \mu_\theta, \Sigma(t)))\right]$$

$$= \mathbb{E}_{q(x_t|x_0)}\left[\frac{1}{2}\left[\log\frac{\det(\Sigma(t))}{\det(\Sigma(t))} - d + tr(\Sigma(t)^{-1}\Sigma(t)) + (\mu_\theta - \tilde{\mu}_t)^T \Sigma(t)^{-1}(\mu_\theta - \tilde{\mu}_t)\right]\right]$$

$$= \mathbb{E}_{q(x_t|x_0)}\left[\frac{1}{2}\left[-d + d + (\mu_\theta - \tilde{\mu}_t)^T \Sigma(t)^{-1}(\mu_\theta - \tilde{\mu}_t)\right]\right]$$

$$= \mathbb{E}_{q(x_t|x_0)}\left[\frac{1}{2}\left[(\mu_\theta - \tilde{\mu}_t)^T \Sigma(t)^{-1}(\mu_\theta - \tilde{\mu}_t)\right]\right]$$

$$= \mathbb{E}_{q(x_t|x_0)}\left[\frac{1}{2}\left[(\mu_\theta - \tilde{\mu}_t)^T (\sigma_t^2 I)^{-1}(\mu_\theta - \tilde{\mu}_t)\right]\right]$$

$$= \mathbb{E}_{q(x_t|x_0)}\left[\frac{1}{2\sigma_t^2}\|\mu_\theta - \tilde{\mu}_t\|^2\right] \#$$