

Q3 : The equation in 2.2 misses a “+” after const.? Also, how do we get the equation 4?

A3: Thank you for pointing it out! We rewrite the equation 2.2.

For equation 4, we follow [1] and derive this equation as below:

[1] introduces the reparameterized trick to discrete diffusion model, and the backward transition $q(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)}, \mathbf{x}^{(0)})$ can be rewritten as:

$$q(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)}, \mathbf{x}^{(0)}) = \begin{cases} \lambda_{t-1}^{(1)}\mathbf{x}^{(t)} + (1 - \lambda_{t-1}^{(1)})\mathbf{q}_{\text{noise}}, & \text{if } \mathbf{x}^{(t)} = \mathbf{x}^{(0)} \\ \lambda_{t-1}^{(2)}\mathbf{x}^{(t)} + (1 - \lambda_{t-1}^{(2)})\mathbf{q}_{\text{noise}}(\mathbf{x}^{(t)}), & \text{if } \mathbf{x}^{(t)} \neq \mathbf{x}^{(0)} \end{cases}$$

where $\mathbf{q}_{\text{noise}}(\mathbf{x}^{(t)}) = \beta_t\mathbf{x}^{(t)} + (1 - \beta_t)\mathbf{q}_{\text{noise}}$, and both $\lambda_{t-1}^{(1)}$ and $\lambda_{t-1}^{(2)}$ are constants relating to β_t and β_{t-1} .

Sampling from it is equivalent to first sampling from a Bernoulli distribution and then the corresponding component distribution:

$$\begin{aligned} v_{t-1}^{(1)} &\sim \text{Bernoulli}(\lambda_{t-1}^{(1)}), & \mathbf{u}_t^{(1)} &\sim \text{Cat}(\mathbf{u}; \mathbf{p} = \mathbf{q}_{\text{noise}}) \\ v_{t-1}^{(2)} &\sim \text{Bernoulli}(\lambda_{t-1}^{(2)}), & \mathbf{u}_t^{(2)} &\sim \text{Cat}(\mathbf{u}; \mathbf{p} = \mathbf{q}_{\text{noise}}(\mathbf{x}_t)) \end{aligned}$$

$$\mathbf{x}_{t-1} = \begin{cases} v_{t-1}^{(1)}\mathbf{x}_t + (1 - v_{t-1}^{(1)})\mathbf{u}_t^{(1)}, & \text{if } \mathbf{x}_t = \mathbf{x}_0 \\ v_{t-1}^{(2)}\mathbf{x}_t + (1 - v_{t-1}^{(2)})\mathbf{u}_t^{(2)}, & \text{if } \mathbf{x}_t \neq \mathbf{x}_0 \end{cases}$$

This reparameterizes the backward transitions $q(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)}, \mathbf{x}^{(0)})$ and $p_\theta(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)})$ into $q(\mathbf{x}^{(t-1)}, \mathbf{v}^{(t-1)}|\mathbf{x}^{(t)}, \mathbf{x}^{(0)})$ and $p_\theta(\mathbf{x}^{(t-1)}, \mathbf{v}^{(t-1)}|\mathbf{x}^{(t)})$, respectively.

Since each token is modeled **conditionally independently**, so we consider the backward transition for **each token**, and sum the losses for them.

For i-th position, the backward transition is $q(\mathbf{x}_i^{(t-1)}, \mathbf{v}_i^{(t-1)}|\mathbf{x}_i^{(t)}, \mathbf{x}_i^{(0)})$.

As shown in [1] (appendix C), the loss at i-th token can be written as below:

$$\mathcal{J}_{t,i} = \mathbf{E}_{q(\mathbf{v}_i^{(t-1)})} \left[KL[q(\mathbf{x}_i^{(t-1)}|\mathbf{v}_i^{(t-1)}, \mathbf{x}_i^{(t)}, \mathbf{x}_i^{(0)})||p_\theta(\mathbf{x}_i^{(t-1)}|\mathbf{v}_i^{(t-1)}, \mathbf{x}_i^{(t)})] \right]$$

Let $b_i(t) = \mathbf{1}_{\mathbf{x}_i^{(t)} = \mathbf{x}_i^{(0)}}$, $q(\mathbf{x}_i^{(t-1)}|\mathbf{v}_i^{(t-1)}, \mathbf{x}_i^{(t)}, \mathbf{x}_i^{(0)})$ can be written as:

$$\begin{aligned}
& q(\mathbf{x}_i^{(t-1)} | \mathbf{v}_i^{(t-1)}, \mathbf{x}_i^{(t)}, \mathbf{x}_i^{(0)}) \\
&= \begin{cases} v_{t-1,i}^{(1)} \mathbf{x}_i^{(t)} + (1 - v_{t-1,i}^{(1)}) \mathbf{q}_{\text{noise}} & \text{if } b_i(t) = 0, \\ v_{t-1,i}^{(2)} \mathbf{x}_i^{(0)} + (1 - v_{t-1,i}^{(2)}) \mathbf{q}_{\text{noise}} & \text{if } b_i(t) = 1, \end{cases}
\end{aligned}$$

And $p_\theta(\mathbf{x}_i^{(t-1)} | \mathbf{v}_i^{(t-1)}, \mathbf{x}_i^{(t)})$ can be written as:

$$\begin{aligned}
& p_\theta(\mathbf{x}_i^{(t-1)} | \mathbf{v}_i^{(t-1)}, \mathbf{x}_i^{(t)}) \\
&= \begin{cases} v_{t-1,i}^{(1)} \mathbf{x}_i^{(t)} + (1 - v_{t-1,i}^{(1)}) \mathbf{q}_{\text{noise}} & \text{if } b_i(t) = 0, \\ v_{t-1,i}^{(2)} p_\theta(\mathbf{x}_i^{(0)} | \mathbf{x}^{(t)}) + (1 - v_{t-1,i}^{(2)}) \mathbf{q}_{\text{noise}} & \text{if } b_i(t) = 1, \end{cases}
\end{aligned}$$

Therefore, the loss at i -th token can be computed by enumerating all cases with respect to $\mathbf{v}_i^{(t-1)}$ and $b_i(t)$. As noted in [1], the KL divergence is equal to $-\log p_\theta(\mathbf{x}_i^{(0)} | \mathbf{x}^{(t)})$ when $v_{t-1,i}^{(2)} = 1$ and $b_i(t) = 1$, while in other cases the KL divergence is 0.

So we have:

$$\begin{aligned}
\mathcal{J}_t &= \sum_{1 \leq i \leq L} \mathcal{J}_{t,i} \\
&= \sum_{1 \leq i \leq L} \mathbf{E}_{q(\mathbf{v}_i^{(t-1)})} \left[KL[q(\mathbf{x}_i^{(t-1)} | \mathbf{v}_i^{(t-1)}, \mathbf{x}_i^{(t)}, \mathbf{x}_i^{(0)}) || p_\theta(\mathbf{x}_i^{(t-1)} | \mathbf{v}_i^{(t-1)}, \mathbf{x}_i^{(t)})] \right] \\
&= \sum_{1 \leq i \leq L} q(\mathbf{v}_i^{(t-1)} = 1) (-\log p_\theta(\mathbf{x}_i^{(0)} | \mathbf{x}^{(t)})) \\
&= -\lambda^{(t)} \sum_{1 \leq i \leq L} b_i(t) \cdot \log p_\theta(\mathbf{x}_i^{(0)} | \mathbf{x}^{(t)})
\end{aligned}$$

[1] Zheng, L., Yuan, J., Yu, L., and Kong, L. A reparameterized discrete diffusion model for text generation. arXiv preprint arXiv:2302.05737