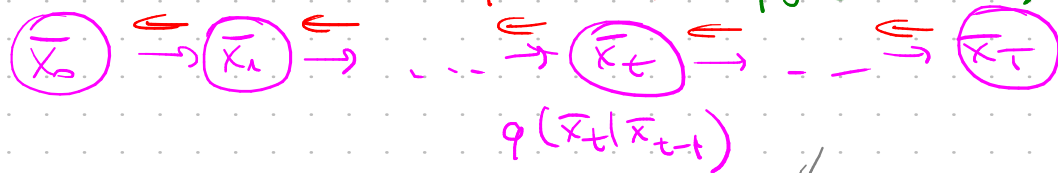


# Diffusion models

$$q(\bar{x}_0) = p(\bar{x}_0)$$

$$q(\bar{x}_{t-1} | \bar{x}_t) \approx p_\theta(\bar{x}_{t-1} | \bar{x}_t)$$



$$q(\bar{x}_t | \bar{x}_{t+1})$$

$$\alpha_t = 1 - \beta_t$$

$$q(\bar{x}_t | \bar{x}_{t-1}) = \mathcal{N}(\bar{x}_t | \sqrt{1 - \beta_t} \bar{x}_{t-1}, \beta_t I)$$

$$q(\bar{x}_1 \dots \bar{x}_T | \bar{x}_0) = q(\bar{x}_1 | \bar{x}_0) q(\bar{x}_2 | \bar{x}_1) \dots q(\bar{x}_T | \bar{x}_{T-1})$$

$$q(\bar{x}_t | \bar{x}_0) = ?$$

$$\bar{\epsilon}_{t-1} \sim \mathcal{N}(\bar{0}, I)$$

$$\bar{x}_t = \sqrt{1 - \beta_t} \bar{x}_{t-1} + \sqrt{\beta_t} \bar{\epsilon}_{t-1} =$$

$$= \sqrt{1 - \beta_t} (\sqrt{1 - \beta_{t-1}} \bar{x}_{t-2} + \sqrt{\beta_{t-1}} \bar{\epsilon}_{t-2}) + \sqrt{\beta_t} \bar{\epsilon}_{t-1} =$$

$$= \sqrt{\alpha_t \alpha_{t-1}} \bar{x}_{t-2} + \sqrt{1 - \alpha_t} \bar{\epsilon}_{t-1} + \sqrt{\alpha_t (1 - \alpha_{t-1})} \bar{\epsilon}_{t-2} =$$

$$(\sqrt{\alpha_t \alpha_{t-1}} \bar{x}_{t-2} + \sqrt{1 - \alpha_t} \bar{\epsilon}_{t-1}) \sim \mathcal{N}(\bar{0}, (1 - \alpha_t) I) + \mathcal{N}(\bar{0}, \alpha_t (1 - \alpha_{t-1}) I) =$$

$$= \mathcal{N}(\bar{0}, (1 - \alpha_t + \alpha_t - \alpha_t \alpha_{t-1}) I) =$$

$$= \sqrt{\alpha_t \alpha_{t-1}} \bar{x}_{t-2} +$$

$$(1 - \alpha_{t-2}) +$$

$$+ \sqrt{1 - \alpha_t \alpha_{t-1}} \bar{\epsilon} =$$

$$+ \alpha_{t-2} (1 - \alpha_t \alpha_{t-1})$$

$$\mathcal{N}(\bar{0}, (1 - \alpha_t \alpha_{t-1}) I)$$

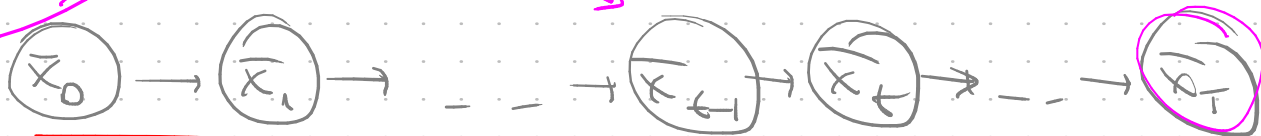
$$= \dots = \sqrt{\alpha_t \alpha_{t-1} \dots \alpha_1} \bar{x}_0 + \sqrt{1 - \alpha_t \alpha_{t-1} \dots \alpha_1} \bar{\epsilon}$$

$$A_t = \alpha_1 \alpha_2 \dots \alpha_t$$

$$q(\bar{x}_t | \bar{x}_0) = \mathcal{N}(\bar{x}_t | \sqrt{A_t} \bar{x}_0, (1 - A_t) I)$$

$$p(\bar{x}_0)$$

$$q(\bar{x}_T) \approx \mathcal{N}(\bar{x}_T)$$



$$q(\bar{x}_t | \bar{x}_0)$$

$$q(\bar{x}_0, \dots, \bar{x}_T) = \underbrace{q(\bar{x}_T)}_{\sim N(\bar{x}_T | 0, I)} q(\bar{x}_{T-1} | \bar{x}_T) \dots q(\bar{x}_0 | \bar{x}_1)$$

$$q(\bar{x}_0 | \bar{x}_T) = \frac{q(\bar{x}_0) q(\bar{x}_T | \bar{x}_0)}{q(\bar{x}_T)}$$

$$q(\bar{x}_{t-1} | \bar{x}_t, \bar{x}_0) = \frac{q(\bar{x}_{t-1} | \bar{x}_0) q(\bar{x}_t | \bar{x}_{t-1}, \bar{x}_0)}{q(\bar{x}_t | \bar{x}_0)} =$$

$$= \frac{N(\bar{x}_{t-1} | \sqrt{A_{t-1}} \bar{x}_0, \sqrt{1-A_{t-1}} I) \cdot N(\bar{x}_t | \sqrt{A_t} \bar{x}_{t-1}, \beta_t I)}{N(\bar{x}_t | \sqrt{A_t} \bar{x}_0, \sqrt{1-A_t} I)} =$$

$$= \text{Const} \cdot \exp \left( -\frac{1}{2} \left( \frac{(\bar{x}_{t-1} - \sqrt{A_{t-1}} \bar{x}_0)^2}{1-A_{t-1}} + \frac{(\bar{x}_t - \sqrt{A_t} \bar{x}_{t-1})^2}{\beta_t} - \frac{(\bar{x}_t - \sqrt{A_t} \bar{x}_0)^2}{1-A_t} \right) \right)$$

$$= \frac{1}{1-A_{t-1}} \left( \bar{x}_{t-1}^T \bar{x}_{t-1} - 2\sqrt{A_{t-1}} \bar{x}_{t-1}^T \bar{x}_0 + A_{t-1} \bar{x}_0^T \bar{x}_0 \right) +$$

$$+ \frac{1}{\beta_t} \left( \bar{x}_t^T \bar{x}_t - 2\sqrt{A_t} \bar{x}_t^T \bar{x}_{t-1} + A_t \bar{x}_{t-1}^T \bar{x}_{t-1} \right) -$$

$$- \frac{1}{1-A_t} \left( \bar{x}_t^T \bar{x}_t - 2\sqrt{A_t} \bar{x}_t^T \bar{x}_0 + A_t \bar{x}_0^T \bar{x}_0 \right) =$$

$$= \bar{x}_{t-1}^T \bar{x}_{t-1} \left( \frac{1}{1-A_{t-1}} + \frac{A_t}{\beta_t} \right) - 2\bar{x}_{t-1}^T \left( \frac{\sqrt{A_t}}{\beta_t} \bar{x}_t + \frac{\sqrt{A_{t-1}}}{1-A_{t-1}} \bar{x}_0 \right) +$$

$$= \frac{1}{\tilde{\beta}_t} \left( \bar{x}_{t-1} - \tilde{\mu}(\bar{x}_t, \bar{x}_0) \right)^2 + \text{const}$$

$$\tilde{\beta}_t = \frac{1}{\frac{1}{1-A_{t-1}} + \frac{\alpha_t}{\beta_t}} = \frac{\beta_t(1-A_{t-1})}{\beta_t + \alpha_t(1-A_{t-1})} = \beta_t \cdot \frac{1-A_{t-1}}{1-A_t}$$

$\frac{1}{1-\alpha_t + \alpha_t + \alpha_t A_{t-1}} = A_t$

$$\bar{x}_t = \sqrt{A_t} \cdot \bar{x}_0 + \sqrt{1-A_t} \cdot \bar{\epsilon}$$

$$\tilde{\mu}(\bar{x}_t, \bar{x}_0) = \frac{1-A_{t-1}}{1-A_t} \cdot \sqrt{\alpha_t} \cdot \bar{x}_t + \beta_t \cdot \frac{\sqrt{A_{t-1}}}{1-A_t} \cdot \bar{x}_0 =$$

$$= \frac{1-A_{t-1}}{1-A_t} \cdot \sqrt{\alpha_t} \cdot \bar{x}_t + \beta_t \cdot \frac{\sqrt{A_{t-1}}}{1-A_t} \cdot \frac{1}{\sqrt{A_t}} \left( \bar{x}_t - \sqrt{1-A_t} \cdot \bar{\epsilon} \right) =$$

$A_t = A_{t-1} \cdot \alpha_t$   
 $A_t = \alpha_t - \alpha_t^2$

$$= \bar{x}_t \left( \frac{1-A_{t-1}}{1-A_t} \sqrt{\alpha_t} + \beta_t \cdot \frac{\sqrt{A_{t-1}}}{1-A_t} \cdot \frac{1}{\sqrt{A_t}} \right) - \beta_t \sqrt{\frac{A_{t-1}}{(1-A_t)A_t}} \cdot \bar{\epsilon}$$

$$\frac{(1-A_{t-1})\alpha_t + 1-\alpha_t}{(1-A_t)\sqrt{\alpha_t}} = \frac{1-A_{t-1}\alpha_t}{(1-A_t)\sqrt{\alpha_t}} = \frac{1}{\sqrt{\alpha_t}}$$

$$= \frac{1}{\sqrt{\alpha_t}} \cdot \bar{x}_t - \frac{1-\alpha_t}{\sqrt{\alpha_t}(1-A_t)} \cdot \bar{\epsilon}$$

$$q(\bar{x}_{t+1} | \bar{x}_t) \approx p_\theta(\bar{x}_{t+1} | \bar{x}_t)$$

$$\frac{q(\bar{x}_{t+1} | \bar{x}_t, \bar{x}_0)}{q(\bar{x}_t | \bar{x}_{t-1})} = \mathcal{N}\left(\bar{x}_{t+1} \mid \frac{1}{\sqrt{\alpha_t}} \left( \bar{x}_t - \frac{1-\alpha_t}{\sqrt{1-A_t}} \bar{\epsilon} \right), \beta_t \frac{1-A_{t-1}}{1-A_t} \cdot \mathbb{I}\right)$$

$$\cancel{q(\bar{x}_1, \dots, \bar{x}_T | \bar{x}_0) \approx p_\theta(\bar{x}_1, \dots, \bar{x}_T | \bar{x}_0)}$$

$$p_\theta(\bar{x}_0) \approx q(\bar{x}_0)$$

$$KL(q(\bar{x}_0) \parallel p_\theta(\bar{x}_0)) \rightarrow \min$$

$$\int q \log \frac{q}{p_\theta} d\bar{x}_0 = \int q \log q d\bar{x}_0 - \int q(\bar{x}_0) \log p_\theta(\bar{x}_0) d\bar{x}_0$$

$$\begin{aligned}
 -E_{q(\bar{x}_0)}[\log p_\theta(\bar{x}_0)] &= -E_{q(\bar{x}_0)}\left[\log \int p_\theta(\bar{x}_0, \bar{x}_1, \dots, \bar{x}_T) d\bar{x}_1 \dots d\bar{x}_T\right] \\
 &= -E_{q(\bar{x}_0)}\left[\log \int q(\bar{x}_1, \bar{x}_T | \bar{x}_0) \cdot \frac{p_\theta(\bar{x}_0, \bar{x}_1, \dots, \bar{x}_T)}{q(\bar{x}_1, \bar{x}_T | \bar{x}_0)} d\bar{x}_1 \dots d\bar{x}_T\right]
 \end{aligned}$$

$$\log E \geq E \log$$

$$= -E_{q(\bar{x}_0)}\left[\log E_{q(\bar{x}_1, \bar{x}_T | \bar{x}_0)}\left[\frac{p_\theta(\bar{x}_0, \bar{x}_1, \dots, \bar{x}_T)}{q(\bar{x}_1, \bar{x}_T | \bar{x}_0)}\right]\right] \leq$$

$$\leq -E_{q(\bar{x}_0)}\left[E_{q(\bar{x}_1, \bar{x}_T | \bar{x}_0)}\left[\log \frac{p_\theta(\bar{x}_0, \bar{x}_1, \dots, \bar{x}_T)}{q(\bar{x}_1, \bar{x}_T | \bar{x}_0)}\right]\right]$$

$$= E_{q(\bar{x}_0, \bar{x}_T)}\left[\log \frac{q(\bar{x}_1, \bar{x}_T | \bar{x}_0)}{p_\theta(\bar{x}_0, \bar{x}_1, \dots, \bar{x}_T)}\right] \rightarrow \min$$

$$E_q\left[\log \frac{q(\bar{x}_1 | \bar{x}_0) q(\bar{x}_2 | \bar{x}_1, \bar{x}_0) q(\bar{x}_3 | \bar{x}_2, \bar{x}_0) \dots q(\bar{x}_T | \bar{x}_{T-1}, \bar{x}_0)}{p_\theta(\bar{x}_T) p_\theta(\bar{x}_{T-1} | \bar{x}_T) \dots p_\theta(\bar{x}_0 | \bar{x}_1)}\right] =$$

$$= E_q\left[-\log p_\theta(\bar{x}_T) + \sum_{t=2}^T \log \frac{q(\bar{x}_t | \bar{x}_{t-1}, \bar{x}_0)}{p_\theta(\bar{x}_{t-1} | \bar{x}_t)} + \log \frac{q(\bar{x}_1 | \bar{x}_0)}{p_\theta(\bar{x}_0 | \bar{x}_1)}\right]$$

$$\log \frac{q(\bar{x}_2 | \bar{x}_0)}{q(\bar{x}_1 | \bar{x}_0)} \frac{q(\bar{x}_3 | \bar{x}_0)}{q(\bar{x}_2 | \bar{x}_0)} \dots \frac{q(\bar{x}_{t-1} | \bar{x}_t, \bar{x}_0)}{p_\theta(\bar{x}_{t-1} | \bar{x}_t)} \cdot \frac{q(\bar{x}_t | \bar{x}_0)}{q(\bar{x}_{t-1} | \bar{x}_0)}$$

$$\begin{aligned}
 &= E_q\left[-\log p_\theta(\bar{x}_T) + \sum_{t=2}^T \log \frac{q(\bar{x}_{t-1} | \bar{x}_t, \bar{x}_0)}{p_\theta(\bar{x}_{t-1} | \bar{x}_t)} + \log \frac{q(\bar{x}_T | \bar{x}_0)}{q(\bar{x}_1 | \bar{x}_0)} + \log \frac{q(\bar{x}_1 | \bar{x}_0)}{p_\theta(\bar{x}_0 | \bar{x}_1)}\right] =
 \end{aligned}$$

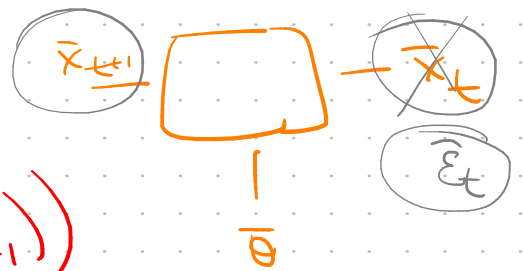
$$= \underbrace{E_q \left[ \log \frac{q(\bar{x}_T | \bar{x}_0)}{p_\theta(\bar{x}_T)} \right]}_{L_T} + \sum_{t=2}^T \log \frac{q(\bar{x}_{t-1} | \bar{x}_t, \bar{x}_0)}{p_\theta(\bar{x}_{t-1} | \bar{x}_t)} - \log p_\theta(\bar{x}_0 | \bar{x}_1)$$

$$E \left[ \log \frac{q(\bar{x}_T | \bar{x}_0)}{p_\theta(\bar{x}_T)} \right] = \text{KL}(q(\bar{x}_T | \bar{x}_0) \| p_\theta(\bar{x}_T))$$

$$= E_q \left[ \underbrace{\text{KL}(q(\bar{x}_T | \bar{x}_0) \| p_\theta(\bar{x}_T))}_{L_T} + \sum_{t=2}^T \overbrace{\text{KL}(q(\bar{x}_{t-1} | \bar{x}_t, \bar{x}_0) \| p_\theta(\bar{x}_{t-1} | \bar{x}_t))}^{L_{t-1}} - \log p_\theta(\bar{x}_0 | \bar{x}_1) \right]_{L_0}$$

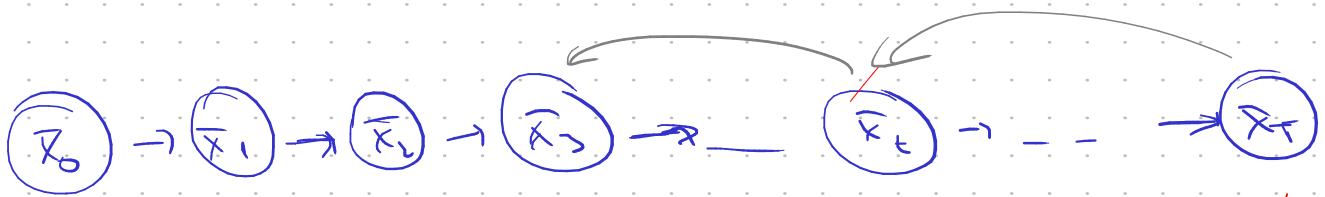
$$L = L_0 + L_1 + L_2 + \dots + L_T, \text{ where}$$

$$L_0 = -\log p_\theta(\bar{x}_0 | \bar{x}_1)$$



$$L_t = \text{KL}(q(\bar{x}_t | \bar{x}_{t+1}, \bar{x}_0) \| p_\theta(\bar{x}_t | \bar{x}_{t+1}))$$

$$L_T = \text{KL}(q(\bar{x}_T | \bar{x}_0) \| p_\theta(\bar{x}_T))$$



$$p_\theta(\bar{x}_{t-1} | \bar{x}_t) = \mathcal{N}(\bar{x}_{t-1} | \underbrace{\bar{\mu}_\theta(\bar{x}_t, t)}_{\bar{\mu}(\bar{x}_t, \bar{x}_0)}, \Sigma_\theta(\bar{x}_t, t))$$

$$\approx \tilde{\mu}(\bar{x}_t, \bar{x}_0) = \frac{1}{\sqrt{\alpha_t}} \left( \bar{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \bar{\epsilon} \right)$$

$$L_t = E \left[ \frac{1}{2 \| \Sigma_\theta \|_2^2} \| \tilde{\mu}(\bar{x}_t, \bar{x}_0) - \bar{\mu}_\theta(\bar{x}_t, t) \|^2 \right] =$$

$$= E \left[ \frac{1}{2 \|\xi_0\|_2^2} \left\| \frac{1}{\sqrt{\alpha_t}} \left( \bar{x}_t + \frac{1-\alpha_t}{\sqrt{1-\alpha_t}} \bar{\xi}_t \right) - \frac{1}{\sqrt{\alpha_t}} \left( \bar{x}_t - \bar{\xi}_0 \right) \right\|^2 \right]$$

$$= E \left[ \frac{(1-\alpha_t)^2}{2(1-\alpha_t) \|\xi_0\|_2^2} \cdot \|\bar{\xi}_t - \bar{\xi}_0(\bar{x}_t, t)\|^2 \right]$$