Diffusion Model

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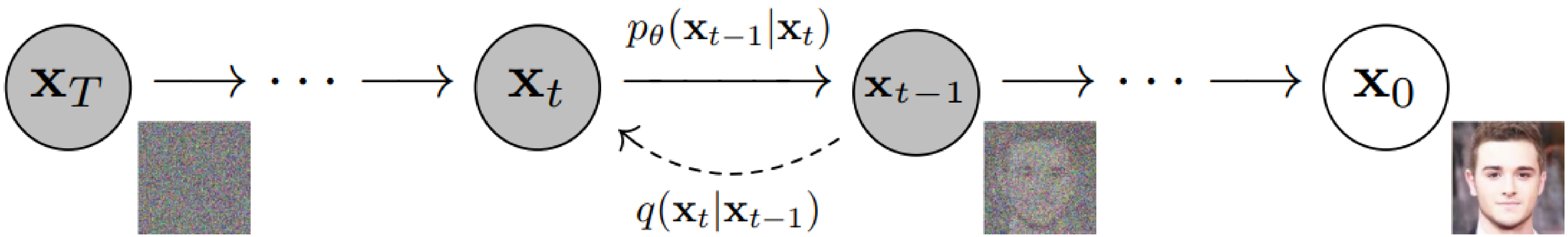
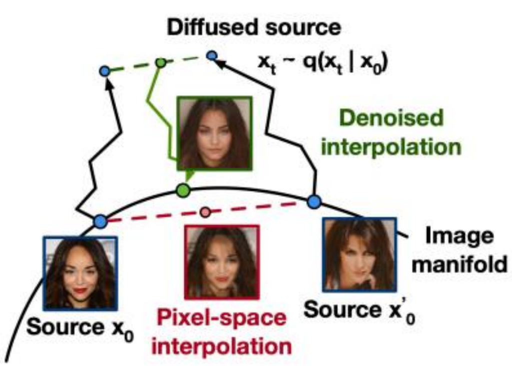
Diffusion模型家族

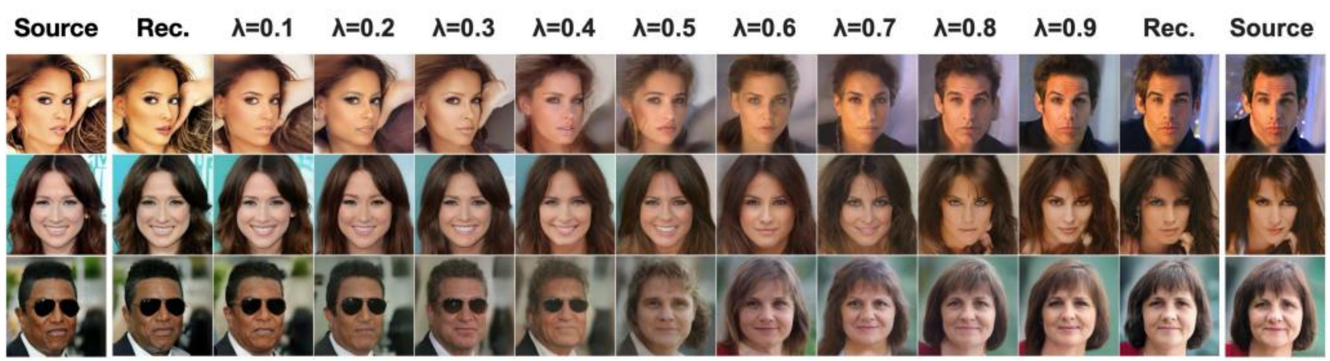
- DDPM
- Score-based生成模型
- 条件DDPM

DDPM



- 线性组合：$\bar{\mathbf{x}}_t = (1-\lambda)\mathbf{x}_0 + \lambda \mathbf{x}'_0$
- 前向加噪：$\mathbf{x}'_t \sim q(\mathbf{x}_t|\mathbf{x}_0)$
- 逆向合成：$\bar{\mathbf{x}}_0 \sim p(\mathbf{x}_0|\bar{\mathbf{x}}_t)$

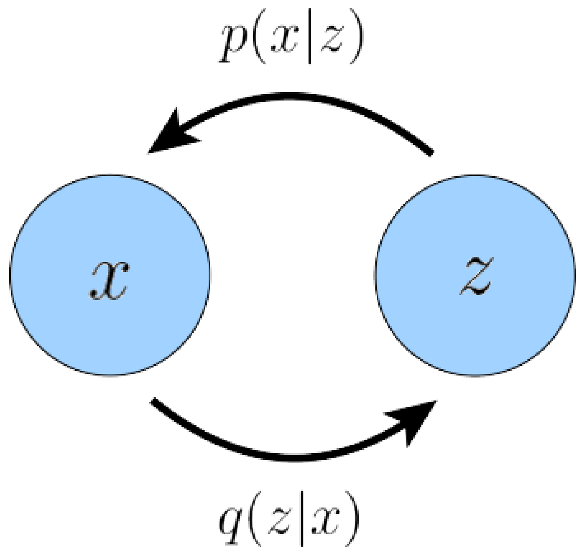




数学背景：ELBO

$$
\begin{aligned}
\log p(\boldsymbol{x}) &= \log p(\boldsymbol{x}) \int q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) dz \\
&= \int q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) (\log p(\boldsymbol{x})) dz \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} [\log p(\boldsymbol{x})] \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{p(\boldsymbol{z}|\boldsymbol{x})}\right] \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}) q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p(\boldsymbol{z}|\boldsymbol{x}) q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right] \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right] + \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p(\boldsymbol{z}|\boldsymbol{x})}\right] \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right] + D_{\mathrm{KL}}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z}|\boldsymbol{x})) \\
&\geq \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right]
\end{aligned}
$$

模型背景：VAE

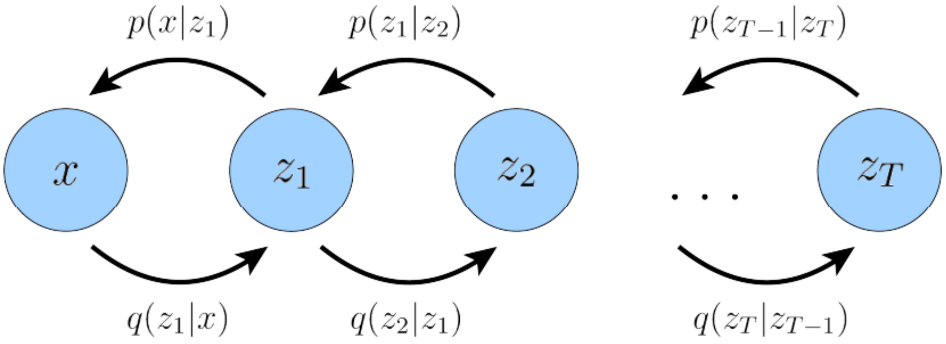


$$\begin{aligned}
\mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x},\boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right] &= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right] \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})\right] + \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right] \\
&= \underbrace{\mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})\right]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z}))}_{\text{prior matching term}}
\end{aligned}$$

$$\begin{aligned}
q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) &= \mathcal{N}(\boldsymbol{z}; \boldsymbol{\mu}_{\phi}(\boldsymbol{x}), \boldsymbol{\sigma}^2_{\phi}(\boldsymbol{x})\mathbf{I}) \\
p(\boldsymbol{z}) &= \mathcal{N}(\boldsymbol{z}; \mathbf{0}, \mathbf{I})
\end{aligned}$$

$$\underset{\boldsymbol{\phi},\boldsymbol{\theta}}{\arg\max}\, \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})\right] - D_{\mathrm{KL}}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z})) \approx \underset{\boldsymbol{\phi},\boldsymbol{\theta}}{\arg\max} \sum_{l=1}^{L} \log p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}^{(l)}) - D_{\mathrm{KL}}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z}))$$

模型背景：HVAE



$$p(\boldsymbol{x}, \boldsymbol{z}_{1:T}) = p(\boldsymbol{z}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}_1) \prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{z}_{t-1}|\boldsymbol{z}_t)$$

$$q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x}) = q_{\boldsymbol{\phi}}(\boldsymbol{z}_1|\boldsymbol{x}) \prod_{t=2}^{T} q_{\boldsymbol{\phi}}(\boldsymbol{z}_t|\boldsymbol{z}_{t-1})$$

$$\begin{aligned}
\log p(\boldsymbol{x}) &= \log \int p(\boldsymbol{x}, \boldsymbol{z}_{1:T}) d\boldsymbol{z}_{1:T} \\
&= \log \int \frac{p(\boldsymbol{x}, \boldsymbol{z}_{1:T}) q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x})} d\boldsymbol{z}_{1:T} \\
&= \log \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x})} \left[\frac{p(\boldsymbol{x}, \boldsymbol{z}_{1:T})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x})} \right] \\
&\geq \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}_{1:T})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x})} \right]
\end{aligned}$$

$$\mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}_{1:T})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x})} \right] = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{z}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}_1) \prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{z}_{t-1}|\boldsymbol{z}_t)}{q_{\boldsymbol{\phi}}(\boldsymbol{z}_1|\boldsymbol{x}) \prod_{t=2}^{T} q_{\boldsymbol{\phi}}(\boldsymbol{z}_t|\boldsymbol{z}_{t-1})} \right]$$

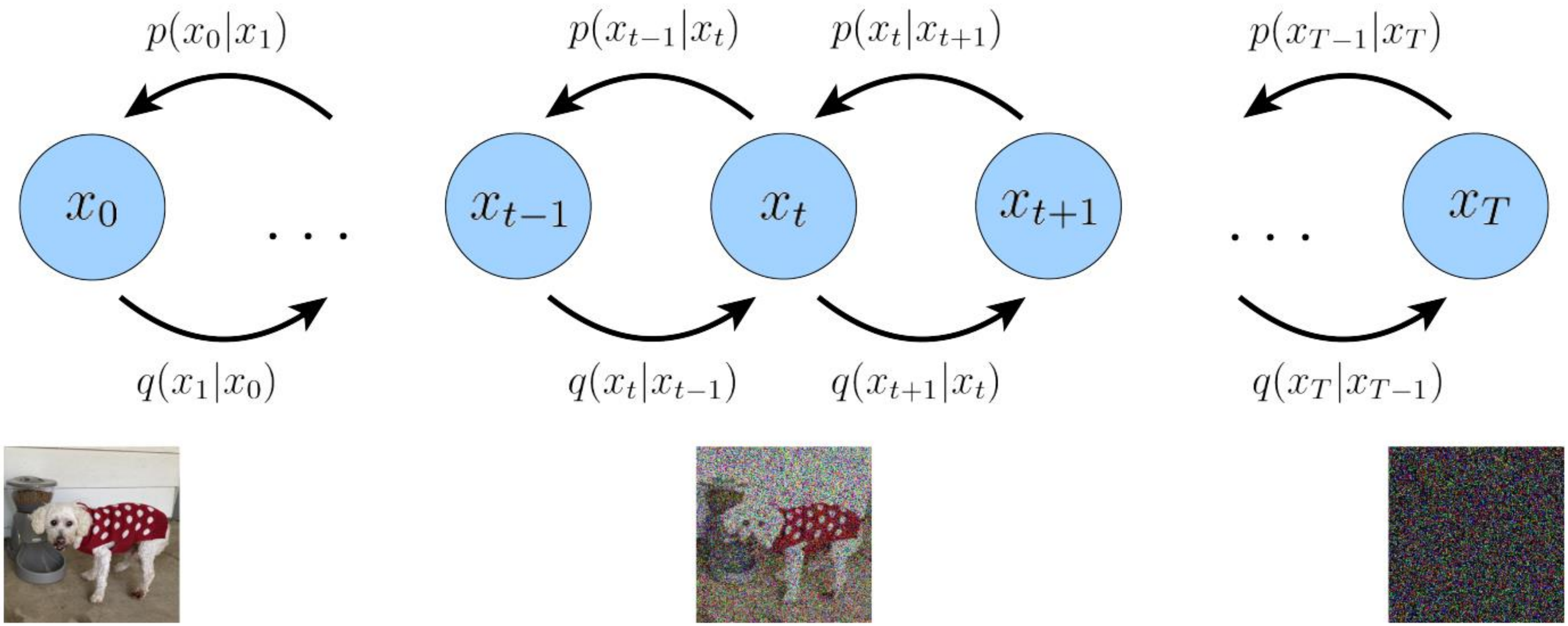
Variational Diffusion Models

$$q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0) = \prod_{t=1}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})$$

$$q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\alpha_t}\boldsymbol{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

$$p(\boldsymbol{x}_{0:T}) = p(\boldsymbol{x}_T)\prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$$

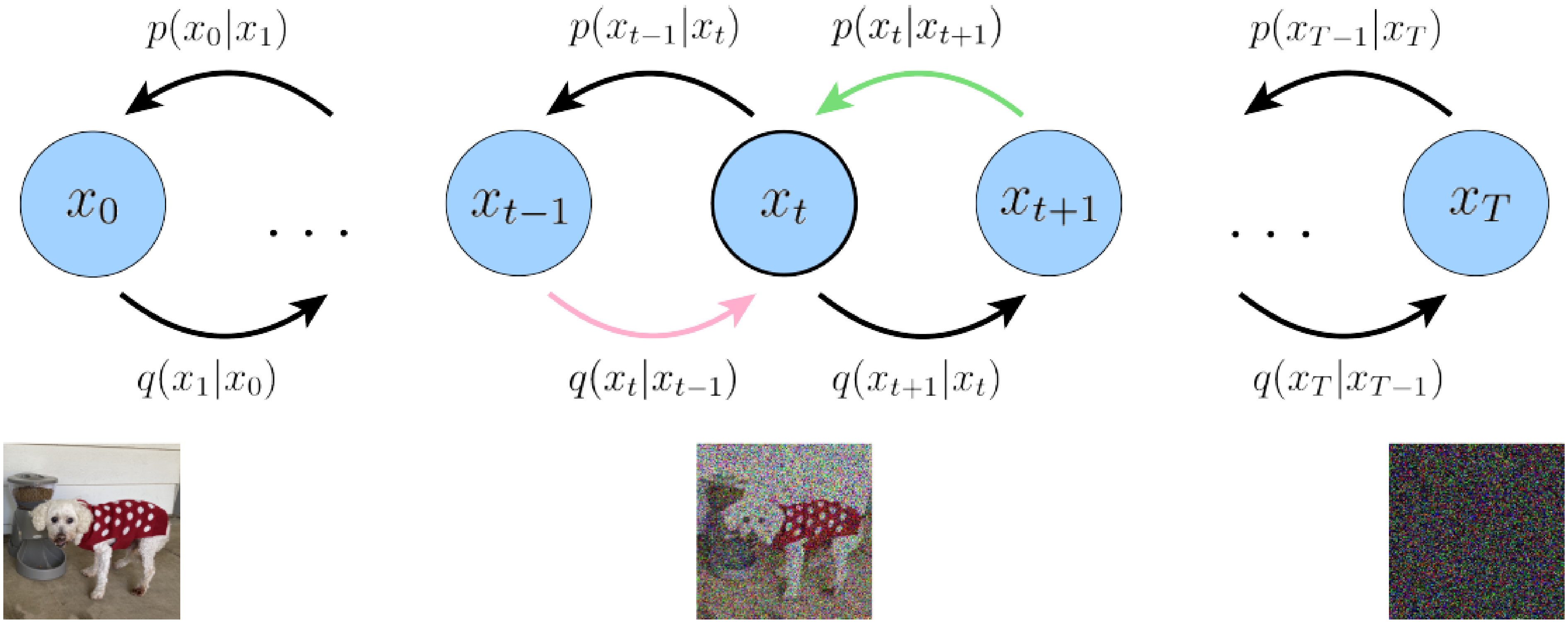
$$p(\boldsymbol{x}_T) = \mathcal{N}(\boldsymbol{x}_T; \mathbf{0}, \mathbf{I})$$



Diffusion模型的ELBO

$$
\begin{aligned}
\log p(\boldsymbol{x}) &= \log \int p(\boldsymbol{x}_{0:T}) d\boldsymbol{x}_{1:T} \\
&= \log \int \frac{p(\boldsymbol{x}_{0:T}) q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} d\boldsymbol{x}_{1:T} \\
&= \log \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \right] \\
&\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) \prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\prod_{t=1}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1) \prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1}) \prod_{t=1}^{T-1} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1) \prod_{t=1}^{T-1} p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1}) \prod_{t=1}^{T-1} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1})} \right] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \prod_{t=1}^{T-1} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} [\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1})} \right] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\sum_{t=1}^{T-1} \log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} [\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1})} \right] + \sum_{t=1}^{T-1} \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} [\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)] + \mathbb{E}_{q(\boldsymbol{x}_{T-1},\boldsymbol{x}_T|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1})} \right] + \sum_{t=1}^{T-1} \mathbb{E}_{q(\boldsymbol{x}_{t-1},\boldsymbol{x}_t,\boldsymbol{x}_{t+1}|\boldsymbol{x}_0)} \left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} [\log p_{\theta}(\boldsymbol{x}_0|\boldsymbol{x}_1)]}_{\text{reconstruction term}} - \underbrace{\mathbb{E}_{q(\boldsymbol{x}_{T-1}|\boldsymbol{x}_0)} [D_{\mathrm{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1}) \parallel p(\boldsymbol{x}_T))]}_{\text{prior matching term}} \\
&\quad - \sum_{t=1}^{T-1} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_{t-1},\boldsymbol{x}_{t+1}|\boldsymbol{x}_0)} [D_{\mathrm{KL}}(q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) \parallel p_{\theta}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1}))]}_{\text{consistency term}}
\end{aligned}
$$

优化目标



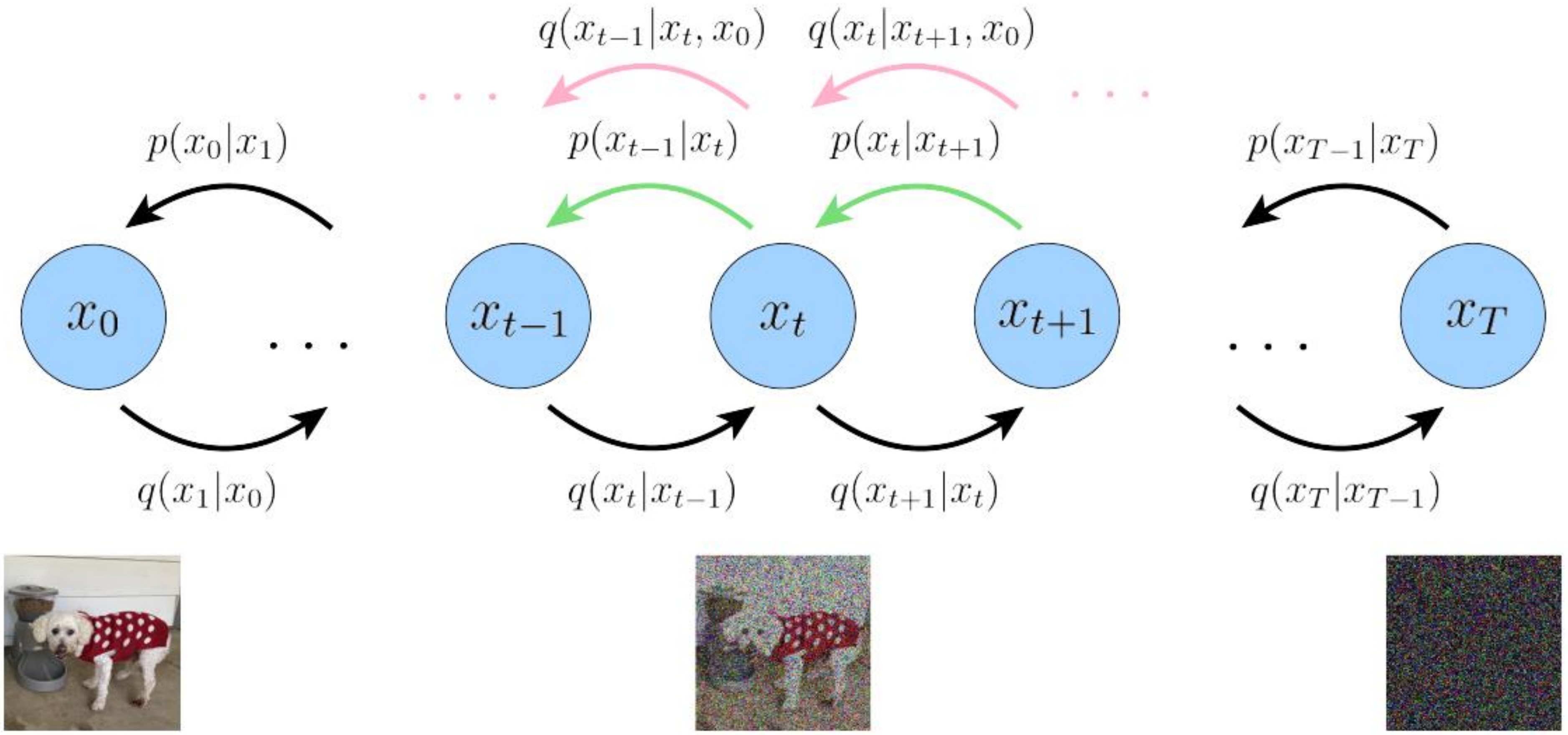
$p(x_0|x_1)$
$p(x_{t-1}|x_t)$
$p(x_t|x_{t+1})$
$p(x_{T-1}|x_T)$
x_0
x_{t-1}
x_t
x_{t+1}
x_T
$q(x_1|x_0)$
$q(x_t|x_{t-1})$
$q(x_{t+1}|x_t)$
$q(x_T|x_{T-1})$

Diffusion模型重写的ELBO

$$
\begin{aligned}
\log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)\prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\prod_{t=1}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)\prod_{t=2}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)\prod_{t=2}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)q(\boldsymbol{x}_t|\boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\cancel{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}}{\cancel{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{\cancel{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}} + \log \frac{\cancel{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)} + \sum_{t=2}^{T} \log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right] + \mathbb{E}_{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_t,\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_0)\parallel p(\boldsymbol{x}_T))}_{\text{prior matching term}} - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\right]}_{\text{denoising matching term}}
\end{aligned}
$$

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

基于重写的优化目标



$q(x_{t-1}|x_t, x_0)$
$q(x_t|x_{t+1}, x_0)$
$p(x_0|x_1)$
$p(x_{t-1}|x_t)$
$p(x_t|x_{t+1})$
$p(x_{T-1}|x_T)$
x_0
x_{t-1}
x_t
x_{t+1}
x_T
$q(x_1|x_0)$
$q(x_t|x_{t-1})$
$q(x_{t+1}|x_t)$
$q(x_T|x_{T-1})$

去噪匹配项

$$\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\right]$$

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

$$\begin{aligned}
\boldsymbol{x}_t &= \sqrt{\alpha_t}\boldsymbol{x}_{t-1}+\sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1}^*\\
&= \sqrt{\alpha_t}\left(\sqrt{\alpha_{t-1}}\boldsymbol{x}_{t-2}+\sqrt{1-\alpha_{t-1}}\boldsymbol{\epsilon}_{t-2}^*\right)+\sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1}^*\\
&= \sqrt{\alpha_t\alpha_{t-1}}\boldsymbol{x}_{t-2}+\sqrt{\alpha_t-\alpha_t\alpha_{t-1}}\boldsymbol{\epsilon}_{t-2}^*+\sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1}^*\\
&= \sqrt{\alpha_t\alpha_{t-1}}\boldsymbol{x}_{t-2}+\sqrt{\sqrt{\alpha_t-\alpha_t\alpha_{t-1}}^2+\sqrt{1-\alpha_t}^2}\boldsymbol{\epsilon}_{t-2}\\
&= \sqrt{\alpha_t\alpha_{t-1}}\boldsymbol{x}_{t-2}+\sqrt{\alpha_t-\alpha_t\alpha_{t-1}+1-\alpha_t}\boldsymbol{\epsilon}_{t-2}\\
&= \sqrt{\alpha_t\alpha_{t-1}}\boldsymbol{x}_{t-2}+\sqrt{1-\alpha_t\alpha_{t-1}}\boldsymbol{\epsilon}_{t-2}\\
&= \ldots\\
&= \sqrt{\prod_{i=1}^{t}\alpha_i}\boldsymbol{x}_0+\sqrt{1-\prod_{i=1}^{t}\alpha_i}\boldsymbol{\epsilon}_0\\
&= \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0+\sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_0\\
&\sim \mathcal{N}(\boldsymbol{x}_t;\sqrt{\bar{\alpha}_t}\boldsymbol{x}_0,(1-\bar{\alpha}_t)\mathbf{I})
\end{aligned}$$

去噪匹配项

$$
\begin{aligned}
q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0) &= \frac{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\\
&= \frac{\mathcal{N}(\boldsymbol{x}_t;\sqrt{\alpha_t}\boldsymbol{x}_{t-1},(1-\alpha_t)\mathbf{I})\mathcal{N}(\boldsymbol{x}_{t-1};\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_0,(1-\bar\alpha_{t-1})\mathbf{I})}{\mathcal{N}(\boldsymbol{x}_t;\sqrt{\bar\alpha_t}\boldsymbol{x}_0,(1-\bar\alpha_t)\mathbf{I})}\\
&\propto \exp\left\{-\left[\frac{(\boldsymbol{x}_t-\sqrt{\alpha_t}\boldsymbol{x}_{t-1})^2}{2(1-\alpha_t)}+\frac{(\boldsymbol{x}_{t-1}-\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_0)^2}{2(1-\bar\alpha_{t-1})}-\frac{(\boldsymbol{x}_t-\sqrt{\bar\alpha_t}\boldsymbol{x}_0)^2}{2(1-\bar\alpha_t)}\right]\right\}\\
&= \exp\left\{-\frac{1}{2}\left[\frac{(\boldsymbol{x}_t-\sqrt{\alpha_t}\boldsymbol{x}_{t-1})^2}{1-\alpha_t}+\frac{(\boldsymbol{x}_{t-1}-\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_0)^2}{1-\bar\alpha_{t-1}}-\frac{(\boldsymbol{x}_t-\sqrt{\bar\alpha_t}\boldsymbol{x}_0)^2}{1-\bar\alpha_t}\right]\right\}\\
&= \exp\left\{-\frac{1}{2}\left[\frac{(-2\sqrt{\alpha_t}\boldsymbol{x}_t\boldsymbol{x}_{t-1}+\alpha_t\boldsymbol{x}_{t-1}^2)}{1-\alpha_t}+\frac{(\boldsymbol{x}_{t-1}^2-2\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_{t-1}\boldsymbol{x}_0)}{1-\bar\alpha_{t-1}}+C(\boldsymbol{x}_t,\boldsymbol{x}_0)\right]\right\}\\
&\propto \exp\left\{-\frac{1}{2}\left[-\frac{2\sqrt{\alpha_t}\boldsymbol{x}_t\boldsymbol{x}_{t-1}}{1-\alpha_t}+\frac{\alpha_t\boldsymbol{x}_{t-1}^2}{1-\alpha_t}+\frac{\boldsymbol{x}_{t-1}^2}{1-\bar\alpha_{t-1}}-\frac{2\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_{t-1}\boldsymbol{x}_0}{1-\bar\alpha_{t-1}}\right]\right\}\\
&= \exp\left\{-\frac{1}{2}\left[(\frac{\alpha_t}{1-\alpha_t}+\frac{1}{1-\bar\alpha_{t-1}})\boldsymbol{x}_{t-1}^2-2\left(\frac{\sqrt{\alpha_t}\boldsymbol{x}_t}{1-\alpha_t}+\frac{\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_0}{1-\bar\alpha_{t-1}}\right)\boldsymbol{x}_{t-1}\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})}\boldsymbol{x}_{t-1}^2-2\left(\frac{\sqrt{\alpha_t}\boldsymbol{x}_t}{1-\alpha_t}+\frac{\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_0}{1-\bar\alpha_{t-1}}\right)\boldsymbol{x}_{t-1}\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})}\boldsymbol{x}_{t-1}^2-2\left(\frac{\sqrt{\alpha_t}\boldsymbol{x}_t}{1-\alpha_t}+\frac{\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_0}{1-\bar\alpha_{t-1}}\right)\boldsymbol{x}_{t-1}\right]\right\}\\
&= \exp\left\{-\frac{1}{2}\left[\frac{1-\bar\alpha_t}{(1-\alpha_t)(1-\bar\alpha_{t-1})}\boldsymbol{x}_{t-1}^2-2\left(\frac{\sqrt{\alpha_t}\boldsymbol{x}_t}{1-\alpha_t}+\frac{\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_0}{1-\bar\alpha_{t-1}}\right)\boldsymbol{x}_{t-1}\right]\right\}\\
&= \exp\left\{-\frac{1}{2}\left(\frac{1-\bar\alpha_t}{(1-\alpha_t)(1-\bar\alpha_{t-1})}\right)\left[\boldsymbol{x}_{t-1}^2-2\frac{\left(\frac{\sqrt{\alpha_t}\boldsymbol{x}_t}{1-\alpha_t}+\frac{\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_0}{1-\bar\alpha_{t-1}}\right)}{\frac{1-\bar\alpha_t}{(1-\alpha_t)(1-\bar\alpha_{t-1})}}\boldsymbol{x}_{t-1}\right]\right\}\\
&= \exp\left\{-\frac{1}{2}\left(\frac{1-\bar\alpha_t}{(1-\alpha_t)(1-\bar\alpha_{t-1})}\right)\left[\boldsymbol{x}_{t-1}^2-2\frac{\left(\frac{\sqrt{\alpha_t}\boldsymbol{x}_t}{1-\alpha_t}+\frac{\sqrt{\bar\alpha_{t-1}}\boldsymbol{x}_0}{1-\bar\alpha_{t-1}}\right)(1-\alpha_t)(1-\bar\alpha_{t-1})}{1-\bar\alpha_t}\boldsymbol{x}_{t-1}\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[\boldsymbol{x}_{t-1}^2-2\frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})\boldsymbol{x}_t+\sqrt{\bar\alpha_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar\alpha_t}\boldsymbol{x}_{t-1}\right]\right\}\\
&\propto \mathcal{N}(\boldsymbol{x}_{t-1};\underbrace{\frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})\boldsymbol{x}_t+\sqrt{\bar\alpha_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar\alpha_t}}_{\mu_q(\boldsymbol{x}_t,\boldsymbol{x}_0)},\underbrace{\frac{(1-\alpha_t)(1-\bar\alpha_{t-1})}{1-\bar\alpha_t}\mathbf{I}}_{\boldsymbol{\Sigma}_q(t)})
\end{aligned}
$$

去噪匹配项

$$
\begin{aligned}
&\arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\\
=&\arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}(\mathcal{N}(\boldsymbol{x}_{t-1};\boldsymbol{\mu}_q,\boldsymbol{\Sigma}_q(t))\parallel\mathcal{N}(\boldsymbol{x}_{t-1};\boldsymbol{\mu}_{\boldsymbol{\theta}},\boldsymbol{\Sigma}_q(t)))\\
=&\arg\min_{\boldsymbol{\theta}}\frac{1}{2}\left[\log\frac{|\boldsymbol{\Sigma}_q(t)|}{|\boldsymbol{\Sigma}_q(t)|}-d+\mathrm{tr}(\boldsymbol{\Sigma}_q(t)^{-1}\boldsymbol{\Sigma}_q(t))+(\boldsymbol{\mu}_{\boldsymbol{\theta}}-\boldsymbol{\mu}_q)^T\boldsymbol{\Sigma}_q(t)^{-1}(\boldsymbol{\mu}_{\boldsymbol{\theta}}-\boldsymbol{\mu}_q)\right]\\
=&\arg\min_{\boldsymbol{\theta}}\frac{1}{2}\left[\log 1-d+d+(\boldsymbol{\mu}_{\boldsymbol{\theta}}-\boldsymbol{\mu}_q)^T\boldsymbol{\Sigma}_q(t)^{-1}(\boldsymbol{\mu}_{\boldsymbol{\theta}}-\boldsymbol{\mu}_q)\right]\\
=&\arg\min_{\boldsymbol{\theta}}\frac{1}{2}\left[(\boldsymbol{\mu}_{\boldsymbol{\theta}}-\boldsymbol{\mu}_q)^T\boldsymbol{\Sigma}_q(t)^{-1}(\boldsymbol{\mu}_{\boldsymbol{\theta}}-\boldsymbol{\mu}_q)\right]\\
=&\arg\min_{\boldsymbol{\theta}}\frac{1}{2}\left[(\boldsymbol{\mu}_{\boldsymbol{\theta}}-\boldsymbol{\mu}_q)^T\left(\sigma_q^2(t)\mathbf{I}\right)^{-1}(\boldsymbol{\mu}_{\boldsymbol{\theta}}-\boldsymbol{\mu}_q)\right]\\
=&\arg\min_{\boldsymbol{\theta}}\frac{1}{2\sigma_q^2(t)}\left[\left\|\boldsymbol{\mu}_{\boldsymbol{\theta}}-\boldsymbol{\mu}_q\right\|_2^2\right]
\end{aligned}
$$

$$
\boldsymbol{\mu}_q(\boldsymbol{x}_t,\boldsymbol{x}_0)=\frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})\boldsymbol{x}_t+\sqrt{\bar\alpha_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar\alpha_t}
$$

$$
\boldsymbol{\mu}_{\boldsymbol{\theta}}(\boldsymbol{x}_t,t)=\frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})\boldsymbol{x}_t+\sqrt{\bar\alpha_{t-1}}(1-\alpha_t)\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t,t)}{1-\bar\alpha_t}
$$

$$
\begin{aligned}
&\arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\\
=&\arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}(\mathcal{N}(\boldsymbol{x}_{t-1};\boldsymbol{\mu}_q,\boldsymbol{\Sigma}_q(t))\parallel\mathcal{N}(\boldsymbol{x}_{t-1};\boldsymbol{\mu}_{\boldsymbol{\theta}},\boldsymbol{\Sigma}_q(t)))\\
=&\arg\min_{\boldsymbol{\theta}}\frac{1}{2\sigma_q^2(t)}\left[\left\|\frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})\boldsymbol{x}_t+\sqrt{\bar\alpha_{t-1}}(1-\alpha_t)\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t,t)}{1-\bar\alpha_t}-\frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})\boldsymbol{x}_t+\sqrt{\bar\alpha_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar\alpha_t}\right\|_2^2\right]\\
=&\arg\min_{\boldsymbol{\theta}}\frac{1}{2\sigma_q^2(t)}\left[\left\|\frac{\sqrt{\bar\alpha_{t-1}}(1-\alpha_t)\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t,t)}{1-\bar\alpha_t}-\frac{\sqrt{\bar\alpha_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar\alpha_t}\right\|_2^2\right]\\
=&\arg\min_{\boldsymbol{\theta}}\frac{1}{2\sigma_q^2(t)}\left[\left\|\frac{\sqrt{\bar\alpha_{t-1}}(1-\alpha_t)}{1-\bar\alpha_t}\left(\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t,t)-\boldsymbol{x}_0\right)\right\|_2^2\right]\\
=&\arg\min_{\boldsymbol{\theta}}\frac{1}{2\sigma_q^2(t)}\frac{\bar\alpha_{t-1}(1-\alpha_t)^2}{(1-\bar\alpha_t)^2}\left[\left\|\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t,t)-\boldsymbol{x}_0\right\|_2^2\right]
\end{aligned}
$$

$$
\arg\min_{\boldsymbol{\theta}}\mathbb{E}_{t\sim U\{2,T\}}\left[\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\right]\right]
$$

去噪匹配项

$$\begin{aligned}
\boldsymbol{\mu}_q(\boldsymbol{x}_t, \boldsymbol{x}_0) &= \frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})\boldsymbol{x}_t + \sqrt{\bar\alpha_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar\alpha_t} \\
&= \frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})\boldsymbol{x}_t + \sqrt{\bar\alpha_{t-1}}(1-\alpha_t)\frac{\boldsymbol{x}_t - \sqrt{1-\bar\alpha_t}\boldsymbol{\epsilon}_0}{\sqrt{\bar\alpha_t}}}{1-\bar\alpha_t} \\
&= \frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})\boldsymbol{x}_t + (1-\alpha_t)\frac{\boldsymbol{x}_t - \sqrt{1-\bar\alpha_t}\boldsymbol{\epsilon}_0}{\sqrt{\alpha_t}}}{1-\bar\alpha_t} \\
&= \frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})\boldsymbol{x}_t}{1-\bar\alpha_t} + \frac{(1-\alpha_t)\boldsymbol{x}_t}{(1-\bar\alpha_t)\sqrt{\alpha_t}} - \frac{(1-\alpha_t)\sqrt{1-\bar\alpha_t}\boldsymbol{\epsilon}_0}{(1-\bar\alpha_t)\sqrt{\alpha_t}} \\
&= \left(\frac{\sqrt{\alpha_t}(1-\bar\alpha_{t-1})}{1-\bar\alpha_t} + \frac{1-\alpha_t}{(1-\bar\alpha_t)\sqrt{\alpha_t}}\right)\boldsymbol{x}_t - \frac{(1-\alpha_t)\sqrt{1-\bar\alpha_t}}{(1-\bar\alpha_t)\sqrt{\alpha_t}}\boldsymbol{\epsilon}_0 \\
&= \left(\frac{\alpha_t(1-\bar\alpha_{t-1})}{(1-\bar\alpha_t)\sqrt{\alpha_t}} + \frac{1-\alpha_t}{(1-\bar\alpha_t)\sqrt{\alpha_t}}\right)\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}\sqrt{\alpha_t}}\boldsymbol{\epsilon}_0 \\
&= \frac{\alpha_t - \bar\alpha_t + 1 - \alpha_t}{(1-\bar\alpha_t)\sqrt{\alpha_t}}\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}\sqrt{\alpha_t}}\boldsymbol{\epsilon}_0 \\
&= \frac{1-\bar\alpha_t}{(1-\bar\alpha_t)\sqrt{\alpha_t}}\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}\sqrt{\alpha_t}}\boldsymbol{\epsilon}_0 \\
&= \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}\sqrt{\alpha_t}}\boldsymbol{\epsilon}_0
\end{aligned}$$

$$\boldsymbol{x}_0 = \frac{\boldsymbol{x}_t - \sqrt{1-\bar\alpha_t}\boldsymbol{\epsilon}_0}{\sqrt{\bar\alpha_t}}$$

$$\begin{aligned}
&\arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)) \\
&= \arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}(\mathcal{N}(\boldsymbol{x}_{t-1}; \boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q(t)) \parallel \mathcal{N}(\boldsymbol{x}_{t-1}; \boldsymbol{\mu}_{\boldsymbol{\theta}}, \boldsymbol{\Sigma}_q(t))) \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)}\left[\left\|\frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}\sqrt{\alpha_t}}\hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) - \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t + \frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}\sqrt{\alpha_t}}\boldsymbol{\epsilon}_0\right\|_2^2\right] \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)}\left[\left\|\frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}\sqrt{\alpha_t}}\boldsymbol{\epsilon}_0 - \frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}\sqrt{\alpha_t}}\hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t)\right\|_2^2\right] \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)}\left[\left\|\frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}\sqrt{\alpha_t}}(\boldsymbol{\epsilon}_0 - \hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t))\right\|_2^2\right] \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)}\frac{(1-\alpha_t)^2}{(1-\bar\alpha_t)\alpha_t}\left[\left\|\boldsymbol{\epsilon}_0 - \hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t)\right\|_2^2\right]
\end{aligned}$$

$$\boldsymbol{\mu}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}\sqrt{\alpha_t}}\hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t)$$

训练与采样算法

$$\mathbf{x}_{t-1} \sim p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$$

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z} \qquad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \ldots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

实验结果

Table 1: CIFAR10 results. NLL measured in bits/dim.

Model	IS	FID	NLL Test (Train)
Conditional			
EBM [11]	8.30	37.9	
JEM [17]	8.76	38.4	
BigGAN [3]	9.22	14.73	
StyleGAN2 + ADA (v1) [29]	**10.06**	**2.67**	
Unconditional			
Diffusion (original) [53]			≤ 5.40
Gated PixelCNN [59]	4.60	65.93	3.03 (2.90)
Sparse Transformer [7]			**2.80**
PixelIQN [43]	5.29	49.46	
EBM [11]	6.78	38.2	
NCSNv2 [56]		31.75	
NCSN [55]	8.87 ± 0.12	25.32	
SNGAN [39]	8.22 ± 0.05	21.7	
SNGAN-DDLS [4]	9.09 ± 0.10	15.42	
StyleGAN2 + ADA (v1) [29]	$\mathbf{9.74} \pm 0.05$	3.26	
Ours (L, fixed isotropic $\mathbf{\Sigma}$)	7.67 ± 0.13	13.51	≤ 3.70 (3.69)
Ours (L_{simple})	9.46 ± 0.11	**3.17**	≤ 3.75 (3.72)

DDPM实现 1

Denoise Diffusion

```python
class DenoiseDiffusion:
```

- `eps_model` is $\epsilon_\theta(x_t, t)$ model
- `n_steps` is t
- `device` is the device to place constants on

```python
    def __init__(self, eps_model: nn.Module, n_steps: int, device: torch.device):
```

```python
        super().__init__()
        self.eps_model = eps_model
```

Create $\beta_1, \dots, \beta_T$ linearly increasing variance schedule

```python
        self.beta = torch.linspace(0.0001, 0.02, n_steps).to(device)
```

$\alpha_t = 1 - \beta_t$

```python
        self.alpha = 1. - self.beta
```

$\bar\alpha_t = \prod_{s=1}^t \alpha_s$

```python
        self.alpha_bar = torch.cumprod(self.alpha, dim=0)
```

T

```python
        self.n_steps = n_steps
```

$\sigma^2 = \beta$

```python
        self.sigma2 = self.beta
```

Get $q(x_t|x_0)$ distribution

$$q(x_t|x_0) = \mathcal{N}\Big(x_t; \sqrt{\bar\alpha_t} x_0, (1-\bar\alpha_t) \mathbf{I}\Big)$$

```python
    def q_xt_x0(self, x0: torch.Tensor, t: torch.Tensor) -> Tuple[torch.Tensor, torch.Tensor]:
```

gather α_t and compute $\sqrt{\bar\alpha_t} x_0$

```python
        mean = gather(self.alpha_bar, t) ** 0.5 * x0
```

$(1-\bar\alpha_t) \mathbf{I}$

```python
        var = 1 - gather(self.alpha_bar, t)
```

```python
        return mean, var
```

Sample from $q(x_t|x_0)$

$$q(x_t|x_0) = \mathcal{N}\Big(x_t; \sqrt{\bar\alpha_t} x_0, (1-\bar\alpha_t) \mathbf{I}\Big)$$

```python
    def q_sample(self, x0: torch.Tensor, t: torch.Tensor, eps: Optional[torch.Tensor] = None):
```

$\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

```python
        if eps is None:
            eps = torch.randn_like(x0)
```

get $q(x_t|x_0)$

```python
        mean, var = self.q_xt_x0(x0, t)
```

Sample from $q(x_t|x_0)$

```python
        return mean + (var ** 0.5) * eps
```

DDPM实现 2

Sample from $p_\theta(x_{t-1}|x_t)$

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}\big(x_{t-1}; \mu_\theta(x_t,t), \sigma_t^2 \mathbf{I}\big)$$
$$\mu_\theta(x_t,t) = \frac{1}{\sqrt{\alpha_t}}\Big(x_t - \frac{\beta_t}{\sqrt{1-\bar\alpha_t}}\epsilon_\theta(x_t,t)\Big)$$

```python
def p_sample(self, xt: torch.Tensor, t: torch.Tensor):
```

$\epsilon_\theta(x_t,t)$

```python
    eps_theta = self.eps_model(xt, t)
```

gather $\bar\alpha_t$

```python
    alpha_bar = gather(self.alpha_bar, t)
```

α_t

```python
    alpha = gather(self.alpha, t)
```

$\frac{\beta}{\sqrt{1-\bar\alpha_t}}$

```python
    eps_coef = (1 - alpha) / (1 - alpha_bar) ** .5
```

$$\frac{1}{\sqrt{\alpha_t}}\Big(x_t - \frac{\beta_t}{\sqrt{1-\bar\alpha_t}}\epsilon_\theta(x_t,t)\Big)$$

```python
    mean = 1 / (alpha ** 0.5) * (xt - eps_coef * eps_theta)
```

σ^2

```python
    var = gather(self.sigma2, t)
```

$\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

```python
    eps = torch.randn(xt.shape, device=xt.device)
```

Sample

```python
    return mean + (var ** .5) * eps
```

Simplified Loss

$$L_{\text{simple}}(\theta) = \mathbb{E}_{t,x_0,\epsilon}\Bigg[\bigg\|\epsilon - \epsilon_\theta\big(\sqrt{\bar\alpha_t}x_0 + \sqrt{1-\bar\alpha_t}\epsilon, t\big)\bigg\|^2\Bigg]$$

```python
def loss(self, x0: torch.Tensor, noise: Optional[torch.Tensor] = None):
```

Get batch size

```python
    batch_size = x0.shape[0]
```

Get random t for each sample in the batch

```python
    t = torch.randint(0, self.n_steps, (batch_size,), device=x0.device, dtype=torch.long)
```

$\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

```python
    if noise is None:
        noise = torch.randn_like(x0)
```

Sample x_t for $q(x_t|x_0)$

```python
    xt = self.q_sample(x0, t, eps=noise)
```

Get $\epsilon_\theta(\sqrt{\bar\alpha_t}x_0 + \sqrt{1-\bar\alpha_t}\epsilon, t)$

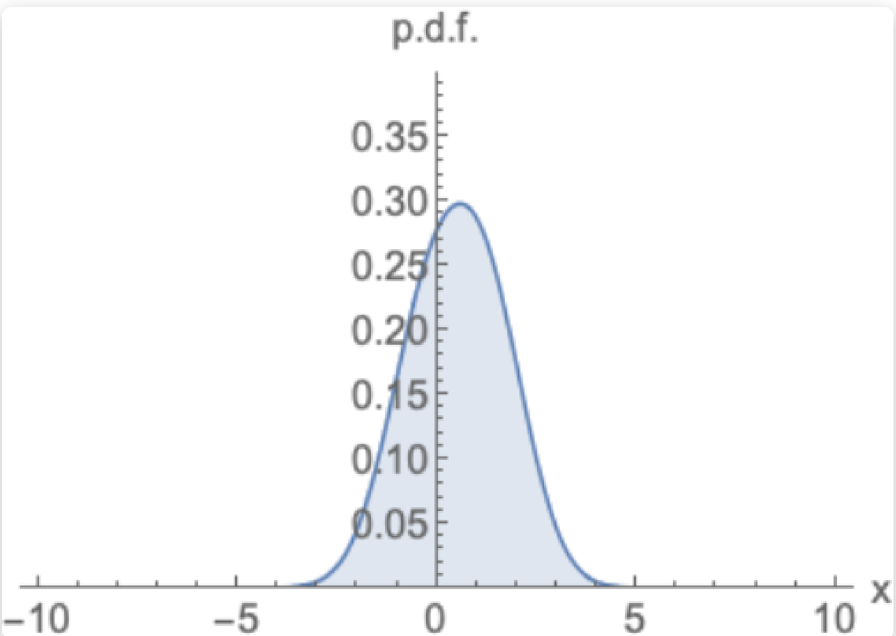
```python
    eps_theta = self.eps_model(xt, t)
```

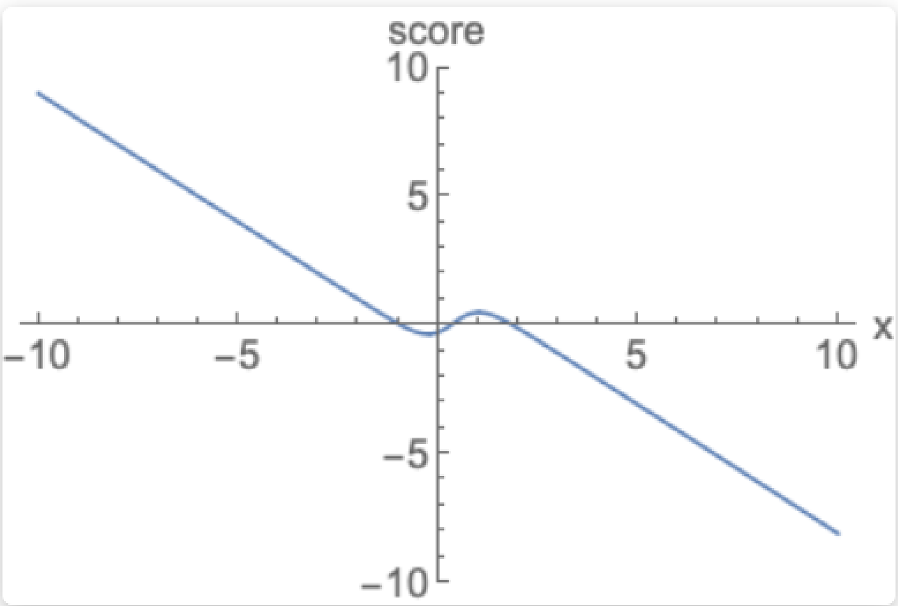
MSE loss

```python
    return F.mse_loss(noise, eps_theta)
```

Score-based生成模型

$$\mathbf{s}_\theta(\mathbf{x}) = \nabla_\mathbf{x} \log p_\theta(\mathbf{x}) = -\nabla_\mathbf{x} f_\theta(\mathbf{x}) - \underbrace{\nabla_\mathbf{x} \log Z_\theta}_{=0} = -\nabla_\mathbf{x} f_\theta(\mathbf{x}) \qquad p_\theta(\mathbf{x}) = \frac{e^{-f_\theta(\mathbf{x})}}{Z_\theta}$$



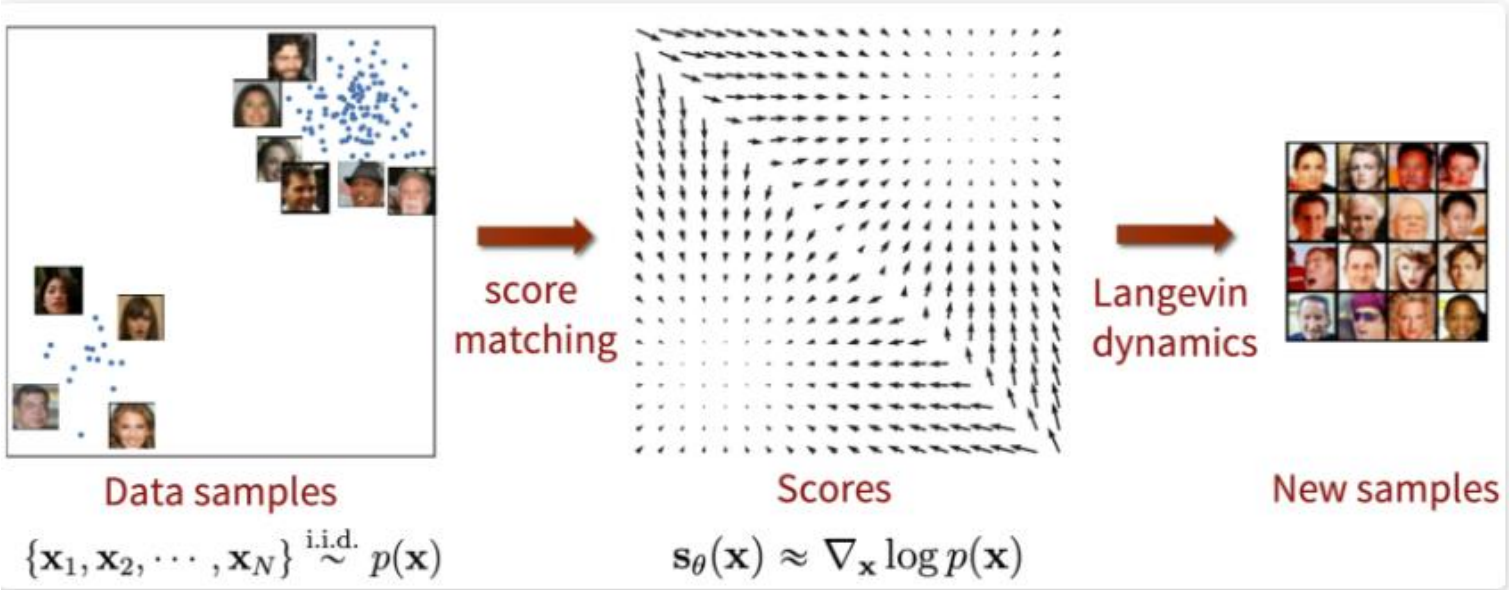


数据生成（Langevin dynamics）

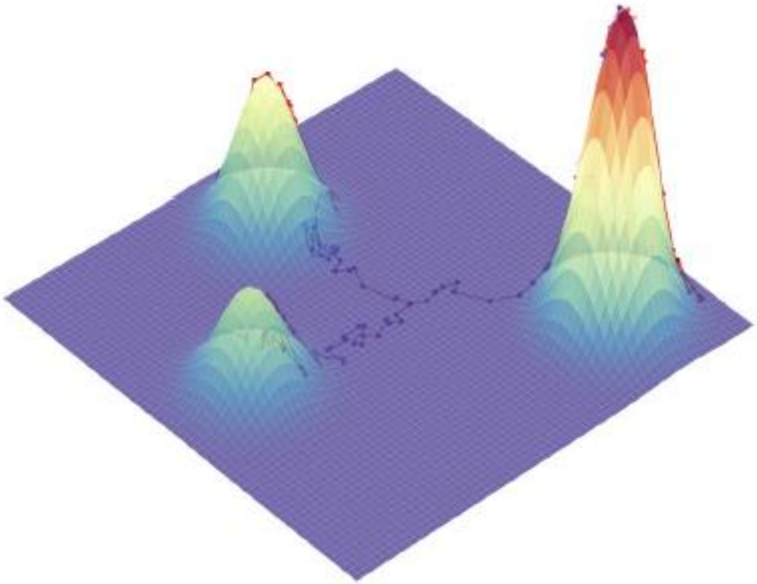
$$\mathcal{L}(\theta) = \mathbb{E}_{\mathbf{x}\sim p(\mathbf{x})}\left[\left\|\mathbf{s}(\mathbf{x};\theta) - \nabla_{\mathbf{x}}\log p(\mathbf{x})\right\|^2\right]$$

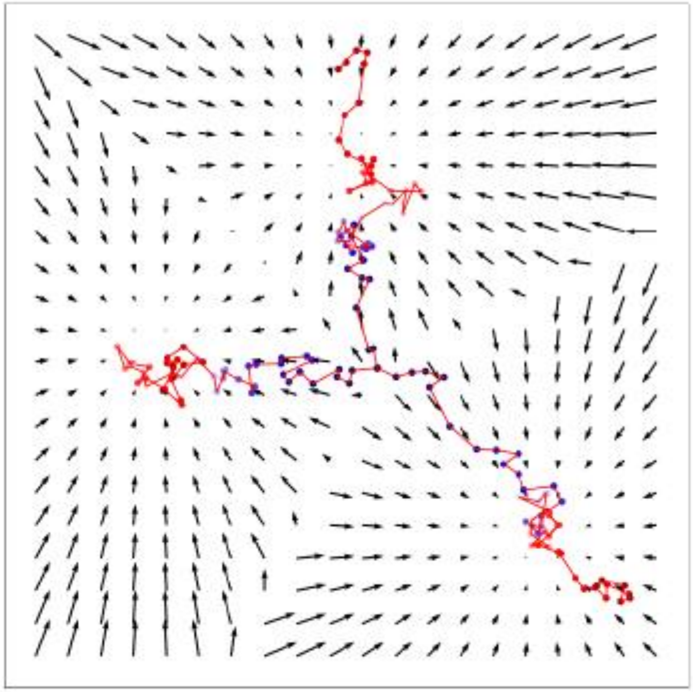
$$\mathcal{L}(\theta) = \mathbb{E}_{\mathbf{x}\sim p(\mathbf{x})}\left[\frac{1}{2}\left\|\mathbf{s}(\mathbf{x};\theta)\right\|^2 + \mathrm{tr}\left(\nabla_{\mathbf{x}}\mathbf{s}(\mathbf{x};\theta)\right) + g(\mathbf{x})\right]$$

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \varepsilon\mathbf{s}(\mathbf{x};\theta) + \sqrt{2\varepsilon}\,\mathbf{z}_i \qquad \mathbf{z}_i \sim \mathcal{N}(\mathbf{0},\mathbf{I})$$



Langevin dynamics可视化





Score-based生成模型实现

```python
# score_network takes input of 2 dimension
score_network = torch.nn.Sequential(
    torch.nn.Linear(2, 64),
    torch.nn.LogSigmoid(),
    torch.nn.Linear(64, 64),
    torch.nn.LogSigmoid(),
    torch.nn.Linear(64, 64),
    torch.nn.LogSigmoid(),
    torch.nn.Linear(64, 2),
)
```

```python
def calc_loss(score_network: torch.nn.Module, x: torch.Tensor)
    # x: (batch_size, 2) is the training data
    score = score_network(x)  # score: (batch_size, 2)

    # first term: half of the squared norm
    term1 = torch.linalg.norm(score, dim=-1) ** 2 * 0.5

    # second term: trace of the Jacobian
    jac = vmap(jacrev(score_network))(x)  # (batch_size, 2, 2)
    term2 = torch.einsum("bii->b", jac)  # compute the trace
    return (term1 + term2).mean()
```

```python
# start the training loop
opt = torch.optim.Adam(score_network.parameters(), lr=3e-4)
dloader = torch.utils.data.DataLoader(dset, batch_size=32, shuffle=True)
for i_epoch in range(5000):
    for data, in dloader:
        # training step
        opt.zero_grad()
        loss = calc_loss(score_network, data)
        loss.backward()
        opt.step()
```

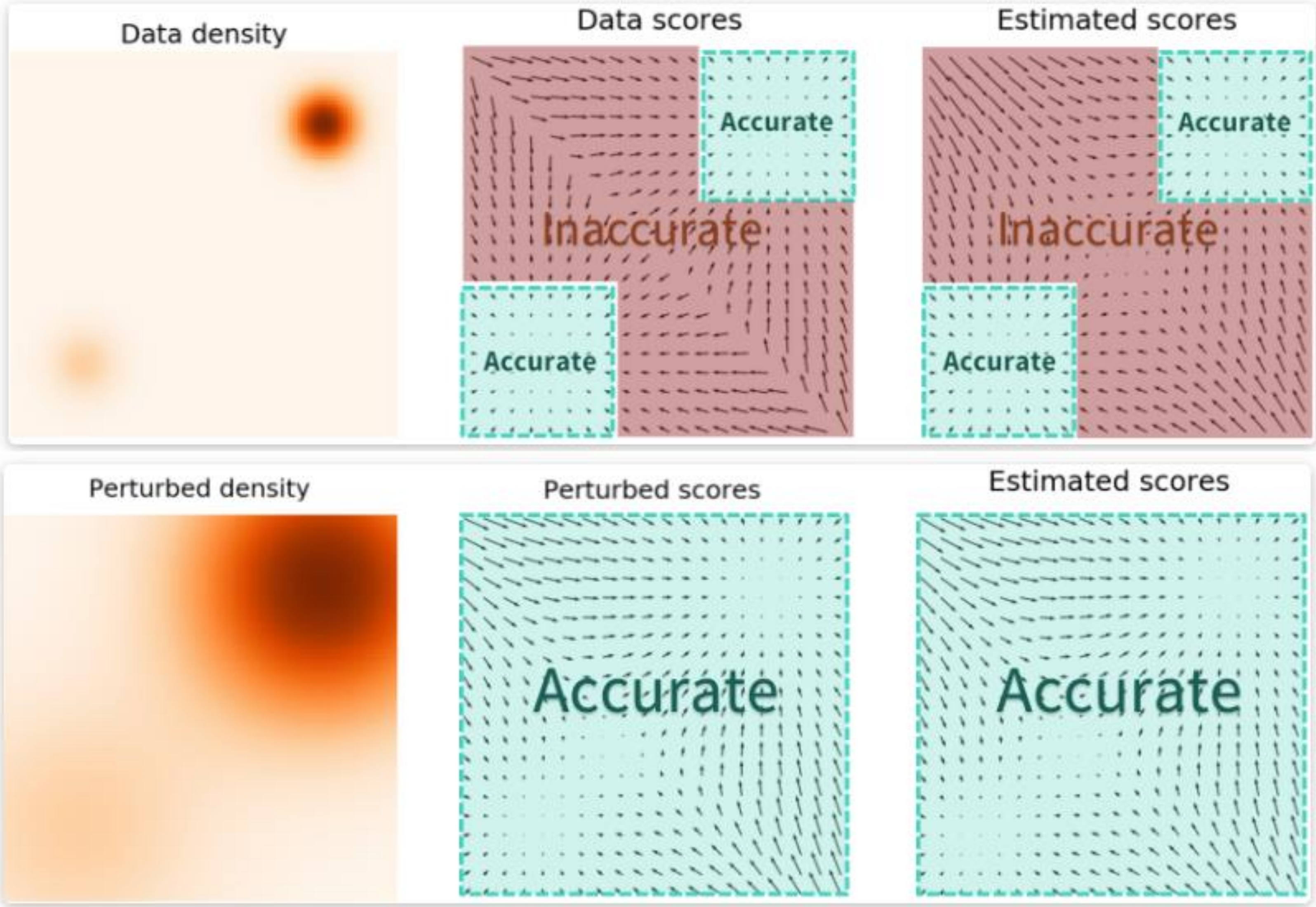
Score-based生成模型实现

- Neural network: n input parameters, $\mathbf{x}$, with n output parameters, $\mathbf{s}(\mathbf{x};\theta)$.
- Training: minimize $\mathcal{L}(\theta) = \mathbb{E}_{\mathbf{x}\sim p(\mathbf{x})}\left[\frac{1}{2}\|\mathbf{s}(\mathbf{x};\theta)\|^2 + \mathrm{tr}\left(\nabla_{\mathbf{x}}\mathbf{s}(\mathbf{x};\theta)\right)\right]$.
- Samples generation: $\mathbf{x}_{i+1} = \mathbf{x}_i + \varepsilon\mathbf{s}(\mathbf{x};\theta) + \sqrt{2\varepsilon}\,\mathbf{z}_i$ for $i = \{0, \ldots, N\}$. with $\mathbf{z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and some small value of ε and reasonable value of $\mathbf{x}_0$.

```python
def generate_samples(score_net: torch.nn.Module, nsamples: int, eps: float = 0.001, nsteps:
    # generate samples using Langevin MCMC
    # x0: (sample_size, nch)
    x0 = torch.rand((nsamples, 2)) * 2 - 1
    for i in range(nsteps):
        z = torch.randn_like(x0)
        x0 = x0 + eps * score_net(x0) + (2 * eps) ** 0.5 * z
    return x0

samples = generate_samples(score_network, 1000).detach()
```

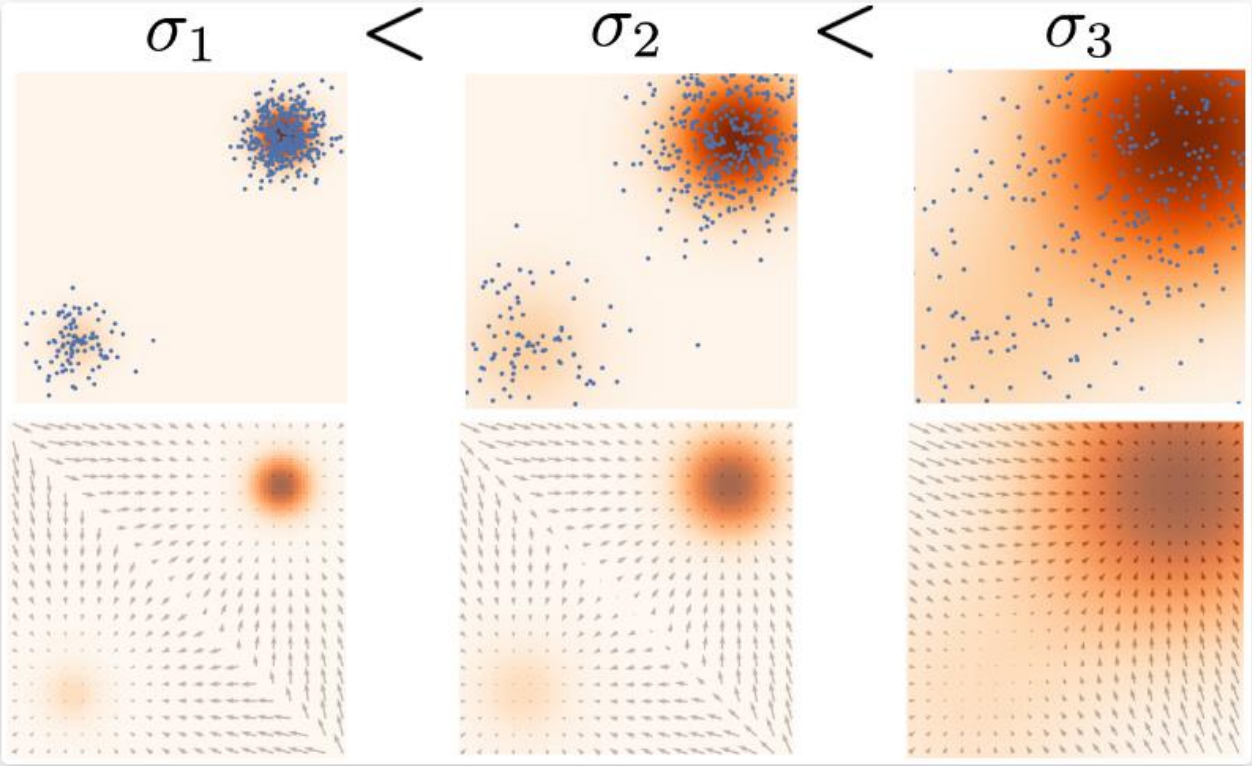
噪声扰动的Score-based生成模型



噪声扰动

$$p_{\sigma_i}(\mathbf{x}) = \int p(\mathbf{y})\mathcal{N}(\mathbf{x}; \mathbf{y}, \sigma_i^2 I)\mathrm{d}\mathbf{y}.$$

$$\mathbf{s}_\theta(\mathbf{x}, i) \approx \nabla_\mathbf{x} \log p_{\sigma_i}(\mathbf{x}) \text{ for all } i = 1, 2, \cdots, L.$$



基于噪声扰动的训练和采样

$$\sum_{i=1}^{L} \lambda(i) \mathbb{E}_{p_{\sigma_i}(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p_{\sigma_i}(\mathbf{x}) - \mathbf{s}_\theta(\mathbf{x}, i)\|_2^2]$$

Algorithm 1 Annealed Langevin dynamics.

Require: $\{\sigma_i\}_{i=1}^{L}, \epsilon, T.$

1: Initialize $\tilde{\mathbf{x}}_0$
2: **for** $i \leftarrow 1$ to L **do**
3: $\quad \alpha_i \leftarrow \epsilon \cdot \sigma_i^2 / \sigma_L^2$ $\quad \triangleright\ \alpha_i$ is the step size.
4: $\quad$ **for** $t \leftarrow 1$ to T **do**
5: $\quad\quad$ Draw $\mathbf{z}_t \sim \mathcal{N}(0, I)$
6: $\quad\quad \tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_{t-1} + \dfrac{\alpha_i}{2} \mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}}_{t-1}, \sigma_i) + \sqrt{\alpha_i}\, \mathbf{z}_t$
7: $\quad$ **end for**
8: $\quad \tilde{\mathbf{x}}_0 \leftarrow \tilde{\mathbf{x}}_T$
9: **end for**
return $\tilde{\mathbf{x}}_T$

基于Score函数的去噪匹配

$$\begin{aligned}
\boldsymbol{\mu}_q(\boldsymbol{x}_t, \boldsymbol{x}_0) &= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t} \\
&= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\frac{\boldsymbol{x}_t + (1-\bar{\alpha}_t)\nabla \log p(\boldsymbol{x}_t)}{\sqrt{\bar{\alpha}_t}}}{1-\bar{\alpha}_t} \\
&= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + (1-\alpha_t)\frac{\boldsymbol{x}_t + (1-\bar{\alpha}_t)\nabla \log p(\boldsymbol{x}_t)}{\sqrt{\alpha_t}}}{1-\bar{\alpha}_t} \\
&= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t}{1-\bar{\alpha}_t} + \frac{(1-\alpha_t)\boldsymbol{x}_t}{(1-\bar{\alpha}_t)\sqrt{\alpha_t}} + \frac{(1-\alpha_t)(1-\bar{\alpha}_t)\nabla \log p(\boldsymbol{x}_t)}{(1-\bar{\alpha}_t)\sqrt{\alpha_t}} \\
&= \left(\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t} + \frac{1-\alpha_t}{(1-\bar{\alpha}_t)\sqrt{\alpha_t}}\right)\boldsymbol{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}}\nabla \log p(\boldsymbol{x}_t) \\
&= \left(\frac{\alpha_t(1-\bar{\alpha}_{t-1})}{(1-\bar{\alpha}_t)\sqrt{\alpha_t}} + \frac{1-\alpha_t}{(1-\bar{\alpha}_t)\sqrt{\alpha_t}}\right)\boldsymbol{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}}\nabla \log p(\boldsymbol{x}_t) \\
&= \frac{\alpha_t - \bar{\alpha}_t + 1 - \alpha_t}{(1-\bar{\alpha}_t)\sqrt{\alpha_t}}\boldsymbol{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}}\nabla \log p(\boldsymbol{x}_t) \\
&= \frac{1-\bar{\alpha}_t}{(1-\bar{\alpha}_t)\sqrt{\alpha_t}}\boldsymbol{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}}\nabla \log p(\boldsymbol{x}_t) \\
&= \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}}\nabla \log p(\boldsymbol{x}_t)
\end{aligned}$$

$$\mathbb{E}\left[\boldsymbol{\mu}_z | \boldsymbol{z}\right] = \boldsymbol{z} + \boldsymbol{\Sigma}_z \nabla_{\boldsymbol{z}} \log p(\boldsymbol{z})$$

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

$$\mathbb{E}\left[\boldsymbol{\mu}_{x_t} | \boldsymbol{x}_t\right] = \boldsymbol{x}_t + (1-\bar{\alpha}_t)\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t)$$

$$\sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 = \boldsymbol{x}_t + (1-\bar{\alpha}_t)\nabla \log p(\boldsymbol{x}_t)$$

$$\therefore \boldsymbol{x}_0 = \frac{\boldsymbol{x}_t + (1-\bar{\alpha}_t)\nabla \log p(\boldsymbol{x}_t)}{\sqrt{\bar{\alpha}_t}}$$

基于Score函数的去噪匹配

$$\boldsymbol{\mu}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}}\boldsymbol{s}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t)$$

$$\begin{aligned}
&\arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)) \\
&= \arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}(\mathcal{N}(\boldsymbol{x}_{t-1}; \boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q(t)) \parallel \mathcal{N}(\boldsymbol{x}_{t-1}; \boldsymbol{\mu}_{\boldsymbol{\theta}}, \boldsymbol{\Sigma}_q(t))) \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)}\left[\left\|\frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}}\boldsymbol{s}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) - \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{\alpha_t}}\nabla\log p(\boldsymbol{x}_t)\right\|_2^2\right] \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)}\left[\left\|\frac{1-\alpha_t}{\sqrt{\alpha_t}}\boldsymbol{s}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) - \frac{1-\alpha_t}{\sqrt{\alpha_t}}\nabla\log p(\boldsymbol{x}_t)\right\|_2^2\right] \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)}\left[\left\|\frac{1-\alpha_t}{\sqrt{\alpha_t}}(\boldsymbol{s}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) - \nabla\log p(\boldsymbol{x}_t))\right\|_2^2\right] \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)}\frac{(1-\alpha_t)^2}{\alpha_t}\left[\|\boldsymbol{s}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) - \nabla\log p(\boldsymbol{x}_t)\|_2^2\right]
\end{aligned}$$

条件DDPM

$$p(\boldsymbol{x}_{0:T}) = p(\boldsymbol{x}_T) \prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$$

$$p(\boldsymbol{x}_{0:T}|y) = p(\boldsymbol{x}_T) \prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, y)$$

- 分类引导

$$\begin{aligned}
\nabla \log p(\boldsymbol{x}_t|y) &= \nabla \log \left(\frac{p(\boldsymbol{x}_t)p(y|\boldsymbol{x}_t)}{p(y)} \right) \\
&= \nabla \log p(\boldsymbol{x}_t) + \nabla \log p(y|\boldsymbol{x}_t) - \nabla \log p(y) \\
&= \underbrace{\nabla \log p(\boldsymbol{x}_t)}_{\text{unconditional score}} + \underbrace{\nabla \log p(y|\boldsymbol{x}_t)}_{\text{adversarial gradient}}
\end{aligned}$$

$$\nabla \log p(\boldsymbol{x}_t|y) = \nabla \log p(\boldsymbol{x}_t) + \gamma \nabla \log p(y|\boldsymbol{x}_t)$$

- 无分类引导

$$\nabla \log p(y|\boldsymbol{x}_t) = \nabla \log p(\boldsymbol{x}_t|y) - \nabla \log p(\boldsymbol{x}_t)$$

$$\begin{aligned}
\nabla \log p(\boldsymbol{x}_t|y) &= \nabla \log p(\boldsymbol{x}_t) + \gamma \left(\nabla \log p(\boldsymbol{x}_t|y) - \nabla \log p(\boldsymbol{x}_t) \right) \\
&= \nabla \log p(\boldsymbol{x}_t) + \gamma \nabla \log p(\boldsymbol{x}_t|y) - \gamma \nabla \log p(\boldsymbol{x}_t) \\
&= \underbrace{\gamma \nabla \log p(\boldsymbol{x}_t|y)}_{\text{conditional score}} + \underbrace{(1-\gamma) \nabla \log p(\boldsymbol{x}_t)}_{\text{unconditional score}}
\end{aligned}$$