生成模型

Diffusion理论发展与应用

常一帆

Diffusion

理论基础
- DDPM
- DDIM
- SDE
- LDM
- Classifier-guided
- Classifier-free

微调
- Dreambooth
- LORA
- Textual inversion

细粒度控制
- controlnet

应用
- Repaint
- Blended-diffusion
- Diffedit
- P2p
- Pnp
- InstructPix2Pix
- Zero-classifier

CVPR24-oral
- 精准控制
- 复杂场景
- …

主要调研图像生成（文生图/图片编辑）的研究，
暂时略过了视频生成等方向

Generative Models

- Given observed samples x from a distribution of interest,
- The goal of a generative model is to learn to *model* its true data distribution $p(x)$

Generative Models

- ELBO(Evidence Lower Bound)
- VAE
- Hierarchical VAE

Luo, C. (2022). Understanding Diffusion Models: A Unified Perspective.

ELBO(Evidence Lower Bound)

- Actually, we try to learn an associated unseen *latent* variable, ***z***
- Model ***x*** and ***z*** by a joint distribution $p(x, z)$
- Maximize the likelihood $p(x)$ of all observed ***x*** , termed "likelihood-based"

ELBO(Evidence Lower Bound)

- Maximize the likelihood p(x) of all observed x ???

$$
\begin{aligned}
\log p(\boldsymbol{x}) &= \log p(\boldsymbol{x}) \int q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}) dz && \text{(Multiply by } 1 = \int q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}) dz\text{)} \\
&= \int q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}) (\log p(\boldsymbol{x})) dz && \text{(Bring evidence into integral)} \\
&= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \left[\log p(\boldsymbol{x}) \right] && \text{(Definition of Expectation)} \\
&= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{p(\boldsymbol{z}|\boldsymbol{x})} \right] && \text{(Apply Equation 2)} \\
&= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}) q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}{p(\boldsymbol{z}|\boldsymbol{x}) q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \right] && \text{(Multiply by } 1 = \frac{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\text{)} \\
&= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \right] + \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}{p(\boldsymbol{z}|\boldsymbol{x})} \right] && \text{(Split the Expectation)} \\
&= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \right] + D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z}|\boldsymbol{x})) && \text{(Definition of KL Divergence)} \\
&\geq \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \right] && \text{(KL Divergence always } \geq 0\text{)}
\end{aligned}
$$

$$
\mathrm{E}(X) = \int_{-\infty}^{\infty} x f(x)\, \mathrm{d}x.
$$

$$
\mathrm{E}(g(X)) = \int_{\Omega} g(x) f(x)\, \mathrm{d}x
$$

$$
p(\boldsymbol{x}) = \frac{p(\boldsymbol{x}, \boldsymbol{z})}{p(\boldsymbol{z}|\boldsymbol{x})}
$$

$$
\mathbb{D}_{\mathrm{KL}}(P||Q) = \int_{-\infty}^{\infty} p(\mathbf{x}) \ln\left(\frac{p(\mathbf{x})}{q(\mathbf{x})}\right) d\mathbf{x}
$$

KL散度非负

1. 非负性

$\mathbb{D}_{\mathrm{KL}}(P||Q) \geq 0$，$\mathbb{D}_{\mathrm{KL}} = 0$当且仅当$P = Q$。

证明（我们仅对离散情况进行证明，对于连续随机变量情况，我们将积分化为求和的极限后可以用相同方式证明）：

我们只需要证明$\sum_i P(i) \ln(\frac{Q(i)}{P(i)}) \leq 0$。采用不等式$\ln(\mathbf{x}) \leq \mathbf{x} - 1, \forall x > 0$，则:

$$\sum_i P(i) \ln(\frac{Q(i)}{P(i)}) \leq \sum_i P(i)(\frac{Q(i)}{P(i)} - 1) = 0$$

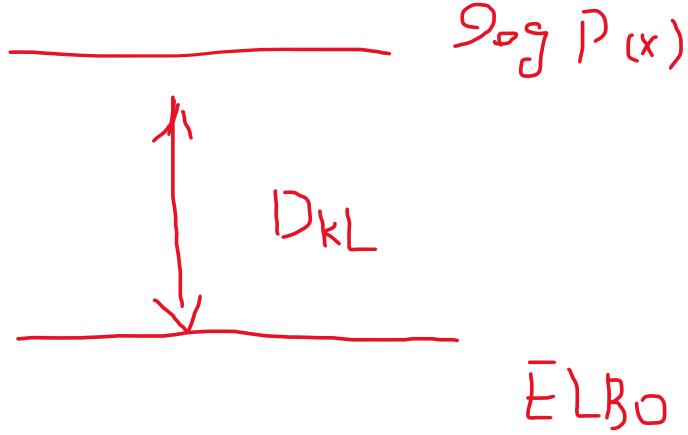
等号当且仅当对于任意的i，$\frac{Q(i)}{P(i)} = 1$时取得，此时有$P = Q$。

ELBO(Evidence Lower Bound)

- Maximize the likelihood p(x) of all observed x ???

$$\log p(\boldsymbol{x}) \geq \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x},\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\right]$$

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



VAE(Variational Autoencoder)

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

- Model

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

VAE(Variational Autoencoder)

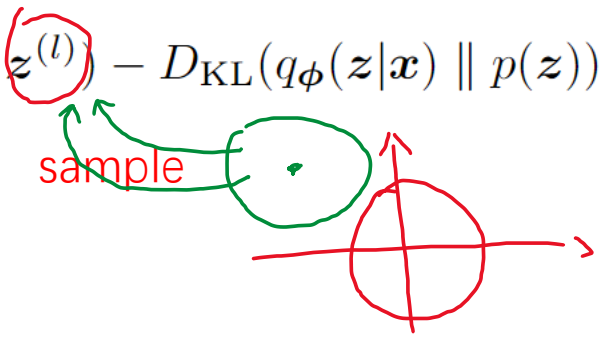
$$\mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x},\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\right] = \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\right] \quad \text{(Chain Rule of Probability)}$$

$$= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})\right] + \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\right] \quad \text{(Split the Expectation)}$$

$$= \underbrace{\mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})\right]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z}))}_{\text{prior matching term}} \quad \text{(Definition of KL Divergence)}$$

- optimize

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



reparameterization

$$\boldsymbol{z} = \boldsymbol{\mu}_{\boldsymbol{\phi}}(\boldsymbol{x}) + \boldsymbol{\sigma}_{\boldsymbol{\phi}}(\boldsymbol{x}) \odot \boldsymbol{\epsilon} \quad \text{with } \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon}; \mathbf{0}, \mathbf{I})$$

```python
latent_dim = 2
input_dim = 28 * 28
inter_dim = 256

class VAE(nn.Module):
    def __init__(self, input_dim=input_dim, inter_dim=inter_dim, latent_dim=latent_dim):
        super(VAE, self).__init__()

        elf.encoder = nn.Sequential(
            nn.Linear(input_dim, inter_dim),
            nn.ReLU(),
            nn.Linear(inter_dim, latent_dim * 2),
        )

        self.decoder =  nn.Sequential(
            nn.Linear(latent_dim, inter_dim),
            nn.ReLU(),
            nn.Linear(inter_dim, input_dim),
            nn.Sigmoid(),
        )

    def reparameterise(self, mu, logvar):
        epsilon = torch.randn_like(mu)
        return mu + epsilon * torch.exp(logvar / 2)

    def forward(self, x):
        org_size = x.size()
        batch = org_size[0]
        x = x.view(batch, -1)

        h = self.encoder(x)
        mu, logvar = h.chunk(2, dim=1)
        z = self.reparameterise(mu, logvar)
        recon_x = self.decoder(z).view(size=org_size)

        return recon_x, mu, logvar
```

coder)

$$= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p_\theta(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\right]$$

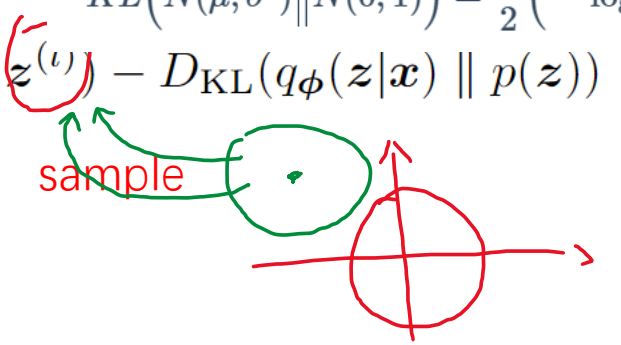
$$= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})\right] + \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\right]$$

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

```python
kl_loss = lambda mu, logvar: -0.5 * torch.sum(1 + logvar - mu.pow(2) - logvar.exp())
recon_loss = lambda recon_x, x: F.binary_cross_entropy(recon_x, x, size_average=False)
```

$$KL\left(N(\mu, \sigma^2)\middle\|N(0,1)\right) = \frac{1}{2}\left(-\log\sigma^2 + \mu^2 + \sigma\right.$$

$$\max_{\phi,\theta} \sum_{l=1}^{L} \log p_\theta(\boldsymbol{x}|\boldsymbol{z}^{(l)}) - D_{\mathrm{KL}}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z}))$$



Rethink VAE && AE

- AE　x -> z -> x
- VAE x->z->x z~N(0,1) 放弃点到点的映射，看重分布关系
- 寻找后验分布p(z|x_i)

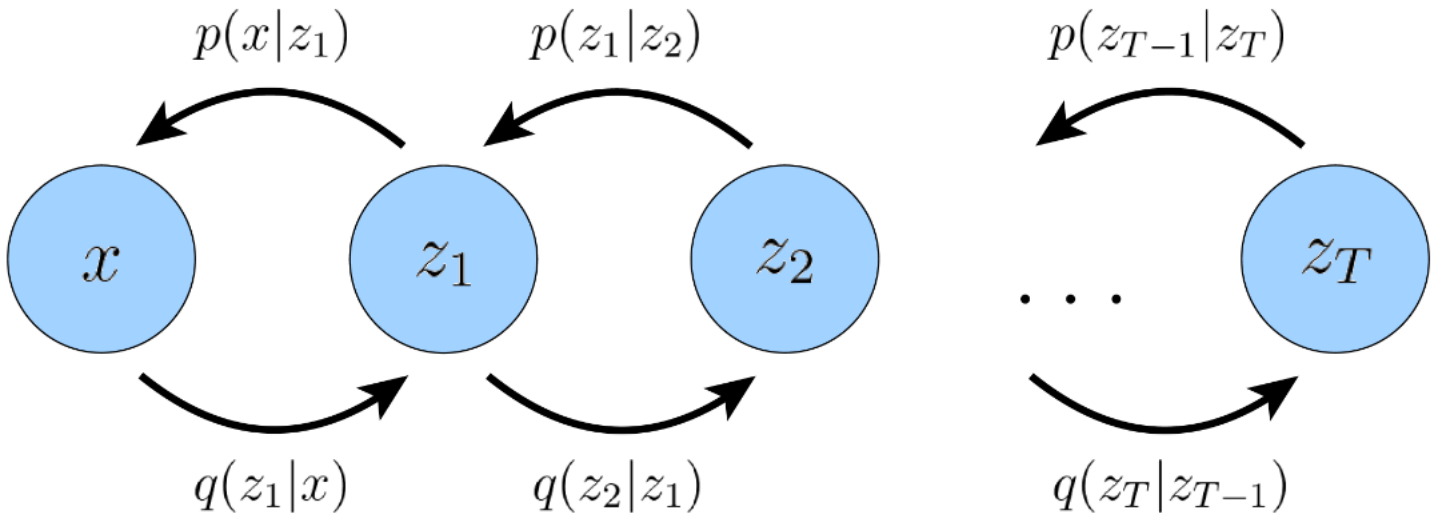
Hierarchical VAE

- generative process is a Markov chain

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

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

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



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

Diffusion Model

- The latent dimension is exactly equal to the data dimension
- Encoder is pre-defined as a linear Gaussian model

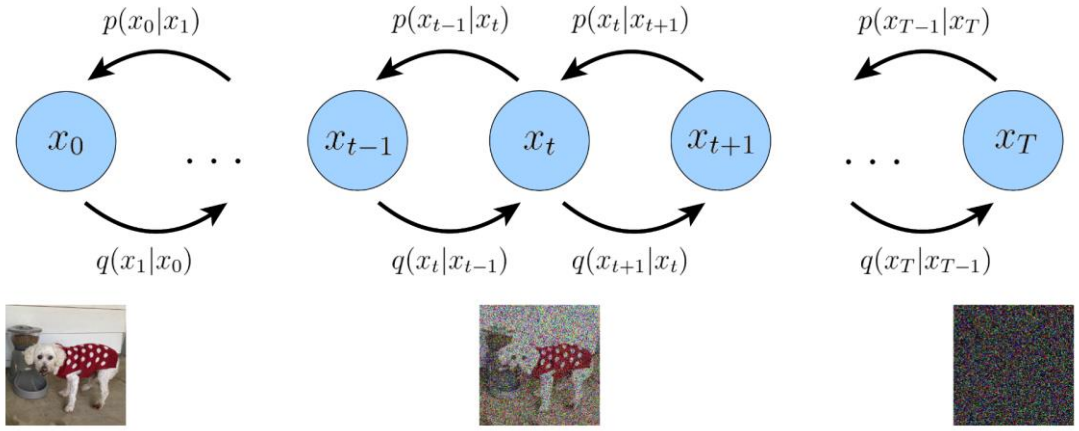
$$q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\alpha_t}\boldsymbol{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

- Distribution of the latent at final timestep T is a standard Gaussian

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

where,

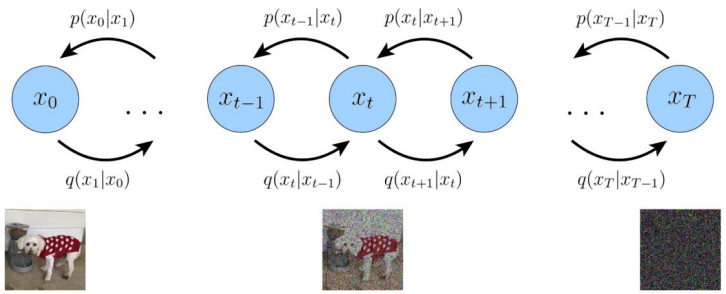
$$p(\boldsymbol{x}_T) = \mathcal{N}(\boldsymbol{x}_T; \mathbf{0}, \mathbf{I})$$



Luo, C. (2022). Understanding Diffusion Models: A Unified Perspective.

Ho, J., Jain, AjayN., & Abbeel, P. (2020). Denoising Diffusion Probabilistic Models. NIPS.

Diffusion Model



$$\log p(\boldsymbol{x}) \geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right]$$

$$= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)\prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\prod_{t=1}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right]$$

$$= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)\prod_{t=2}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right]$$ 提出t=1

$$= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)\prod_{t=2}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)}\right]$$ 前向马尔可夫性质

$$= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log\prod_{t=2}^{T}\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)}\right]$$

$$= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log\prod_{t=2}^{T}\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)q(\boldsymbol{x}_t|\boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}\right]$$

$$= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{\cancel{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}} + \log\frac{\cancel{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)} + \log\prod_{t=2}^{T}\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right]$$

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

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

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

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

$$p(\boldsymbol{x}_{0:T}) = p(\boldsymbol{x}_T)\prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t) \qquad q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0) = \prod_{t=1}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})$$

where,

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

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

贝叶斯公式

$$\cdot \log\prod_{t=2}^{T}\frac{p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)q(\boldsymbol{x}_t|\boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}\Bigg]$$

$$\log\prod_{t=2}^{T}\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}{q(\boldsymbol{x}_t|\boldsymbol{x}_0)} + \log\prod_{t=2}^{T}\frac{p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\Bigg]$$

$$\log\frac{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}{q(\boldsymbol{x}_2|\boldsymbol{x}_0)}\frac{q(\boldsymbol{x}_2|\boldsymbol{x}_0)}{q(\boldsymbol{x}_3|\boldsymbol{x}_0)}\cdots\frac{q(\boldsymbol{x}_{T-1}|\boldsymbol{x}_0)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)} + \log$$

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

1. **贝叶斯公式**:

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

2. **联合概率的分解**:

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

3. **代入联合概率的分解**:

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

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

对任意的归一化概率分布 $p(x,y)$:

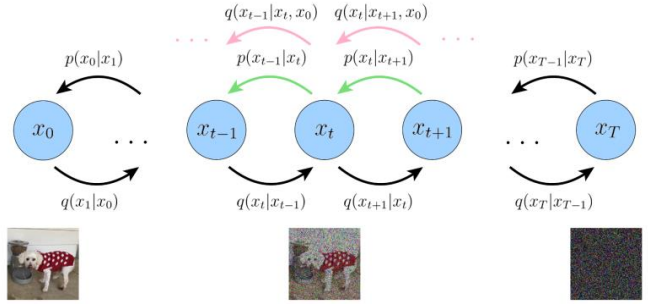
$$\begin{aligned}
\mathbb{E}_{p(x,y)}[f(x)] &= \int p(x,y) f(x) \mathrm{d}x\mathrm{d}y \\
&= \int f(x) \left(\int p(x,y) \mathrm{d}y \right) \mathrm{d}x \\
&= \int p(x) f(x) \mathrm{d}x
\end{aligned}$$

其中，$p(x)$ 是边缘分布（也满足归一化）：

$$p(x) = \int p(x,y) \mathrm{d}y$$

就是一个简单的积分变化而已.

Diffusion Model



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

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

$$\boldsymbol{x}_t = \sqrt{\alpha_t}\boldsymbol{x}_{t-1} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon} \quad \text{with } \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon}; \mathbf{0}, \mathbf{I})$$

$$\mathcal{N}(x; \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^k|\Sigma|}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

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

最后一个问题，为什么我们选择加噪方式为 $x_t = \sqrt{1-\beta_t}x_{t-1} + \beta_t\epsilon$，换言之，若重写为 $x_t = k_t x_{t-1} + \beta_t\epsilon$，为什么要让 $k_t = \sqrt{1-\beta_t}$（i.e. 为什么 $k_t^2 + \beta_t^2 = 1$）？由于我们有式（3） $x_t = \sqrt{\bar{\alpha}_t}x_0 + (1-\bar{\alpha}_t)\epsilon$，我们希望 t 足够大时，$\sqrt{\bar{\alpha}_t}$ 趋近于0，而 $1-\bar{\alpha}_t$ 趋于1，这样我们才能保证 x_T 趋于服从标准正态分布。

若 $x_t = k_t x_{t-1} + \beta_t\epsilon$，那么我们有

$$
\begin{aligned}
x_t &= k_t x_{t-1} + \beta_t\epsilon \\
&= k_t(k_{t-1}x_{t-2} + \beta_{t-1}\epsilon) + \beta_t\epsilon \\
&= \bar{k}_t x_0 + (k_t k_{t-1}\dots k_2\beta_1\epsilon) + (k_t k_{t-1}\dots k_3\beta_2\epsilon) + \dots + (\beta_t\epsilon)
\end{aligned}
$$

其中 $\bar{k}_t = k_1 k_2 \dots k_t$。由于上式括号中每个部分都是正态分布，且均值都是0，因此根据正态分布的可加性，这些括号相加依然是正态分布，且均值为0，方差为 $k_t^2 k_{t-1}^2 \dots k_2^2\beta_1^2 + k_t^2 k_{t-1}^2 \dots k_3^2\beta_2^2 + \dots + \beta_t^2$。而当 $k_t^2 + \beta_t^2 = 1$ 时，我们有 $\beta_t^2 = 1 - k_t^2$，代入上式可得

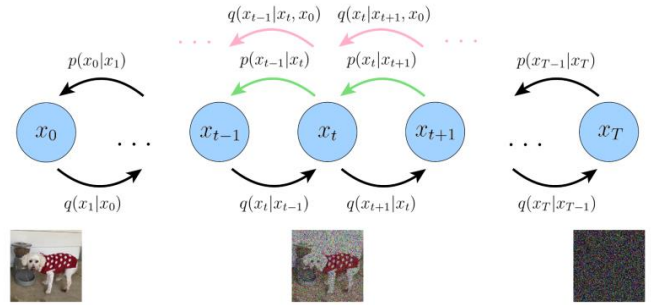
$$
\begin{aligned}
& k_t^2 k_{t-1}^2 \dots k_2^2(1-k_1^2) + k_t^2 k_{t-1}^2 \dots k_3^2(1-k_2^2) + \dots + 1 - k_t^2 \\
=& k_t^2 k_{t-1}^2 \dots k_2^2 - k_t^2 k_{t-1}^2 \dots k_1^2 + k_t^2 k_{t-1}^2 \dots k_3^2 - k_t^2 k_{t-1}^2 \dots k_2^2 + \dots + 1 - k_t^2 \\
=& 1 - \bar{k}_t^2
\end{aligned}
$$

于是满足了我们的需求，即 t 足够大时有 $\bar{k}_t$ 趋近于0，$1-\bar{k}_t^2$ 趋近于1，另外若令 $k_t = \sqrt{\alpha_t}$，我们就得到了式（3）。

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

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

Diffusion Model



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

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

$$\propto \mathcal{N}(\boldsymbol{x}_{t-1}; \underbrace{\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t}}_{\mu_q(\boldsymbol{x}_t, \boldsymbol{x}_0)}, \underbrace{\frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{I}}_{\boldsymbol{\Sigma}_q(t)})$$

- Model $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$ $\mu_\theta(x_t, t)$

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

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

$$\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}\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[\|\boldsymbol{\mu}_{\boldsymbol{\theta}} - \boldsymbol{\mu}_q\|_2^2\right] \\
&= \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}(\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) - \boldsymbol{x}_0)\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[\|\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) - \boldsymbol{x}_0\|_2^2\right]
\end{aligned}$$

Diffusion Model

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

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

$$\propto \mathcal{N}(\boldsymbol{x}_{t-1}; \underbrace{\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t}}_{\mu_q(\boldsymbol{x}_t, \boldsymbol{x}_0)}, \underbrace{\frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{I}}_{\boldsymbol{\Sigma}_q(t)})$$

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

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

- Model $\boldsymbol{\mu}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t)$

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

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

Diffusion Model

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

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

$$\propto \mathcal{N}(\boldsymbol{x}_{t-1}; \underbrace{\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t}}_{\mu_q(\boldsymbol{x}_t, \boldsymbol{x}_0)}, \underbrace{\frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}}_{\boldsymbol{\Sigma}_q(t)} \mathbf{I})$$

- Model $\mu_\theta(x_t, t)$

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

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

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

$$\boldsymbol{\Sigma}_q(t) = \frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}$$

Algorithm 1 Training

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

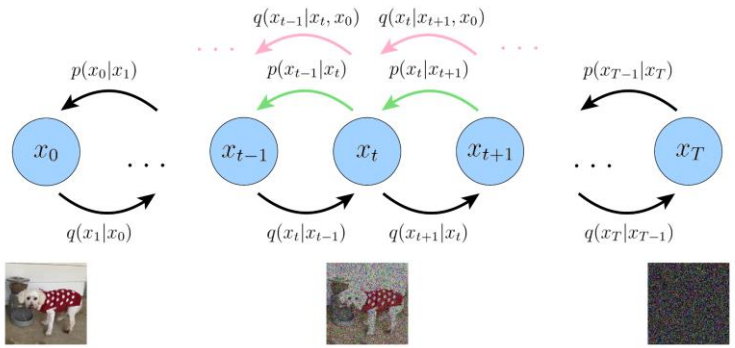
Algorithm 2 Sampling

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

DDIM

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

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



Algorithm 2 Sampling

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

Song, J., Meng, C., & Ermon, S. (2020). Denoising Diffusion Implicit Models. arXiv.

https://www.bilibili.com/video/BV1Ra4y1F73C/?vd_source=26cdccafc07aa98082eae4058dbfcf75

$$q(x_k|x_s, x_0) = \frac{q(x_s|x_k, x_0)q(x_k|x_0)}{q(x_s|x_0)} \qquad k<=s-1$$

$$q(x_k|x_s, x_0) \sim N(kx_0 + mx_s, \sigma^2 I)$$

$$\begin{aligned} x_k &= (kx_0 + mx_s) + \sigma\epsilon \\ &= kx_0 + m(\sqrt{\bar{\alpha}_s}x_0 + \sqrt{1-\bar{\alpha}_s}\epsilon' + \sigma\epsilon) \\ &= (k + m\sqrt{\bar{\alpha}_s})x_0 + \sqrt{m^2(1-\bar{\alpha}_s) + \sigma^2}\epsilon \\ &= \sqrt{\bar{\alpha}_k}x_0 + \sqrt{1-\bar{\alpha}_k}\epsilon \end{aligned}$$

$$m = \frac{\sqrt{1-\bar{\alpha}_k - \sigma^2}}{\sqrt{1-\bar{\alpha}_s}} \qquad k = \sqrt{\bar{\alpha}_k} - \frac{\sqrt{1-\bar{\alpha}_k - \sigma^2}}{\sqrt{1-\bar{\alpha}_s}}\sqrt{\bar{\alpha}_s}$$

$$x_k = (\sqrt{\bar{\alpha}_k} - \frac{\sqrt{1-\bar{\alpha}_k - \sigma^2}}{\sqrt{1-\bar{\alpha}_s}}\sqrt{\bar{\alpha}_s})x_0 + \frac{\sqrt{1-\bar{\alpha}_k - \sigma^2}}{\sqrt{1-\bar{\alpha}_s}}x_s + \sigma\epsilon$$

$$q(x_k|x_s, x_0) \sim N((\sqrt{\bar{\alpha}_k} - \frac{\sqrt{1-\bar{\alpha}_k - \sigma^2}}{\sqrt{1-\bar{\alpha}_s}}\sqrt{\bar{\alpha}_s})x_0 + \frac{\sqrt{1-\bar{\alpha}_k - \sigma^2}}{\sqrt{1-\bar{\alpha}_s}}x_s, \sigma^2 I)$$

$$\begin{aligned} \mu_\theta &= (\sqrt{\bar{\alpha}_k} - \frac{\sqrt{1-\bar{\alpha}_k - \sigma^2}}{\sqrt{1-\bar{\alpha}_s}}\sqrt{\bar{\alpha}_s})x_0 + \frac{\sqrt{1-\bar{\alpha}_k - \sigma^2}}{\sqrt{1-\bar{\alpha}_s}}x_s \\ &= \frac{\sqrt{\bar{\alpha}_k}}{\sqrt{\bar{\alpha}_s}}(x_s - (\sqrt{1-\bar{\alpha}_s} - \frac{\sqrt{\bar{\alpha}_s}}{\sqrt{\bar{\alpha}_k}}\sqrt{1-\bar{\alpha}_k - \sigma^2})\epsilon) \end{aligned}$$

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

DDIM

Table 1: CIFAR10 and CelebA image generation measured in FID. $\eta = 1.0$ and $\hat{\sigma}$ are cases of DDPM (although Ho et al. (2020) only considered $T = 1000$ steps, and $S < T$ can be seen as simulating DDPMs trained with S steps), and $\eta = 0.0$ indicates DDIM.

		CIFAR10 (32 × 32)					CelebA (64 × 64)				
	S	10	20	50	100	1000	10	20	50	100	1000
η	0.0	**13.36**	**6.84**	**4.67**	**4.16**	4.04	**17.33**	**13.73**	**9.17**	**6.53**	3.51
	0.2	14.04	7.11	4.77	4.25	4.09	17.66	14.11	9.51	6.79	3.64
	0.5	16.66	8.35	5.25	4.46	4.29	19.86	16.06	11.01	8.09	4.28
	1.0	41.07	18.36	8.01	5.78	4.73	33.12	26.03	18.48	13.93	5.98
$\hat{\sigma}$		367.43	133.37	32.72	9.99	**3.17**	299.71	183.83	71.71	45.20	**3.26**

$$q(x_k|x_s, x_0) \sim N((\sqrt{\bar{\alpha}_k} - \frac{\sqrt{1-\bar{\alpha}_k-\sigma^2}}{\sqrt{1-\bar{\alpha}_s}}\sqrt{\bar{\alpha}_s})x_0 + \frac{\sqrt{1-\bar{\alpha}_k-\sigma^2}}{\sqrt{1-\bar{\alpha}_s}}x_s, \sigma^2 I)$$

Song, J., Meng, C., & Ermon, S. (2020). Denoising Diffusion Implicit Models. arXiv.

others

- SDE（随机微分方程）
- ODE（常微分方程）

Song, Y., Sohl-Dickstein, J., Kingma, DiederikP., Kumar, A., Ermon, S., & Poole, B. (2020). Score-Based Generative Modeling through Stochastic Differential Equations. arXiv.

Guidance—classifier

- 和前向加噪无关 （论文附录有证明）
- 只需推理时对均值做偏移

Algorithm 1 Classifier guided sampling, given a diffusion model $(\mu_\theta(x_t), \Sigma_\theta(x_t))$, classifier $p_\phi(y|x_t)$, and gradient scale s.

Input: class label y, gradient scale s
$x_0 \leftarrow$ sample from $\mathcal{N}(0, \mathbf{I})$
for all t from T to 1 **do**
  $\mu \leftarrow \mu_\theta(x_t)$
  $\Sigma \leftarrow \Sigma_\theta(x_t)$
  $g \leftarrow s \nabla_{x_t} \log p_\phi(y|x_t)$
  $x_{t-1} \leftarrow$ sample from $\mathcal{N}(\mu + \Sigma g, \Sigma)$
end for
return x_0

Dhariwal, P., & Nichol, A. (2021). Diffusion Models Beat GANs on Image Synthesis. NIPS.

Guidance—classifier

Algorithm 1 Classifier guided sampling, given a diffusion model $(\mu_\theta(x_t), \Sigma_\theta(x_t))$, classifier $p_\phi(y|x_t)$, and gradient scale s.

Input: class label y, gradient scale s
$x_0 \leftarrow$ sample from $\mathcal{N}(0, \mathbf{I})$
for all t from T to 1 **do**
  $\mu \leftarrow \mu_\theta(x_t)$
  $\Sigma \leftarrow \Sigma_\theta(x_t)$
  $g \leftarrow s \nabla_{x_t} \log p_\phi(y|x_t)$
  $x_{t-1} \leftarrow$ sample from $\mathcal{N}(\mu + \Sigma g, \Sigma)$
end for
return x_0

- 只需推理时对均值做偏移

$$q(x_{t-1}|x_t, y) = \frac{q(x_{t-1}|x_t)q(y|x_{t-1}, x_t)}{q(y|x_t)}$$
$$= Zq(x_{t-1}|x_t)q(y|x_{t-1}) \quad \text{（由与前向无关推导得出）}$$

$$p_{\theta,\phi}(x_t|x_{t+1}, y) = Zp_\theta(x_t|x_{t+1})p_\phi(y|x_t)$$

$$\log p_\theta(x_t|x_{t+1}) = -\frac{1}{2}(x_t - \mu)^T\Sigma^{-1}(x_t - \mu) + C$$

$$\log p_\phi(y|x_t) \approx \log p_\phi(y|x_t)|_{x_t=\mu} + (x_t - \mu)\nabla_{x_t} \log p_\phi(y|x_t)|_{x_t=\mu}$$
$$= (x_t - \mu)g + C_1$$

$$\log(p_\theta(x_t|x_{t+1})p_\phi(y|x_t)) \approx -\frac{1}{2}(x_t - \mu)^T\Sigma^{-1}(x_t - \mu) + (x_t - \mu)g + C_2$$
$$= -\frac{1}{2}(x_t - \mu - \Sigma g)^T\Sigma^{-1}(x_t - \mu - \Sigma g) + \frac{1}{2}g^T\Sigma g + C_2$$
$$= -\frac{1}{2}(x_t - \mu - \Sigma g)^T\Sigma^{-1}(x_t - \mu - \Sigma g) + C_3$$
$$= \log p(z) + C_4, z \sim \mathcal{N}(\mu + \Sigma g, \Sigma)$$

https://www.bilibili.com/video/BV1s8411i7cU/?spm_id_from=333.788&vd_source=26cdccafc07aa98082eae4058dbfcf75

https://kexue.fm/archives/9257

Dhariwal, P., & Nichol, A. (2021). Diffusion Models Beat GANs on Image Synthesis. NIPS.

Guidance—classifier in DDIM

Algorithm 1 Classifier guided sampling, given a diffusion model $(\mu_\theta(x_t), \Sigma_\theta(x_t))$, classifier $p_\phi(y|x_t)$, and gradient scale s.

Input: class label y, gradient scale s
$x_0 \leftarrow$ sample from $\mathcal{N}(0, \mathbf{I})$
for all t from T to 1 **do**
  $\mu \leftarrow \mu_\theta(x_t)$
  $\Sigma \leftarrow \Sigma_\theta(x_t)$
  $g \leftarrow s \nabla_{x_t} \log p_\phi(y|x_t)$
  $x_{t-1} \leftarrow$ sample from $\mathcal{N}(\mu + \Sigma g, \Sigma)$
end for
return x_0

$$\nabla_{x_t} \log p_\theta(x_t) = -\frac{1}{\sqrt{1-\bar{\alpha}_t}} \epsilon_\theta(x_t)$$

$$\nabla_{x_t} \log(p_\theta(x_t) p_\phi(y|x_t)) = \nabla_{x_t} \log p_\theta(x_t) + \nabla_{x_t} \log p_\phi(y|x_t)$$

$$-\frac{\hat{\epsilon}}{\sqrt{1-\bar{\alpha}_t}} = -\frac{1}{\sqrt{1-\bar{\alpha}_t}} \epsilon_\theta(x_t) + \nabla_{x_t} \log p_\phi(y|x_t)$$

$$\hat{\epsilon}(x_t) := \epsilon_\theta(x_t) - \sqrt{1-\bar{\alpha}_t}\, \nabla_{x_t} \log p_\phi(y|x_t)$$

$$p(x_t|x_0) \sim N(\sqrt{\bar{\alpha}_t} x_0, 1-\bar{\alpha}_t)$$

$$\nabla log p(x_t|x_0) = -\frac{(x_t - \sqrt{\bar{\alpha}_t} x_0)}{1-\bar{\alpha}_t} = -\frac{\epsilon}{\sqrt{1-\bar{\alpha}_t}}$$

Dhariwal, P., & Nichol, A. (2021). Diffusion Models Beat GANs on Image Synthesis. NIPS.

Guidance—classifier-free

Algorithm 1 Joint training a diffusion model with classifier-free guidance

Require: p_{uncond}: probability of unconditional training

repeat
  $(\mathbf{x}, \mathbf{c}) \sim p(\mathbf{x}, \mathbf{c})$ ▷ Sample data with conditioning from the dataset
  $\mathbf{c} \leftarrow \varnothing$ with probability p_{uncond} ▷ Randomly discard conditioning to train unconditionally
  $\lambda \sim p(\lambda)$ ▷ Sample log SNR value
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  $\mathbf{z}_\lambda = \alpha_\lambda \mathbf{x} + \sigma_\lambda \boldsymbol{\epsilon}$ ▷ Corrupt data to the sampled log SNR value
  Take gradient step on $\nabla_\theta \left\| \boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c}) - \boldsymbol{\epsilon} \right\|^2$ ▷ Optimization of denoising model
until converged

Algorithm 2 Conditional sampling with classifier-free guidance

Require: w: guidance strength
Require: $\mathbf{c}$: conditioning information for conditional sampling
Require: $\lambda_1, \ldots, \lambda_T$: increasing log SNR sequence with $\lambda_1 = \lambda_{\min}, \lambda_T = \lambda_{\max}$

$\mathbf{z}_1 \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = 1, \ldots, T$ **do**
  ▷ Form the classifier-free guided score at log SNR λ_t
  $\tilde{\boldsymbol{\epsilon}}_t = (1 + w)\boldsymbol{\epsilon}_\theta(\mathbf{z}_t, \mathbf{c}) - w\boldsymbol{\epsilon}_\theta(\mathbf{z}_t)$
  ▷ Sampling step (could be replaced by another sampler, e.g. DDIM)
  $\tilde{\mathbf{x}}_t = (\mathbf{z}_t - \sigma_{\lambda_t} \tilde{\boldsymbol{\epsilon}}_t)/\alpha_{\lambda_t}$
  $\mathbf{z}_{t+1} \sim \mathcal{N}(\tilde{\boldsymbol{\mu}}_{\lambda_{t+1}|\lambda_t}(\mathbf{z}_t, \tilde{\mathbf{x}}_t), (\tilde{\sigma}^2_{\lambda_{t+1}|\lambda_t})^{1-v} (\sigma^2_{\lambda_t|\lambda_{t+1}})^v)$ if $t < T$ else $\mathbf{z}_{t+1} = \tilde{\mathbf{x}}_t$
end for
return $\mathbf{z}_{T+1}$

Ho, J., & Salimans, T. (2022). Classifier-Free Diffusion Guidance.

LDM—Stable Diffusion

- Latent Diffusion Model

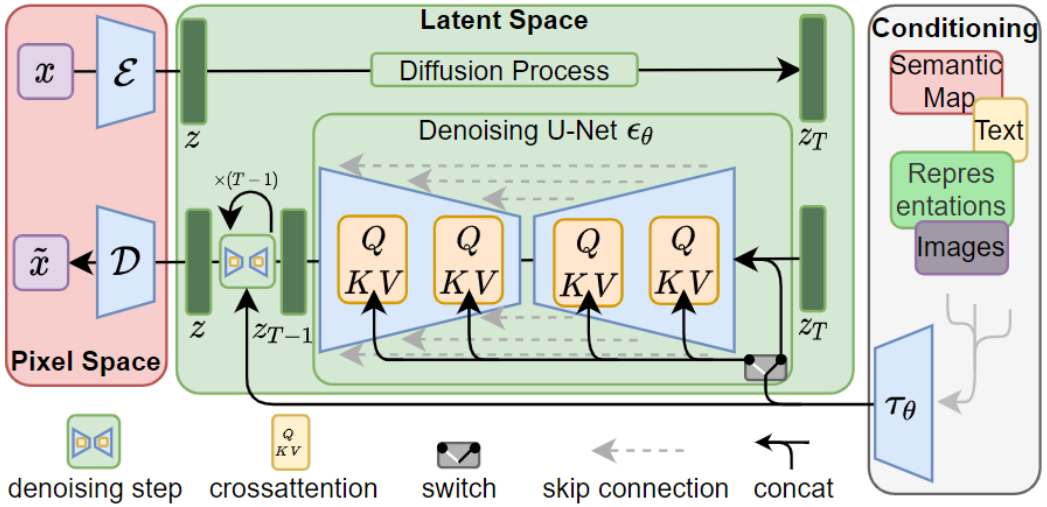


Figure 3. We condition LDMs either via concatenation or by a more general cross-attention mechanism. See Sec. 3.3

- 为什么单独VAE效果不好

1. unkown->N(0,1)

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

Rombach, Robin, Andreas Blattmann, Dominik Lorenz, Patrick Esser, and Bjorn Ommer. 2021. “High-Resolution Image Synthesis with Latent Diffusion Models.” CVPR.

Application

微调

- Dreambooth
- LORA
- Textual inversion

细粒度控制

- controlnet

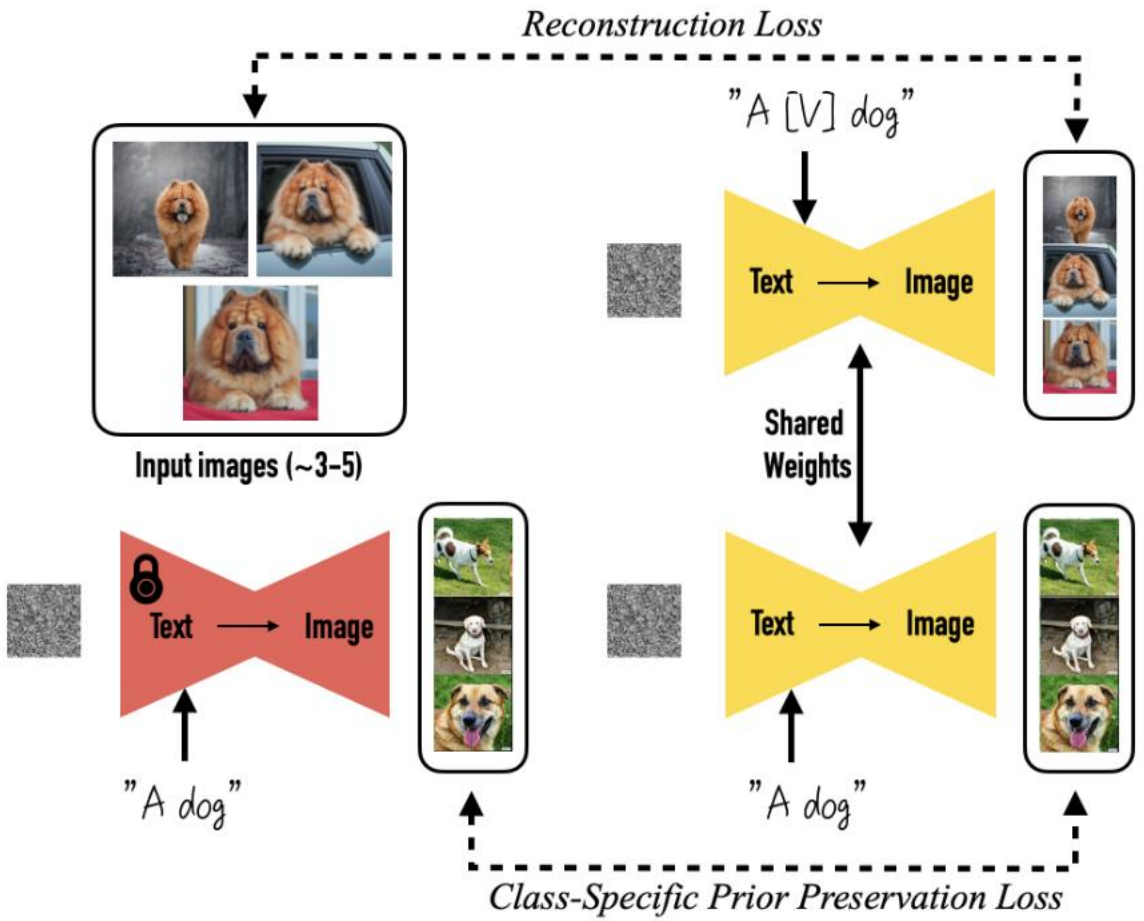
应用

- Repaint
- Blended-diffusion
- Diffedit
- P2p
- Pnp
- InstructPix2Pix
- Zero-classifier

Dreambooth

- Personalization
- Rare-token<->subject

$$\mathbb{E}_{\mathbf{x},\mathbf{c},\boldsymbol{\epsilon},\boldsymbol{\epsilon}',t}[w_t \|\hat{\mathbf{x}}_\theta(\alpha_t \mathbf{x} + \sigma_t \boldsymbol{\epsilon}, \mathbf{c}) - \mathbf{x}\|_2^2 + \lambda w_{t'} \|\hat{\mathbf{x}}_\theta(\alpha_{t'} \mathbf{x}_{\text{pr}} + \sigma_{t'} \boldsymbol{\epsilon}', \mathbf{c}_{\text{pr}}) - \mathbf{x}_{\text{pr}}\|_2^2],$$



Ruiz, N., Li, Y., Jampani, V., Pritch, Y., Rubinstein, M., & Aberman, K. (2022). DreamBooth: Fine Tuning Text-to-Image Diffusion Models for Subject-Driven Generation.

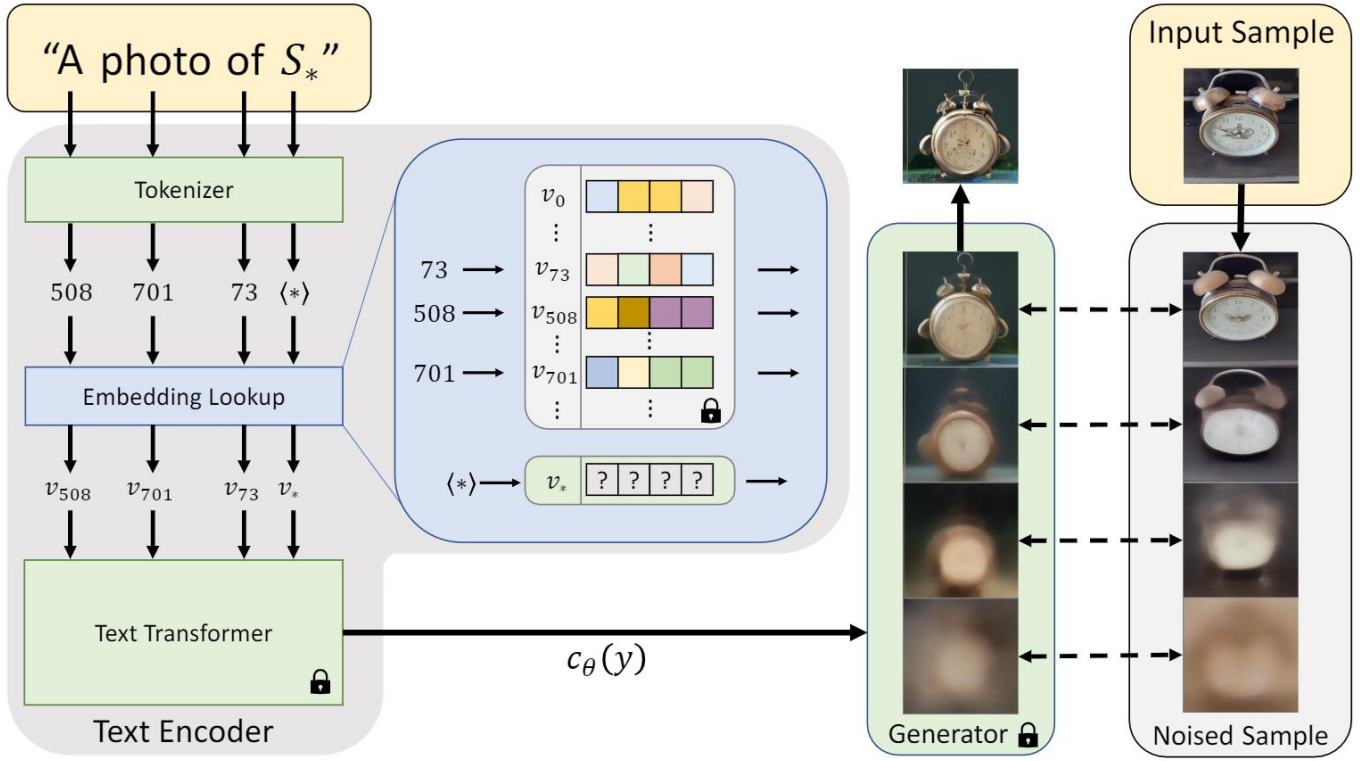
微调

Dreambooth

Ruiz, N., Li, Y., Jampani, V., Pritch, Y., Rubinstein, M., & Aberman, K. (2022). DreamBooth: Fine Tuning Text-to-Image Diffusion Models for Subject-Driven Generation.

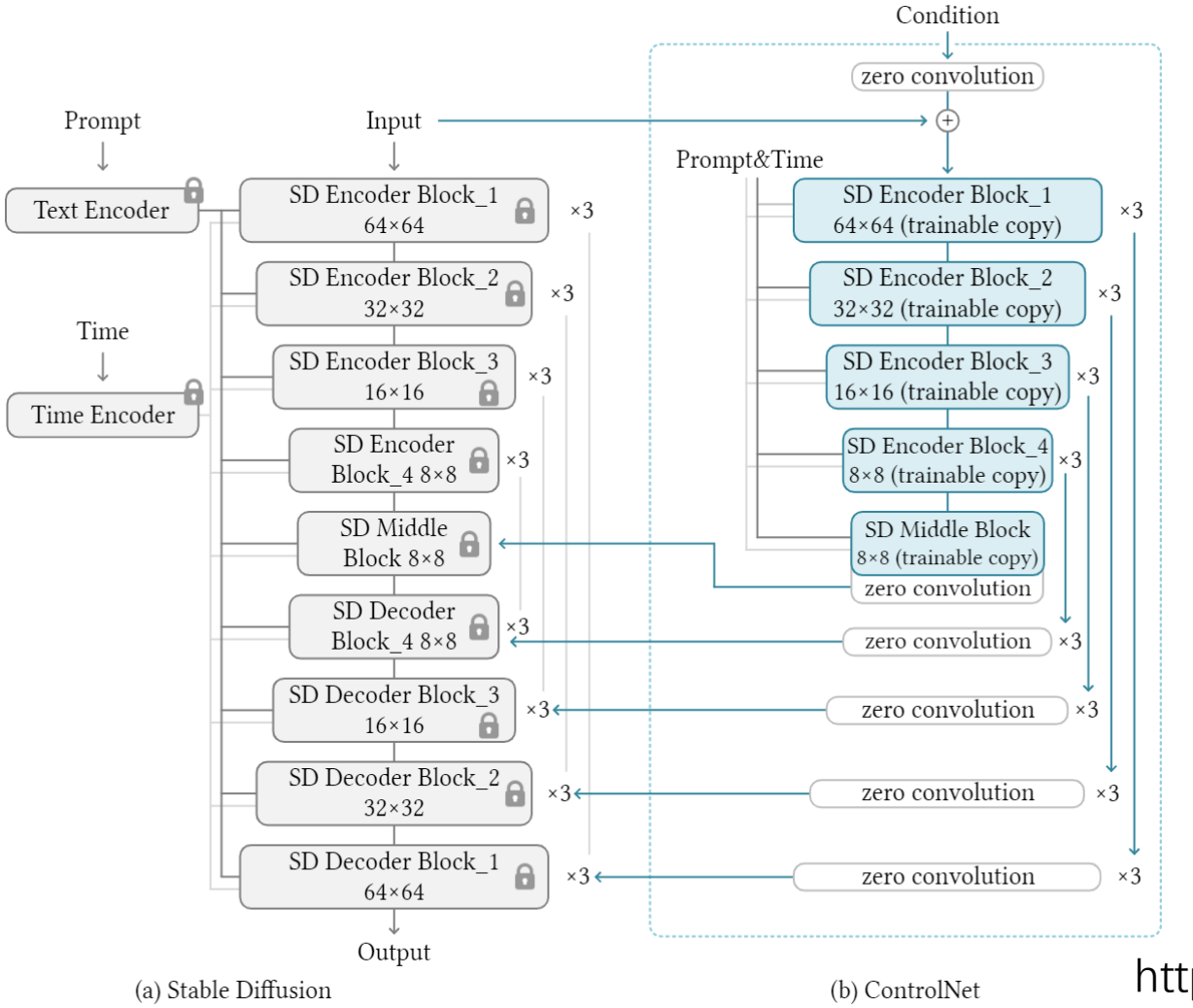
微调

Textual invesion

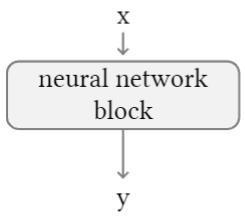


Gal, R., Alaluf, Y., Atzmon, Y., Patashnik, O., Bermano, A., Chechik, G., & Cohen-Or, D. (2022). An Image is Worth One Word: Personalizing Text-to-Image Generation using Textual Inversion.

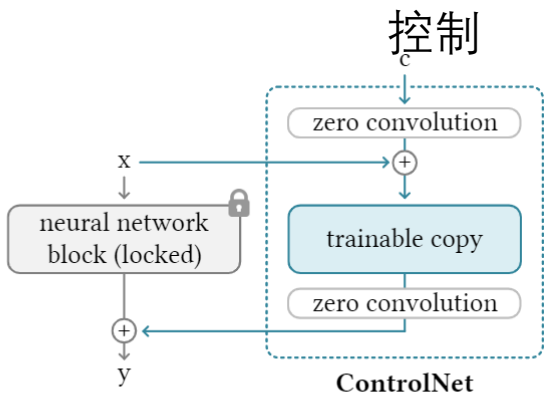
Controlnet



(a) Stable Diffusion (b) ControlNet



(a) Before

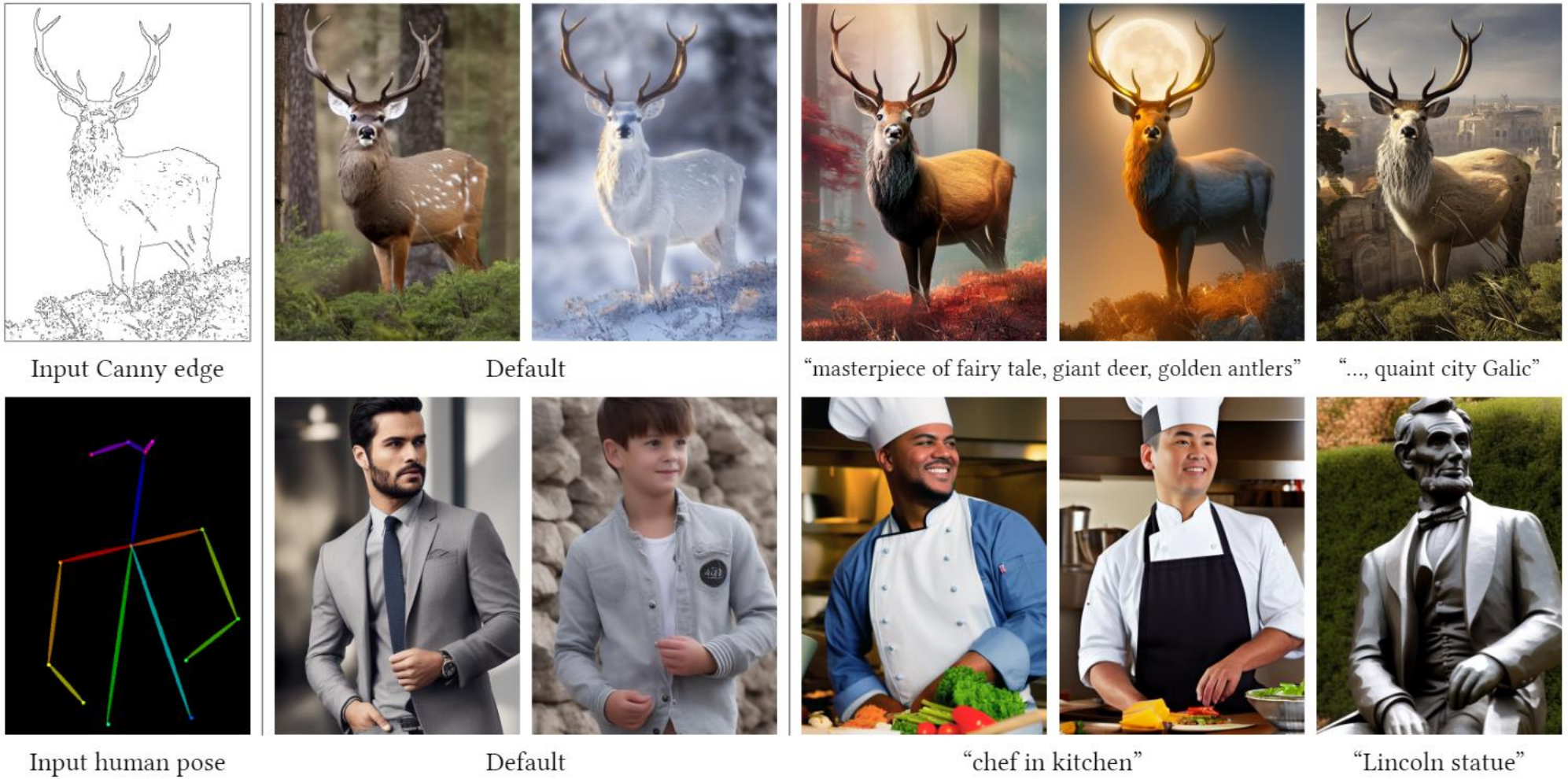


(b) After

https://github.com/lllyasviel/ControlNet/discussions/188

Zhang, L., & Agrawala, M. (2023). Adding Conditional Control to Text-to-Image Diffusion Models.

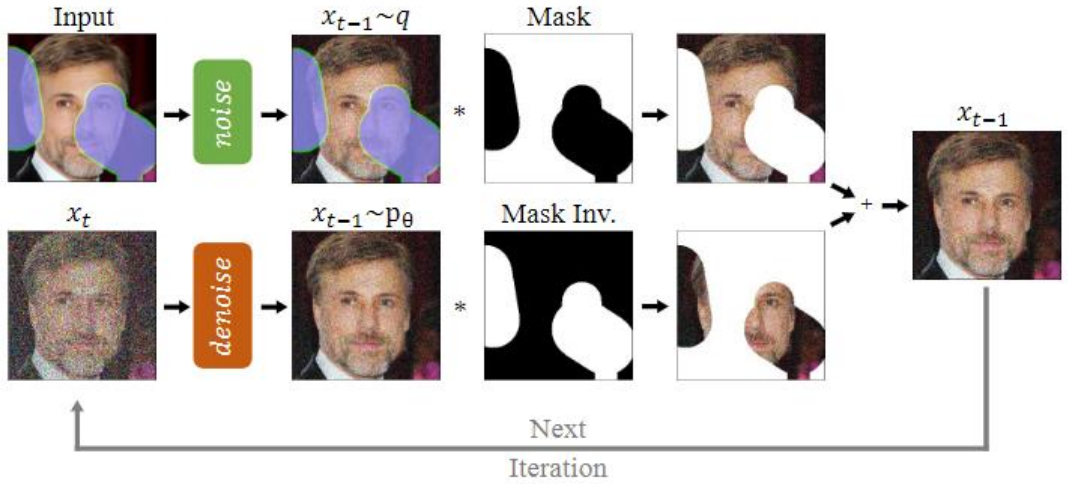
Controlnet


Input Canny edge
Default
"masterpiece of fairy tale, giant deer, golden antlers"
"..., quaint city Galic"
Input human pose
Default
"chef in kitchen"
"Lincoln statue"

Repaint

Algorithm 1 Inpainting using our RePaint approach.

1: $x_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \ldots, 1$ **do**
3: **for** $u = 1, \ldots, U$ **do**
4: $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\epsilon = \mathbf{0}$
5: $x_{t-1}^{\text{known}} = \sqrt{\bar{\alpha}_t} x_0 + (1 - \bar{\alpha}_t)\epsilon$
6: $z \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
7: $x_{t-1}^{\text{unknown}} = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(x_t, t) \right) + \sigma_t z$
8: $x_{t-1} = m \odot x_{t-1}^{\text{known}} + (1 - m) \odot x_{t-1}^{\text{unknown}}$
9: **if** $u < U$ and $t > 1$ **then**
10: $x_t \sim \mathcal{N}(\sqrt{1 - \beta_{t-1}} x_{t-1}, \beta_{t-1}\mathbf{I})$
11: **end if**
12: **end for**
13: **end for**
14: **return** x_0

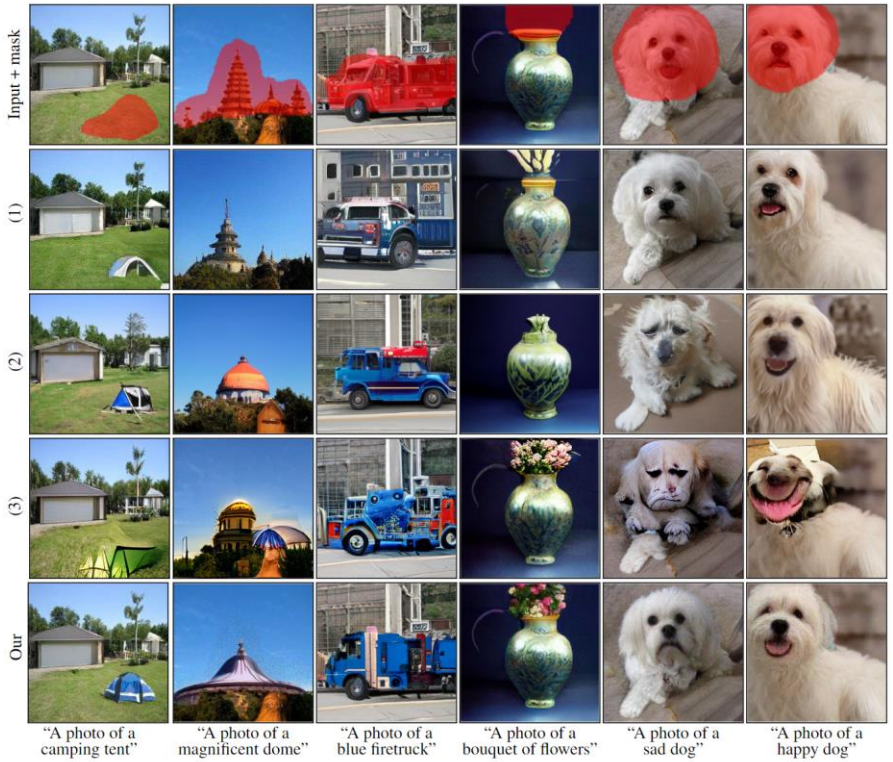


Lugmayr, A., Danelljan, M., Romero, A., Yu, F., Timofte, R., & Van Gool, L. (2022). RePaint: Inpainting using Denoising Diffusion Probabilistic Models. CVPR.

Repaint

Lugmayr, A., Danelljan, M., Romero, A., Yu, F., Timofte, R., & Van Gool, L. (2022). RePaint: Inpainting using Denoising Diffusion Probabilistic Models. CVPR.

Blended-diffusion



Algorithm 1 Local CLIP-guided diffusion, given a diffusion model $(\mu_\theta(x_t), \Sigma_\theta(x_t))$ and *CLIP* model

Input: source image x, target text description d, input mask m, diffusion steps k, background preservation coefficient λ
Output: edited image $\widehat{x}$ that differs from input image x inside area m according to text description d

$x_k \sim \mathcal{N}(\sqrt{\bar{\alpha}_k}x_0, (1-\bar{\alpha}_k)\mathbf{I})$
for all t from k to 1 **do**
  $\mu, \Sigma \leftarrow \mu_\theta(x_t), \Sigma_\theta(x_t)$
  $\widehat{x}_0 \leftarrow \frac{x_t}{\sqrt{\bar{\alpha}_t}} - \frac{\sqrt{1-\bar{\alpha}_t}\epsilon_\theta(x_t,t)}{\sqrt{\bar{\alpha}_t}}$
  $\widehat{x}_{0,aug} \leftarrow ExtendingAugmentations(\widehat{x}_0, N)$
  $\mathcal{L} \leftarrow \mathcal{D}_{CLIP}(\widehat{x}_{0,aug}, d, m) + \lambda\mathcal{D}_{bg}(x, \widehat{x}_{0,aug}, m)$
  $x_{t-1} \sim \mathcal{N}(\mu + \Sigma\nabla_{\widehat{x}_0}\mathcal{L}, \Sigma)$
end for
return x_0

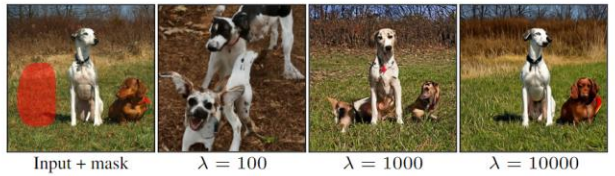


Figure 3. **Effect of λ in local CLIP-guided diffusion.** Given an input image with a mask, and the prompt "a dog": with λ set too low ($\lambda = 100$), the entire image changes completely, while if λ is too high ($\lambda = 10000$), the model fails to change the foreground (and the background preservation is not perfect). Using an intermediate value ($\lambda = 1000$) the model changes the foreground while resembling the original background (zoom for more details).

Algorithm 2 Text-driven blended diffusion: given a diffusion model $(\mu_\theta(x_t), \Sigma_\theta(x_t))$, and *CLIP* model

Input: source image x, target text description d, input mask m, diffusion steps k, number of extending augmentations N
Output: edited image $\widehat{x}$ that differs from input image x inside area m according to text description d

$x_k \sim \mathcal{N}(\sqrt{\bar{\alpha}_k}x_0, (1-\bar{\alpha}_k)\mathbf{I})$
for all t from k to 0 **do**
  $\mu, \Sigma \leftarrow \mu_\theta(x_t), \Sigma_\theta(x_t)$
  $\widehat{x}_0 \leftarrow \frac{x_t}{\sqrt{\bar{\alpha}_t}} - \frac{\sqrt{1-\bar{\alpha}_t}\epsilon_\theta(x_t,t)}{\sqrt{\bar{\alpha}_t}}$
  $\widehat{x}_{0,aug} \leftarrow ExtendingAugmentations(\widehat{x}_0, N)$
  $\nabla_{text} \leftarrow \frac{1}{N}\sum_{i=1}^{N}\nabla_{\widehat{x}_{0,aug}}\mathcal{D}_{CLIP}(\widehat{x}_{0,aug}, d, m)$
  $x_{fg} \sim \mathcal{N}(\mu + \Sigma\nabla_{text}, \Sigma)$
  $x_{bg} \sim \mathcal{N}(\sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_t)\mathbf{I})$
  $x_{t-1} \leftarrow x_{fg} \odot m + x_{bg} \odot (1-m)$
end for
return x_{-1}

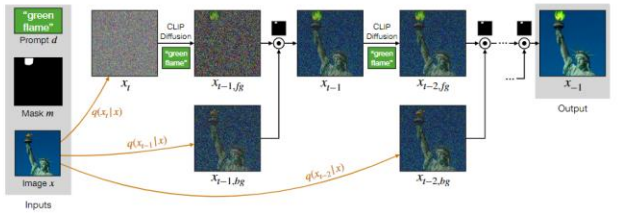
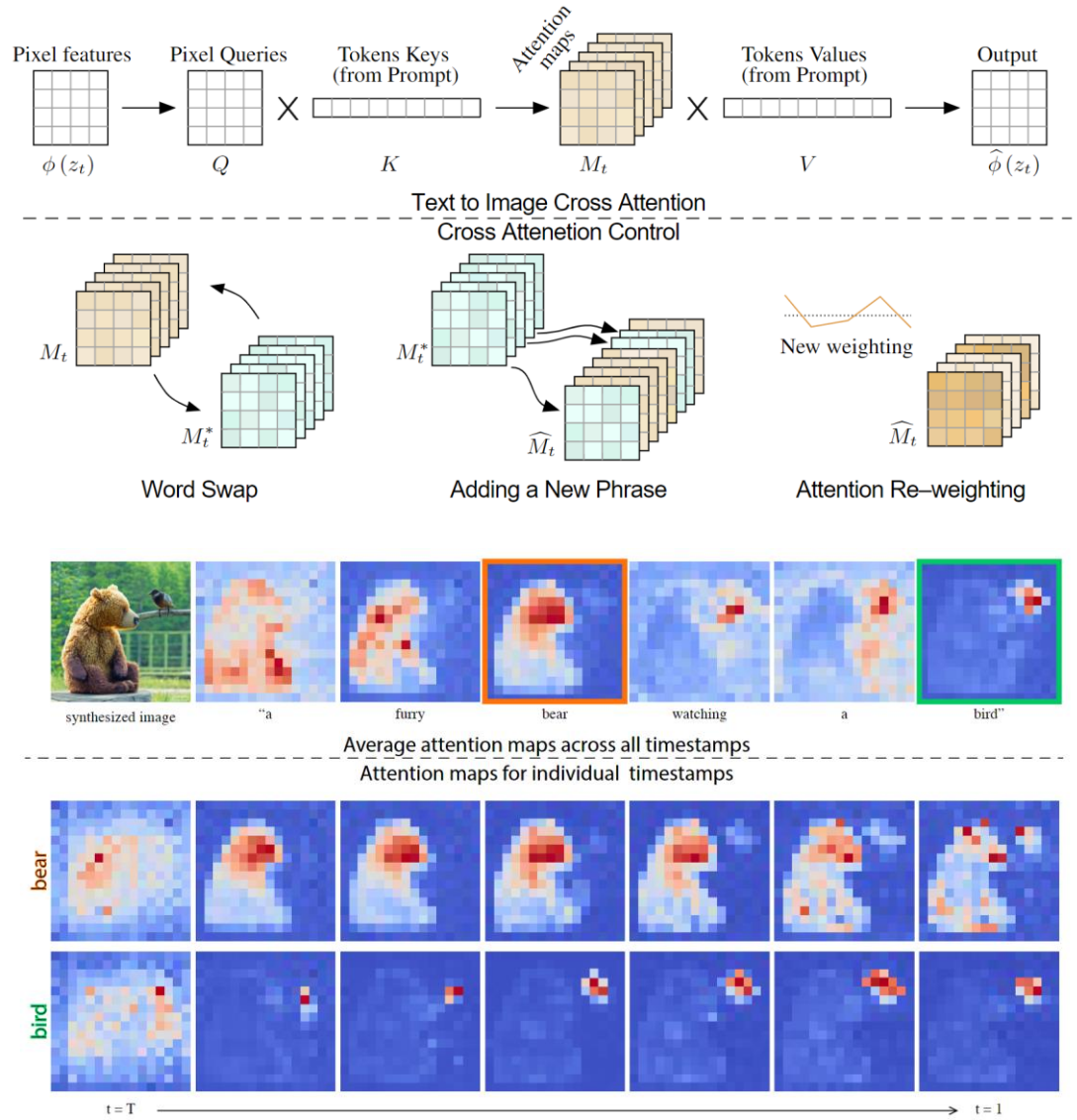


Figure 4. **Text-driven blended diffusion.** Given input image x, input mask m, and a text prompt d, we leverage the diffusion process to edit the image locally and coherently. We denote with $\odot$ the element-wise blending of two images using the input mask m.

Avrahami, O., Lischinski, D., & Fried, O. (2021). Blended Diffusion for Text-driven Editing of Natural Images. 2022(CVPR)

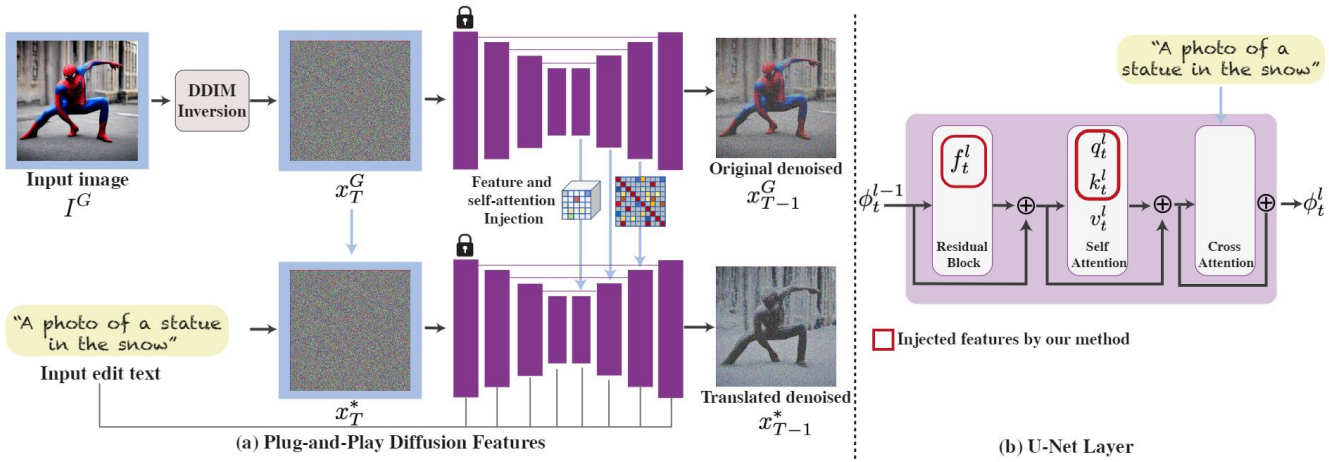
细分应用

P2p



Hertz, A., Mokady, R., Tenenbaum, J., Aberman, K., Pritch, Y., Cohen-Or, D., & Research, G. (2022). Prompt-to-Prompt Image Editing with Cross Attention Control.

Pnp



Algorithm 1 Plug-and-Play Diffusion Features

Inputs:
I^G ▷ real guidance image
P ▷ target text prompt
τ_f, τ_A ▷ injection thresholds

$\boldsymbol{x}_T^G \leftarrow \text{DDIM-inv}(I^G)$
$\boldsymbol{x}_T^* \leftarrow \boldsymbol{x}_T^G$ ▷ Starting from same seed
for $t \leftarrow T \dots 1$ **do**
  $\boldsymbol{z}_{t-1}^G, \boldsymbol{f}_t^4, \left\{\boldsymbol{A}_t^l\right\} \leftarrow \epsilon_\theta\left(\boldsymbol{x}_t^G, \varnothing, t\right)$
  $\boldsymbol{x}_{t-1}^G \leftarrow \text{DDIM-samp}\left(\boldsymbol{x}_t^G, \boldsymbol{z}_{t-1}^G\right)$
  if $t > \tau_f$ **then** $\boldsymbol{f}_t^{*4} \leftarrow \boldsymbol{f}_t^4$ **else** $\boldsymbol{f}_t^{*4} \leftarrow \varnothing$
  if $t > \tau_A$ **then** $\boldsymbol{A}_t^{*l} \leftarrow \boldsymbol{A}_t^l$ **else** $\boldsymbol{A}_t^{*l} \leftarrow \varnothing$
  $\boldsymbol{z}_{t-1}^* \leftarrow \hat{\epsilon}_\theta\left(\boldsymbol{x}_t^*, P, t\,;\, \boldsymbol{f}_t^{*4}, \left\{\boldsymbol{A}_t^{*l}\right\}\right)$
  $\boldsymbol{x}_{t-1}^* \leftarrow \text{DDIM-samp}\left(\boldsymbol{x}_t^*, \boldsymbol{z}_{t-1}^*\right)$
end for
Output: $I^* \leftarrow \boldsymbol{x}_0^*$

Tumanyan, N., Geyer, M., Bagon, S., & Dekel, T. (2022). Plug-and-Play Diffusion Features for Text-Driven Image-to-Image Translation.

InstructPix2Pix

Figure 5. *Mona Lisa* transformed into various artistic mediums.

Figure 6. *The Creation of Adam* with new context and subjects (generated at 768 resolution).

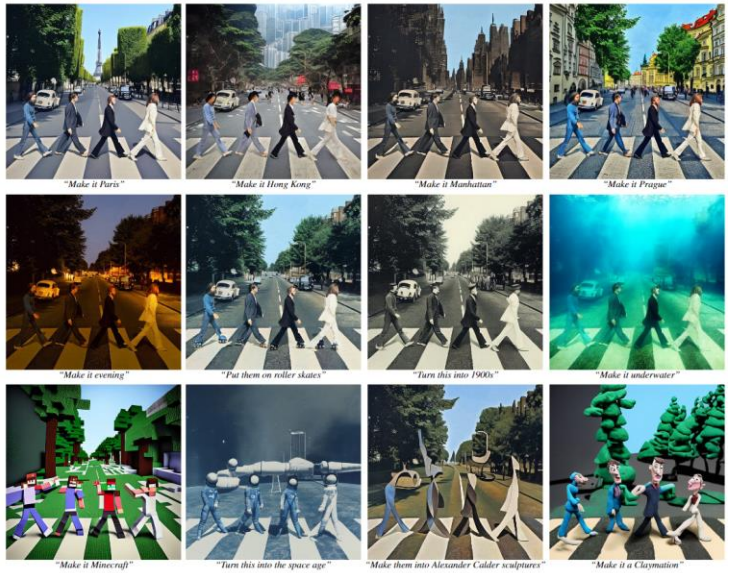
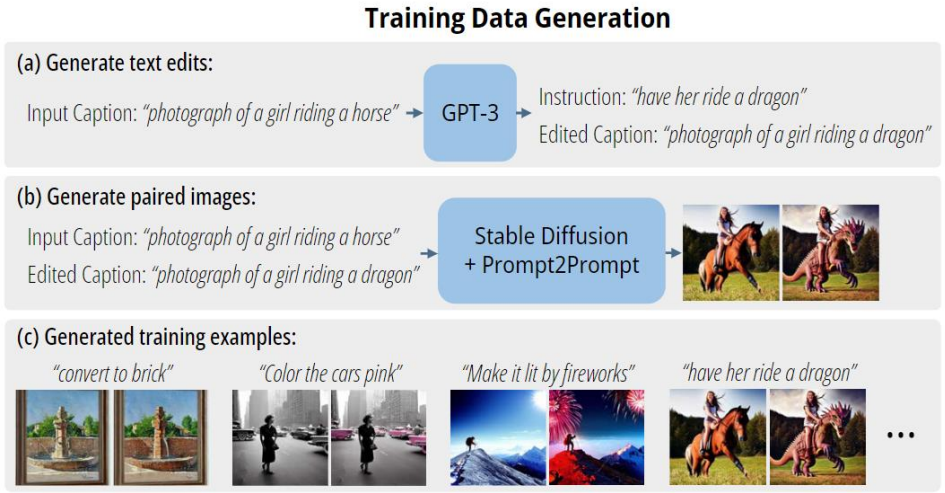
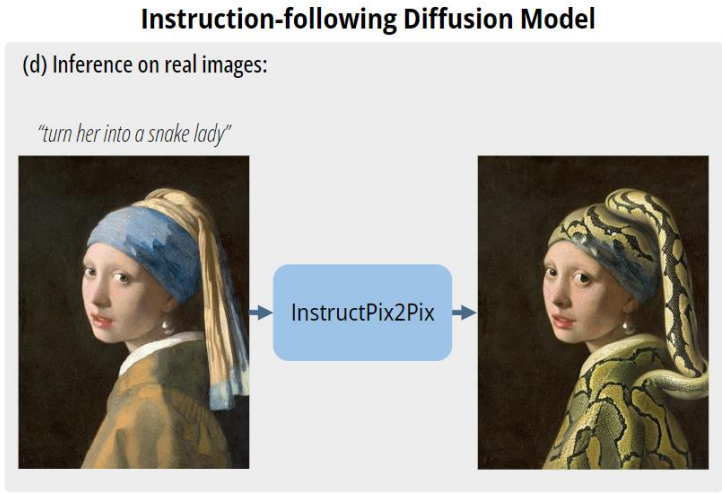


Figure 7. The iconic Beatles *Abbey Road* album cover transformed in a variety of ways.





$$\tilde{e}_\theta(z_t, c_I, c_T) = e_\theta(z_t, \varnothing, \varnothing) + s_I \cdot (e_\theta(z_t, c_I, \varnothing) - e_\theta(z_t, \varnothing, \varnothing)) + s_T \cdot (e_\theta(z_t, c_I, c_T) - e_\theta(z_t, c_I, \varnothing))$$

Brooks, T., Holynski, A., & Efros, AlexeiA. (2022). InstructPix2Pix: Learning to Follow Image Editing Instructions.

InstructPix2Pix

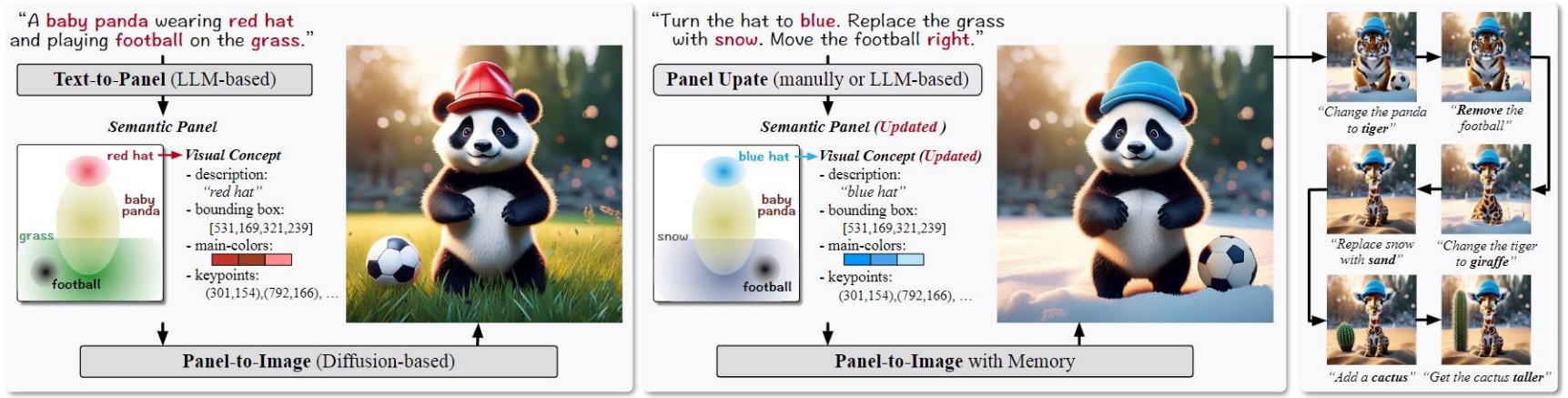
"Zoom into the image" *"Move it to Mars"* *"Color the tie blue"* *"Have the people swap places"*

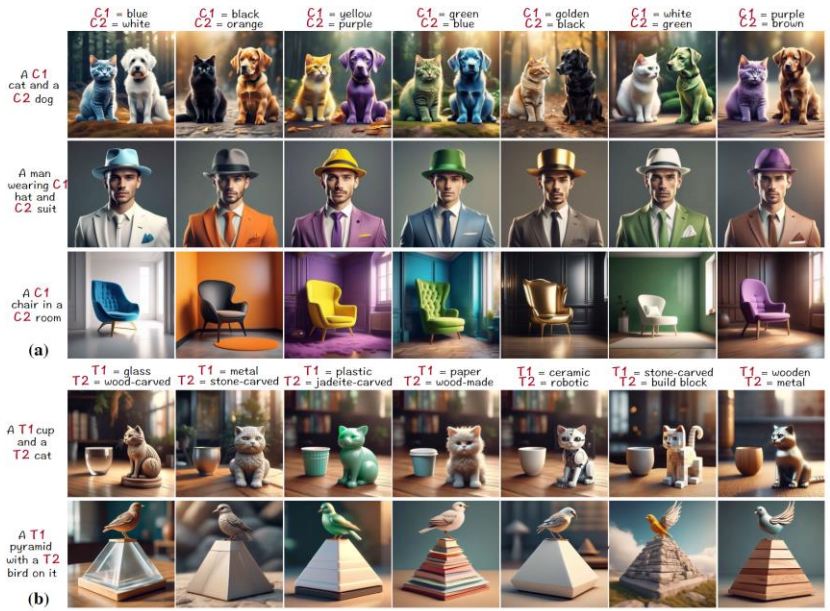
Figure 13. Failure cases. Left to right: our model is not capable of performing viewpoint changes, can make undesired excessive changes to the image, can sometimes fail to isolate the specified object, and has difficulty reorganizing or swapping objects with each other.

CVPR24-oral

- 精准控制
- 复杂场景
- …

Ranni





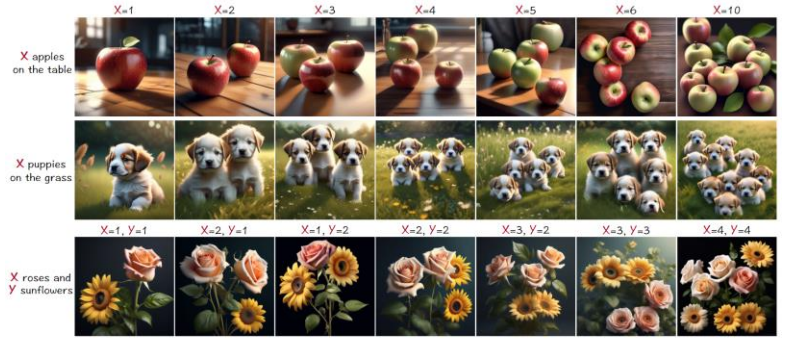
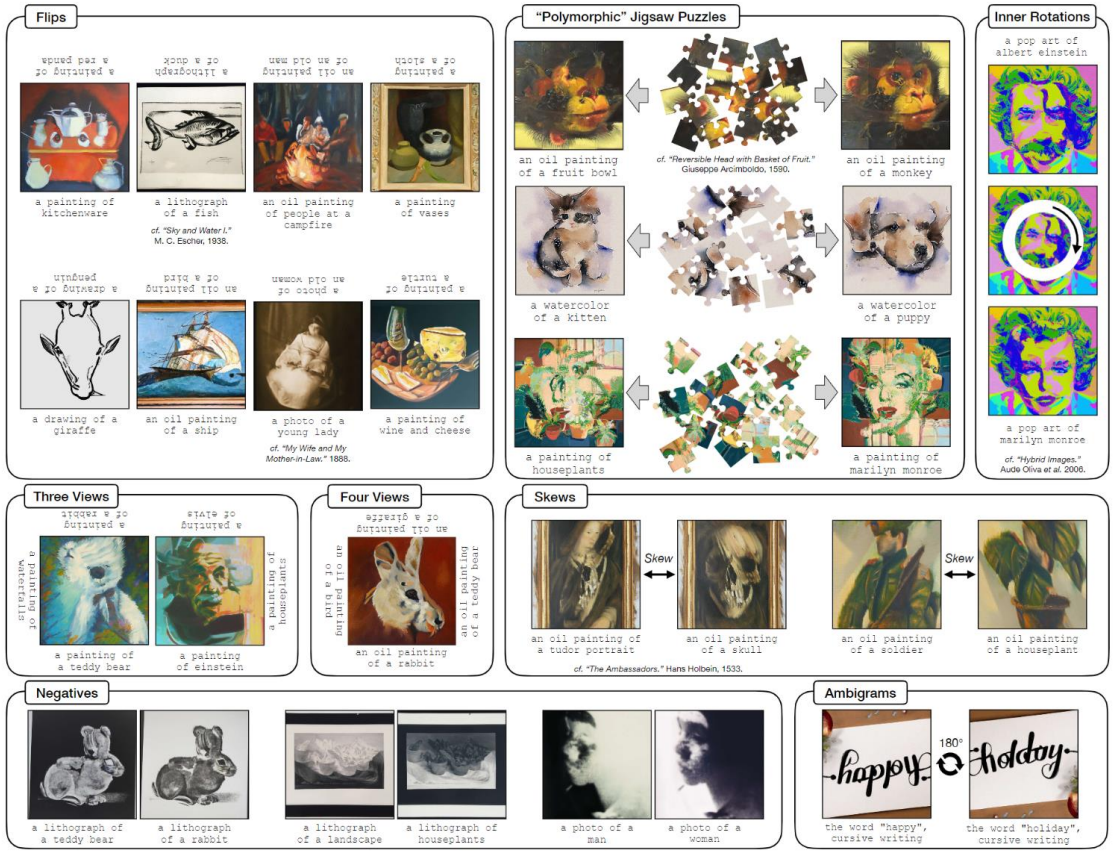


Figure 5. Samples generated by Ranni on **quantity-awareness** prompts.

Figure 6. Samples generated by Ranni on **spatial relationship** prompts.

Feng, Y., Gong, B., Chen, D., Shen, Y., Liu, Y., & Zhou, J. (2023). Ranni: Taming Text-to-Image Diffusion for Accurate Instruction Following.

Visual Anagrams



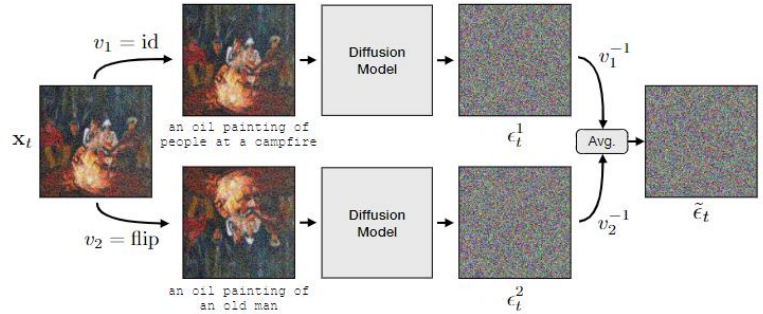
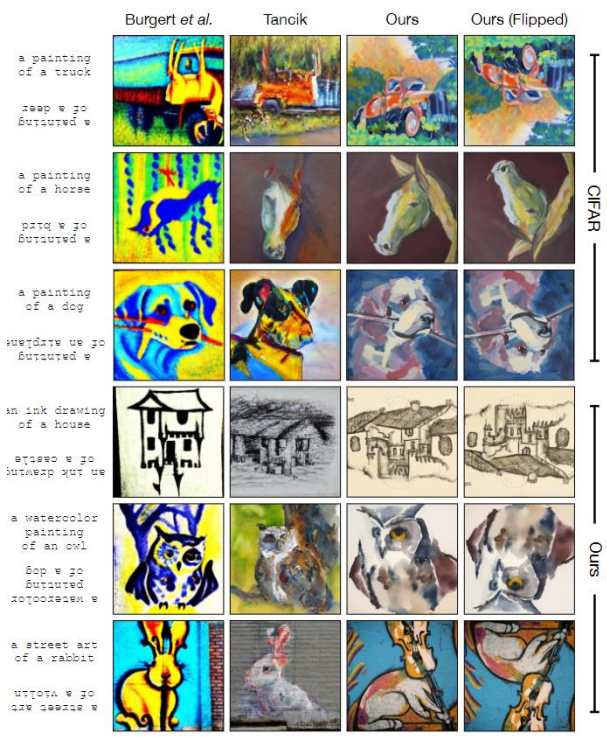


Figure 2. **Algorithm Overview.** Our method works by simultaneously denoising multiple views of an image. Given a noisy image $\mathbf{x}_t$, we compute noise estimates, ϵ_t^i, conditioned on different prompts, after applying views v_i. We then apply the inverse view v_i^{-1} to align estimates, average the estimates, and perform a reverse diffusion step. The final output is an optical illusion.



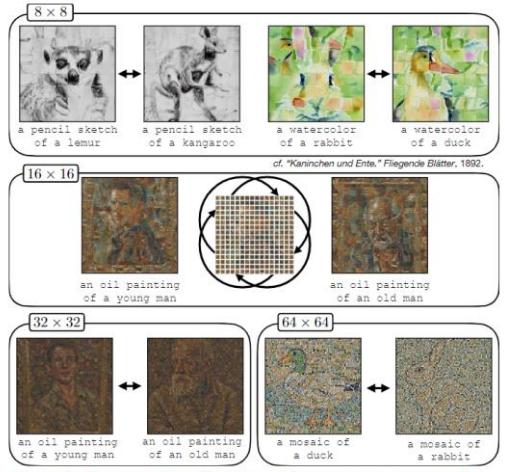
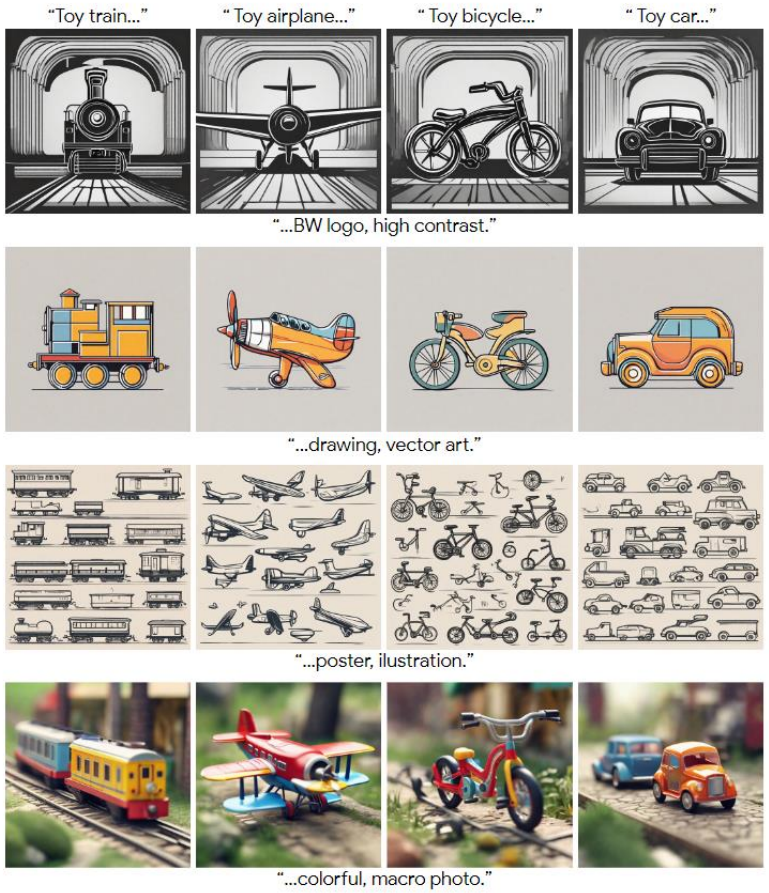


Figure 6. **Permutation Illusions.** We synthesize images whose

Geng, D., Park, I., & Owens, A. (2023). Visual Anagrams: Generating Multi-View Optical Illusions with Diffusion Models.

StyleAligned



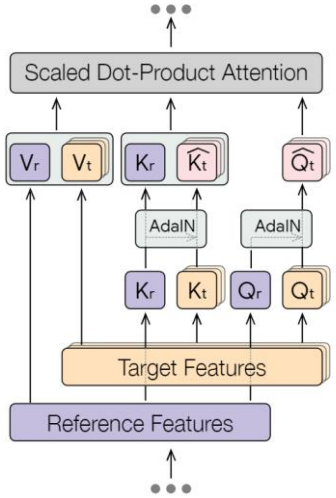


Figure 4. **Shared attention layer.** *The target images attends to the reference image by applying AdaIN over their queries and keys using the reference queries and keys respectively. Then, we apply shared attention where the target features are updated by both the target values V_t and the reference values V_r.*

As illustrated in Fig. 4, to enable balanced attention reference, we normalize the queries Q_t and keys K_t of the target image using the queries Q_r and keys K_r of the reference image using the adaptive normalization operation (AdaIN) [26]:

$$\hat{Q}_t = \text{AdaIN}(Q_t, Q_r) \quad \hat{K}_t = \text{AdaIN}(K_t, K_r),$$

where the AdaIn operation is given by:

$$\text{AdaIN}(x, y) = \sigma(y)\left(\frac{x - \mu(x)}{\sigma(x)}\right) + \mu_y,$$

and $\mu(x), \sigma(x) \in \mathbb{R}^{d_k}$ are the mean and the standard deviation of queries and keys across different pixels. Finally, our shared attention is given by

$$\text{Attention}(\hat{Q}_t, K_{rt}^T, V_{rt}),$$

where $K_{rt} = \begin{bmatrix} K_r \\ \hat{K}_t \end{bmatrix}$ and $V_{rt} = \begin{bmatrix} V_r \\ V_t \end{bmatrix}$.

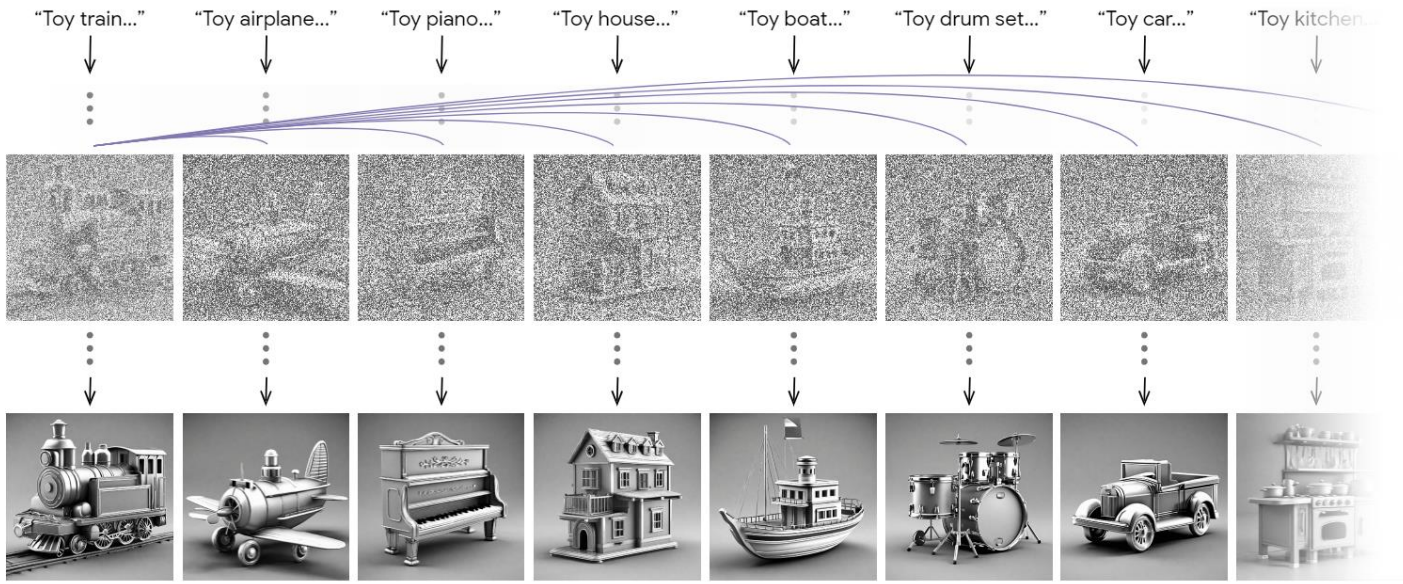


Figure 3. **Style Aligned Diffusion.** *Generation of images with a style aligned to the reference image on the left. In each diffusion denoising step all the images, except the reference, perform a shared self-attention with the reference image.*

Hertz, A., Voynov, A., Fruchter, S., & Cohen-Or, D. (2023). Style Aligned Image Generation via Shared Attention.

Instruct-Imagen

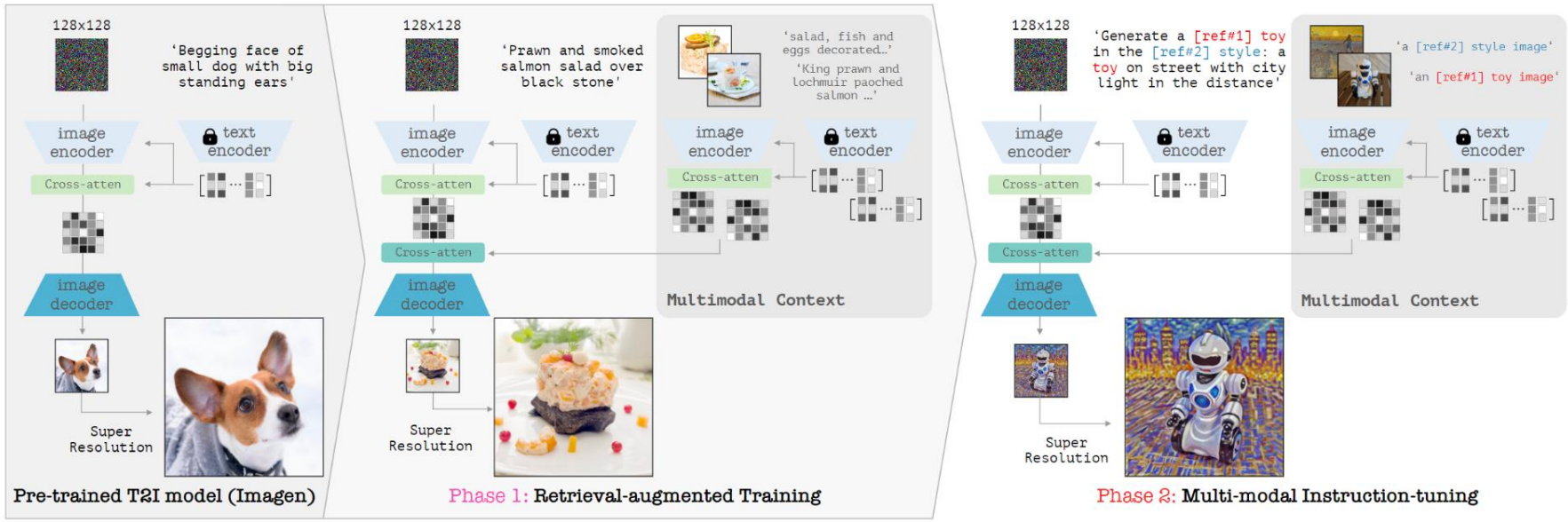
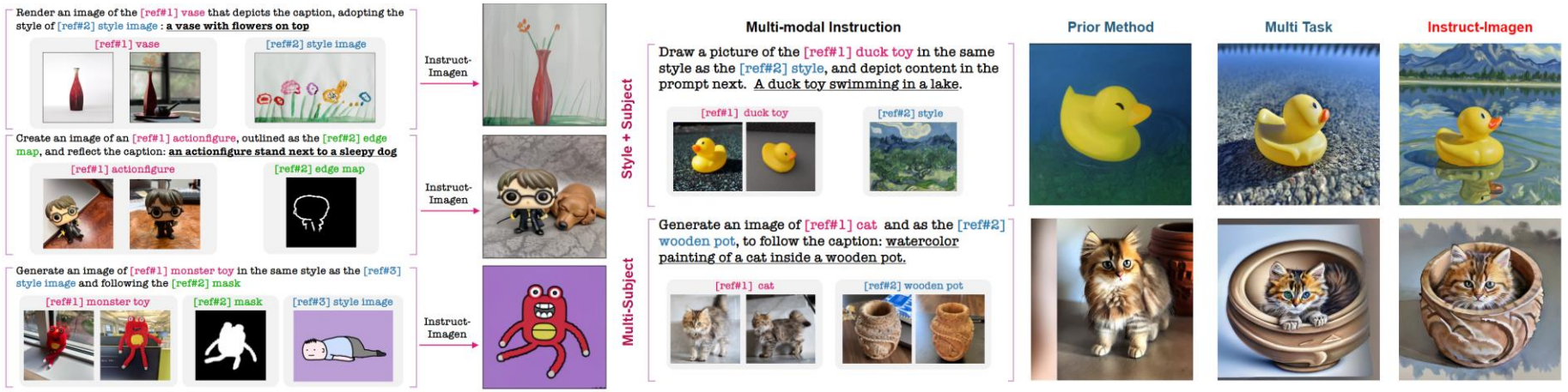


Figure 3. Overview of the two-staged training pipeline for the proposed `Instruct-Imagen` model.



Instruct-Imagen : Image Generation with Multi-modal Instruction. (n.d.).

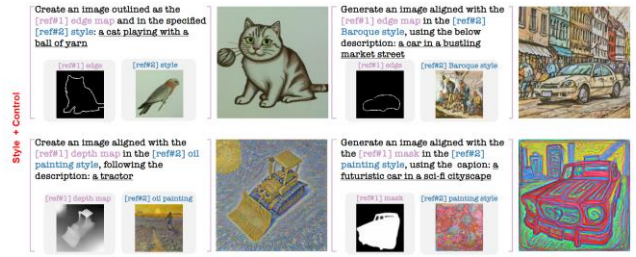


Figure 9. Additional Qualitative Evaluation of `Instruct-Imagen` on Control + Style Generation.

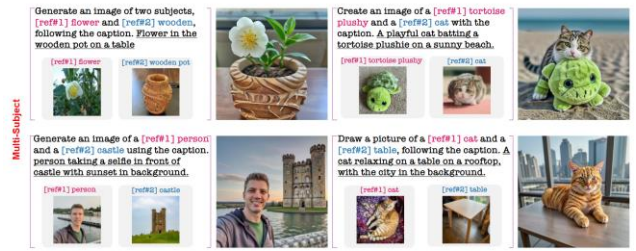
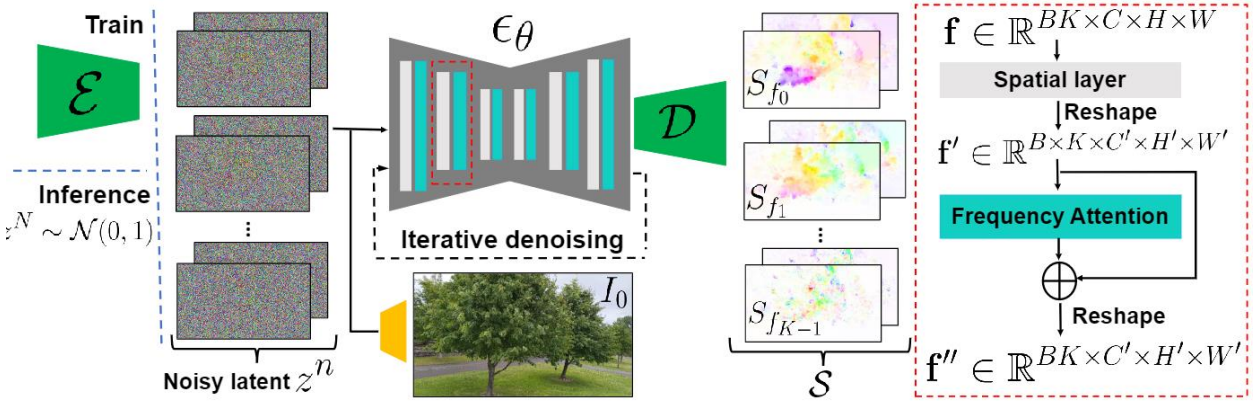


Figure 10. Additional Qualitative Evaluation of `Instruct-Imagen` on Multi-Subject Generation.

Best paper I



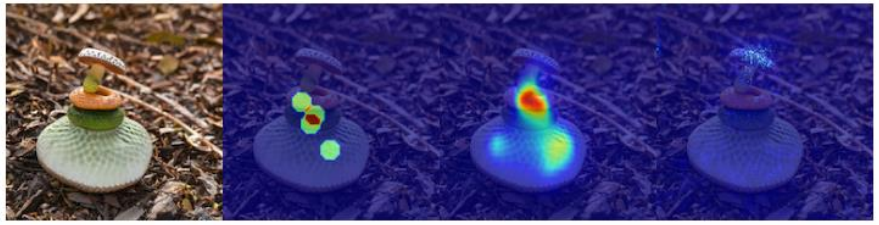
Li, Z., Noah, R., Aleksander, S., & Google, H. (n.d.). Generative Image Dynamics.

Best paper II

Figure 1. **An illustration of our annotation UI**. Annotators mark points on the image to indicate artifact/implausibility regions (red points) or misaligned regions (blue points) w.r.t the text prompt. Then, they click on the words to mark the misaligned keywords (underlined and shaded) and choose the scores for plausibility, text-image alignment, aesthetics, and overall quality (underlined).

(a) Image (b) GT (c) Our model (d) ResNet-50

Figure 5. Examples of implausibility heatmaps. Prompt: *photo of a slim asian little girl ballerina with long hair wearing white tights running on a beach from behind nikon D5*



(a) Image (b) GT (c) Our model (d) CLIP gradient

Figure 6. Examples of misalignment heatmaps. Prompt: *A snake on a mushroom*.

Liang, Y., He, J., Li, G., Li, P., Klimovskiy, A., Carolan, N., ⋯ Navalpakkam, V. (2023). Rich Human Feedback for Text-to-Image Generation.

总结

- 研究广泛但不深入
  - 广泛：多种新奇任务、结合LLM
  - 不深入：设计新模型困难
- 机会仍然很多
  - 精准图像生成/编辑
  - Image-video、text-video
  - Text-3D
  - Text-4D