NỀN TẢNG AI TẠO SINH

(IT5410 – Foundation of Generative AI)

MÔ HÌNH SINH SÂU DIFFUSION

Thân Quang Khoát

Trường CNTT&TT, ĐHBKHN

2025

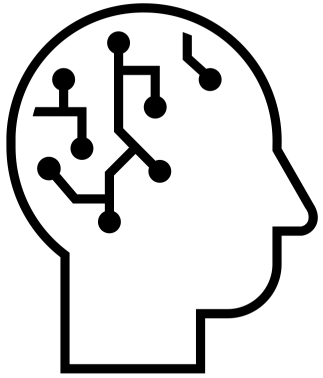
Nội dung

- Mở đầu
- Một số vấn đề của Học sâu
- Một số kiến trúc mạng nơron
- **Mô hình sinh sâu**
- Đánh giá chất lượng
- Học tăng cường

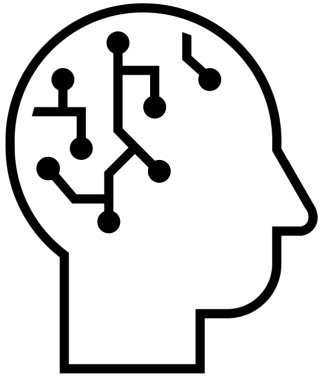
Deep Generative Learning

Samples from a Data Distribution

Train



Neural Network



Sample

Denoising Diffusion Models

Emerging as powerful generative models, outperforming GANs

"Diffusion Models Beat GANs on Image Synthesis" Dhariwal & Nichol, OpenAI, 2021

"Cascaded Diffusion Models for High Fidelity Image Generation" Ho et al., Google, 2021

Text-to-Image Generation

DALL·E 2

“a teddy bear on a skateboard in times square”

[“Hierarchical Text-Conditional Image Generation with CLIP Latents” Ramesh et al., 2022]

Imagen

“ A group of teddy bears in suit in a corporate office celebrating the birthday of their friend. There is a pizza cake on the desk. ”

[“Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding”, Saharia et al., 2022]

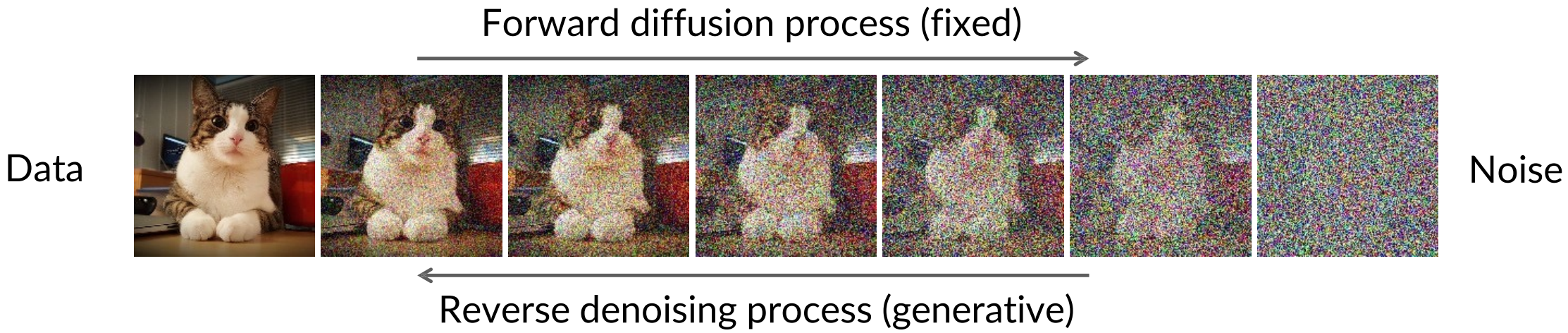
Outline

- Part (1): Denoising Diffusion Probabilistic Models
- Part (2): Conditional Generation and Guidance
- Part (3): Text-to-image Diffusion Models

Part (1): Denoising Diffusion Probabilistic Models

Denoising Diffusion Models

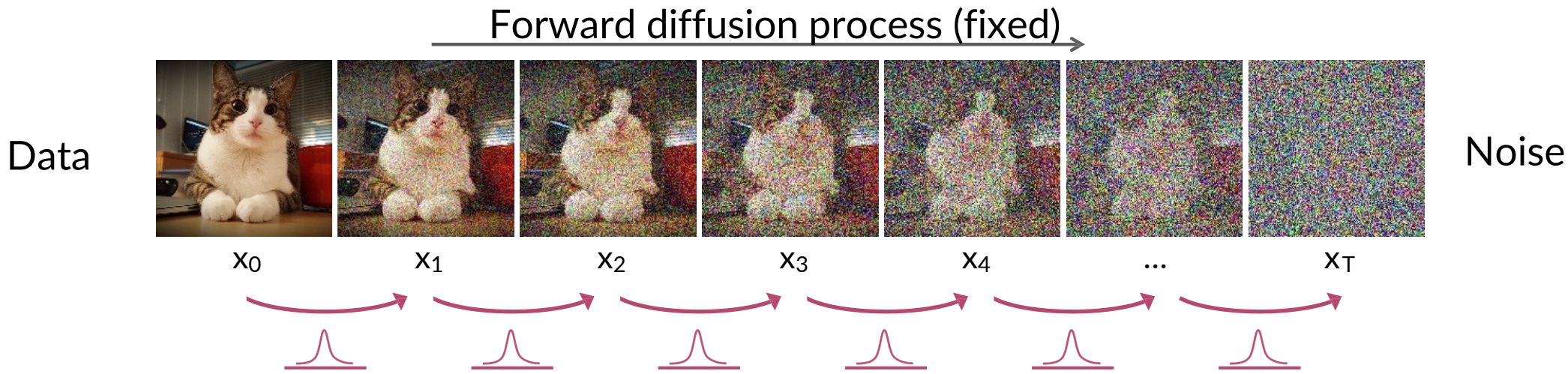
- Denoising diffusion models consist of two processes:
  - Forward diffusion process that gradually adds noise to input
  - Reverse denoising process that learns to generate data by denoising



Sohl-Dickstein et al., Deep Unsupervised Learning using Nonequilibrium Thermodynamics, ICML 2015
Ho et al., Denoising Diffusion Probabilistic Models, NeurIPS 2020
Song et al., Score-Based Generative Modeling through Stochastic Differential Equations, ICLR 2021

Forward Diffusion Process

The formal definition of the forward process in T steps:



Forward process:
add Gaussian noise each step

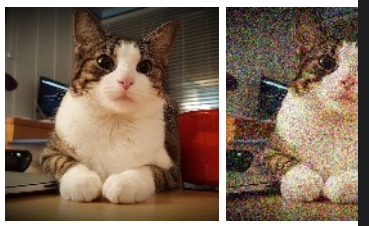
$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I})$$

➡ $$q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$$ (Probability Chain Rule - Markov Chain)

Deep Generative Learning

https://lilianweng.github.io/posts/2021-07-11-diffusion-models/

Data



x_0 x_1

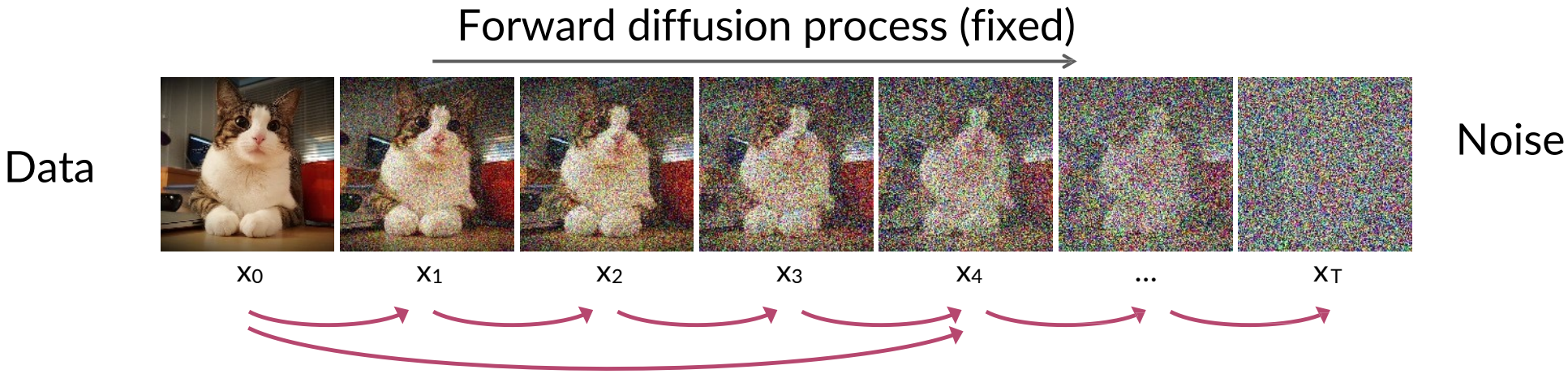
$$
\begin{aligned}
\mathbf{x}_t &= \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1} && \text{;where } \boldsymbol{\epsilon}_{t-1}, \boldsymbol{\epsilon}_{t-2}, \cdots \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \\
&= \sqrt{\alpha_t\alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\bar{\boldsymbol{\epsilon}}_{t-2} && \text{;where } \bar{\boldsymbol{\epsilon}}_{t-2} \text{ merges two Gaussians (*).} \\
&= \cdots \\
&= \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon} \\
q(\mathbf{x}_t|\mathbf{x}_0) &= \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})
\end{aligned}
$$

(*) Recall that when we merge two Gaussians with different variance, $\mathcal{N}(\mathbf{0}, \sigma_1^2\mathbf{I})$ and $\mathcal{N}(\mathbf{0}, \sigma_2^2\mathbf{I})$, the new distribution is $\mathcal{N}(\mathbf{0}, (\sigma_1^2 + \sigma_2^2)\mathbf{I})$. Here the merged standard deviation is $\sqrt{(1-\alpha_t) + \alpha_t(1-\alpha_{t-1})} = \sqrt{1-\alpha_t\alpha_{t-1}}$.

Nice property: samples from an *arbitrary forward step* are also Gaussian-distributed!

Define $\bar{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s)$ ➡ $q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}))$ (Diffusion Kernel)

Diffusion Kernel



Nice property: samples from an *arbitrary forward step* are also Gaussian-distributed!

Define $\bar{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s)$ ➡ $q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}))$ (Diffusion Kernel)

Gaussian reparameterization trick: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\,\epsilon$ where $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

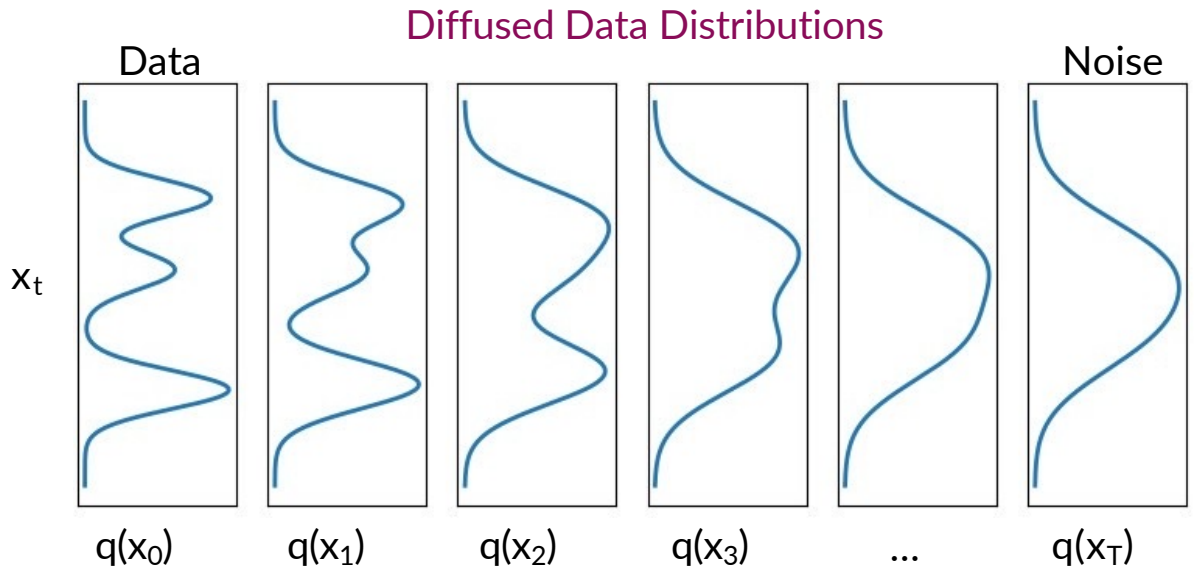
β_t values schedule (i.e., the noise schedule) is designed such that $\bar{\alpha}_T \to 0$ and $q(\mathbf{x}_T|\mathbf{x}_0) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}))$

What happens to a distribution in the forward diffusion?

So far, we discussed the diffusion kernel $q(\mathbf{x}_t|\mathbf{x}_0)$ but what about $q(\mathbf{x}_t)$

$$\underbrace{q(\mathbf{x}_t)}_{\text{Diffused data dist.}} = \int \underbrace{q(\mathbf{x}_0, \mathbf{x}_t)}_{\text{Joint dist.}} d\mathbf{x}_0 = \int \underbrace{q(\mathbf{x}_0)}_{\text{Input data dist.}} \underbrace{q(\mathbf{x}_t|\mathbf{x}_0)}_{\text{Diffusion kernel}} d\mathbf{x}_0$$

The diffusion kernel is Gaussian convolution.



We can sample $\mathbf{x}_t \sim q(\mathbf{x}_t)$ by first sampling $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ and then sampling $\mathbf{x}_t \sim q(\mathbf{x}_t|\mathbf{x}_0)$ (i.e., ancestral sampling).

Generative Learning by Denoising

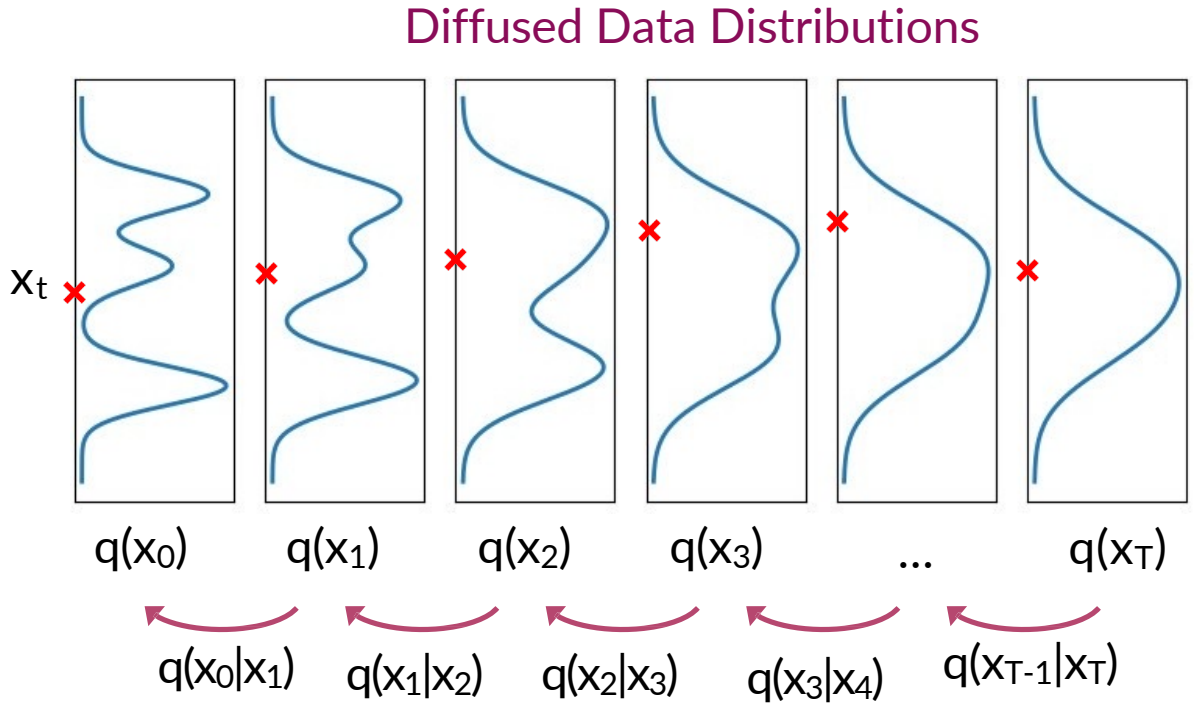
Recall, that the diffusion parameters are designed such that $q(\mathbf{x}_T) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}))$

Generation:

- Sample $\mathbf{x}_T \sim \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$

- Iteratively sample $\mathbf{x}_{t-1} \sim q(\mathbf{x}_{t-1}|\mathbf{x}_t)$

True Denoising Dist.

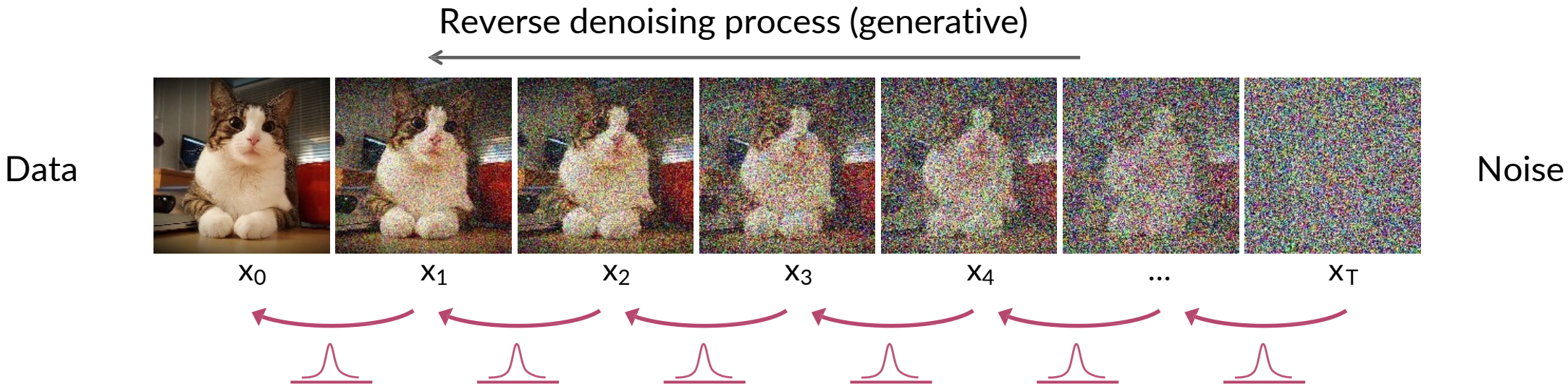


In general, $q(\mathbf{x}_{t-1}|\mathbf{x}_t) \propto q(\mathbf{x}_{t-1})q(\mathbf{x}_t|\mathbf{x}_{t-1})$ is intractable.

Can we approximate $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$?

Reverse Denoising Process

- Reverse processes in T steps:



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

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \underbrace{\mu_\theta(\mathbf{x}_t, t)}, \sigma_t^2\mathbf{I})$$

Trainable network

(U-net, Denoising Autoencoder)

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

Learning Denoising Model - High-level intuition

- Because $q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$ is intractable, we can instead derive a tractable posterior distribution $q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0)$
- Then we can train a neural network $p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$ to match this distribution.
- The learning objective is to minimize:

$$D_{KL}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))$$

Learning Denoising Model: Tractable posterior distribution

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I})$$

Using Bayes' rule:

$$\begin{aligned}
q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) &= q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} \\
&\propto \exp\Big(-\frac{1}{2}\big(\frac{(\mathbf{x}_t - \sqrt{\alpha_t}\mathbf{x}_{t-1})^2}{\beta_t} + \frac{(\mathbf{x}_{t-1} - \sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0)^2}{1-\bar{\alpha}_{t-1}} - \frac{(\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{x}_0)^2}{1-\bar{\alpha}_t}\big)\Big) \\
&= \exp\Big(-\frac{1}{2}\big(\frac{\mathbf{x}_t^2 - 2\sqrt{\alpha_t}\mathbf{x}_t\mathbf{x}_{t-1} + \alpha_t\mathbf{x}_{t-1}^2}{\beta_t} + \frac{\mathbf{x}_{t-1}^2 - 2\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0\mathbf{x}_{t-1} + \bar{\alpha}_{t-1}\mathbf{x}_0^2}{1-\bar{\alpha}_{t-1}} - \frac{(\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{x}_0)^2}{1-\bar{\alpha}_t}\big)\Big) \\
&= \exp\Big(-\frac{1}{2}\big((\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}})\mathbf{x}_{t-1}^2 - (\frac{2\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0)\mathbf{x}_{t-1} + C(\mathbf{x}_t, \mathbf{x}_0)\big)\Big)
\end{aligned}$$

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Following the standard Gaussian density function, we can derive the mean and the variance:

$$\begin{aligned}
\tilde{\beta}_t &= 1/(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}) = 1/(\frac{\alpha_t - \bar{\alpha}_t + \beta_t}{\beta_t(1-\bar{\alpha}_{t-1})}) = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \cdot \beta_t \\
\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) &= (\frac{\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0)/(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}) \\
&= (\frac{\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0)\frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \cdot \beta_t \\
&= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 \\
&= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\frac{1}{\sqrt{\bar{\alpha}_t}}(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_t) = \frac{1}{\sqrt{1-\beta_t}}\Big(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\Big)
\end{aligned}$$

Learning Denoising Model: Variational upper bound

- For training, we can form variational upper bound that is commonly used for training VAEs:

$$
\begin{aligned}
-\log p_\theta(\mathbf{x}_0) &\leq -\log p_\theta(\mathbf{x}_0) + D_{\mathrm{KL}}(q(\mathbf{x}_{1:T}|\mathbf{x}_0)\|p_\theta(\mathbf{x}_{1:T}|\mathbf{x}_0)) \\
&= -\log p_\theta(\mathbf{x}_0) + \mathbb{E}_{\mathbf{x}_{1:T}\sim q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})/p_\theta(\mathbf{x}_0)}\right] \\
&= -\log p_\theta(\mathbf{x}_0) + \mathbb{E}_q\left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})} + \log p_\theta(\mathbf{x}_0)\right] \\
&= \mathbb{E}_q\left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})}\right] \\
\text{Let } L = \mathbb{E}_{q(\mathbf{x}_{0:T})}&\left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})}\right] \geq -\mathbb{E}_{q(\mathbf{x}_0)} \log p_\theta(\mathbf{x}_0)
\end{aligned}
$$

Learning Denoising Model -Variational upper bound

- Sohl-Dickstein et al. ICML 2015 and Ho et al. NeurIPS 2020 show that:

$$
\begin{aligned}
L &= \mathbb{E}_{q(\mathbf{x}_{0:T})}\Big[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})}\Big] \\
&= \mathbb{E}_q\Big[\log \frac{\prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})}{p_\theta(\mathbf{x}_T)\prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}\Big] \\
&= \mathbb{E}_q\Big[-\log p_\theta(\mathbf{x}_T) + \sum_{t=1}^{T}\log \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}\Big] \\
&= \mathbb{E}_q\Big[-\log p_\theta(\mathbf{x}_T) + \sum_{t=2}^{T}\log \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)} + \log \frac{q(\mathbf{x}_1|\mathbf{x}_0)}{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}\Big] \\
&= \mathbb{E}_q\Big[-\log p_\theta(\mathbf{x}_T) + \sum_{t=2}^{T}\log \Big(\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}\cdot\frac{q(\mathbf{x}_t|\mathbf{x}_0)}{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}\Big) + \log \frac{q(\mathbf{x}_1|\mathbf{x}_0)}{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}\Big] \\
&= \mathbb{E}_q\Big[-\log p_\theta(\mathbf{x}_T) + \sum_{t=2}^{T}\log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)} + \sum_{t=2}^{T}\log \frac{q(\mathbf{x}_t|\mathbf{x}_0)}{q(\mathbf{x}_{t-1}|\mathbf{x}_0)} + \log \frac{q(\mathbf{x}_1|\mathbf{x}_0)}{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}\Big] \\
&= \mathbb{E}_q\Big[-\log p_\theta(\mathbf{x}_T) + \sum_{t=2}^{T}\log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)} + \log \frac{q(\mathbf{x}_T|\mathbf{x}_0)}{q(\mathbf{x}_1|\mathbf{x}_0)} + \log \frac{q(\mathbf{x}_1|\mathbf{x}_0)}{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}\Big] \\
&= \mathbb{E}_q\Big[\log \frac{q(\mathbf{x}_T|\mathbf{x}_0)}{p_\theta(\mathbf{x}_T)} + \sum_{t=2}^{T}\log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)} - \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)\Big] \\
&= \mathbb{E}_q[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0)\parallel p_\theta(\mathbf{x}_T))}_{L_T} + \sum_{t=2}^{T}\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)\parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}}\underbrace{-\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}]
\end{aligned}
$$

Total loss

$$
\begin{aligned}
L &= L_T + L_{T-1} + \cdots + L_0 \\
\text{where } L_T &= D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0)\parallel p_\theta(\mathbf{x}_T)) \\
L_{t-1} &= D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)\parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)) \text{ for } 2\le t\le T \\
L_0 &= -\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)
\end{aligned}
$$

Parameterizing the Denoising Model

Since both $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ and $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ are Normal distributions, the KL divergence has a simple form:

$$L_{t-1} = D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)) = \mathbb{E}_q \left[\frac{1}{2\sigma_t^2} ||\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_\theta(\mathbf{x}_t, t)||^2 \right] + C$$

Recall that $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\, \mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\, \epsilon$. Ho et al. NeurIPS 2020 observe that:

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

They propose to represent the mean of the denoising model using a *noise-prediction* network:

$$\mu_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{1-\beta_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon_\theta(\mathbf{x}_t, t) \right)$$

With this parameterization

$$L_{t-1} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[\frac{\beta_t^2}{2\sigma_t^2 (1-\beta_t)(1-\bar{\alpha}_t)} ||\epsilon - \epsilon_\theta(\underbrace{\sqrt{\bar{\alpha}_t}\, \mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\, \epsilon}_{\mathbf{x}_t}, t)||^2 \right] + C$$

Objective Weighting: Trading likelihood for perceptual quality

$$L_{t-1} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[\underbrace{\frac{\beta_t^2}{2\sigma_t^2(1-\beta_t)(1-\bar{\alpha}_t)}}_{\lambda_t} ||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\ \mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\ \epsilon, t)||^2 \right]$$

- The time dependent λ_t ensures that the training objective is weighted properly for the maximum data likelihood training.
- However, this weight is often very large for small t's.
- Ho et al. NeurIPS 2020 observe that simply setting $\lambda_t = 1$ improves sample quality. So, they propose to use:

$$L_{\text{simple}} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), t \sim \mathcal{U}(1,T)} \left[||\epsilon - \epsilon_\theta(\underbrace{\sqrt{\bar{\alpha}_t}\ \mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\ \epsilon}_{\mathbf{x}_t}, t)||^2 \right]$$

For more advanced weighting see Choi et al., Perception Prioritized Training of Diffusion Models, CVPR 2022.

Summary: Training and Sample Generation

Algorithm 1 Training

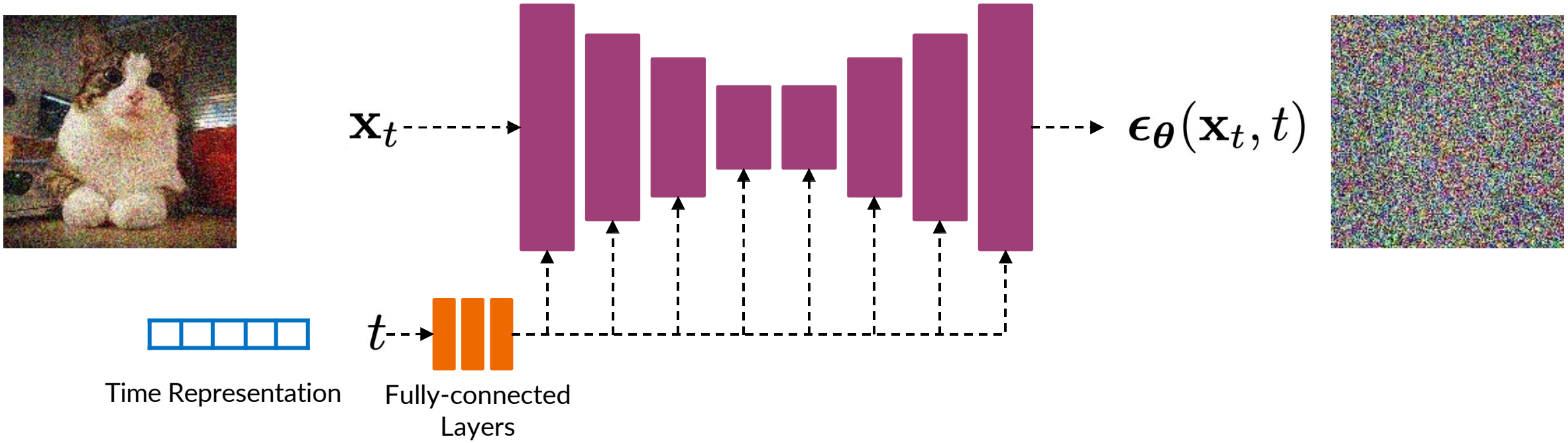
1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(\{1, \dots, T\})$
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: Take gradient descent step on
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0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

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \dots, 1$ **do**
3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
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** $\mathbf{x}_0$

Implementation Considerations - Network Architectures

- Diffusion models often use U-Net architectures with ResNet blocks and self-attention layers for $\epsilon_\theta(\mathbf{x}_t, t)$



Time representation: sinusoidal positional embeddings or random Fourier features.

Time features are fed to the residual blocks using either simple spatial addition or using adaptive group normalization layers. (see Dharivwal and Nichol NeurIPS 2021)

Diffusion Parameters - Noise Schedule

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

Data

Noise

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \sigma_t^2\mathbf{I})$$

β_t and σ_t^2 control the variance of the forward diffusion and reverse denoising processes.

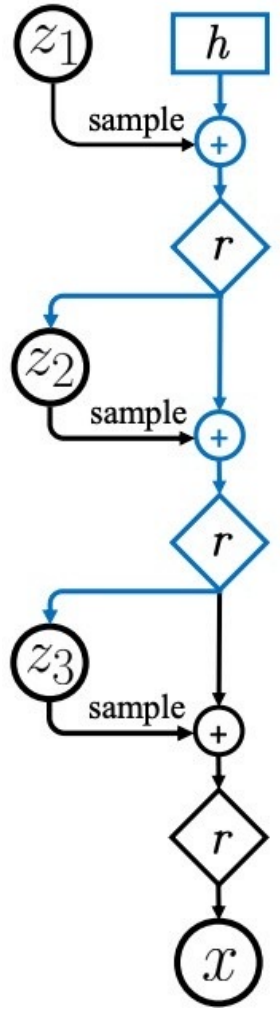
Often a linear schedule is used for β_t. And σ_t^2 is set equal to β_t.

Kingma et al. NeurIPS 2022 introduce a new parameterization of diffusion models using signal-to-noise ratio (SNR) and show how to learn the noise schedule by minimizing the variance of the training objective.

We can also train σ_t^2 while training the diffusion model by minimizing the variational bound (Improved DPM) or after training the diffusion model (Analytic-DPM by Bao et al. ICLR 2022).

Connection to VAEs

- Diffusion models can be considered as a special form of hierarchical VAEs.
- However, in diffusion models:
  - The encoder is fixed
  - The latent variables have the same dimension as the data
  - The denoising model is shared across different timestep
  - The model is trained with some reweighting of the variational bound.



Vahdat and Kautz, NVAE: A Deep Hierarchical Variational Autoencoder, NeurIPS 2020
Sønderby, et al.. Ladder variational autoencoders, NeurIPS 2016.

Summary: Denoising Diffusion Probabilistic Models

- In this part, we reviewed denoising diffusion probabilistic models.
- The model is trained by sampling from the forward diffusion process and training a denoising model to predict the noise. We discussed how the forward process perturbs the data distribution or data samples.
- The devil is in the details:
  - Network architectures
  - Objective weighting
  - Diffusion parameters (i.e., noise schedule)
- See "Elucidating the Design Space of Diffusion-Based Generative Models" by Karras et al. for important design decisions.

Practice

Diffusion Models Tutorial Google Colab

Part (2): Conditional Generation and Guidance

Impressive Results

DALL·E 2

"a propaganda poster depicting a cat dressed as french emperor napoleon holding a piece of cheese"

IMAGEN

"A photo of a raccoon wearing an astronaut helmet, looking out of the window at night."

"Hierarchical Text-Conditional Image Generation with CLIP Latents" Ramesh et al., 2022

"Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", Saharia et al., 2022

How to Control Diffusion Models

Explicit Conditioning

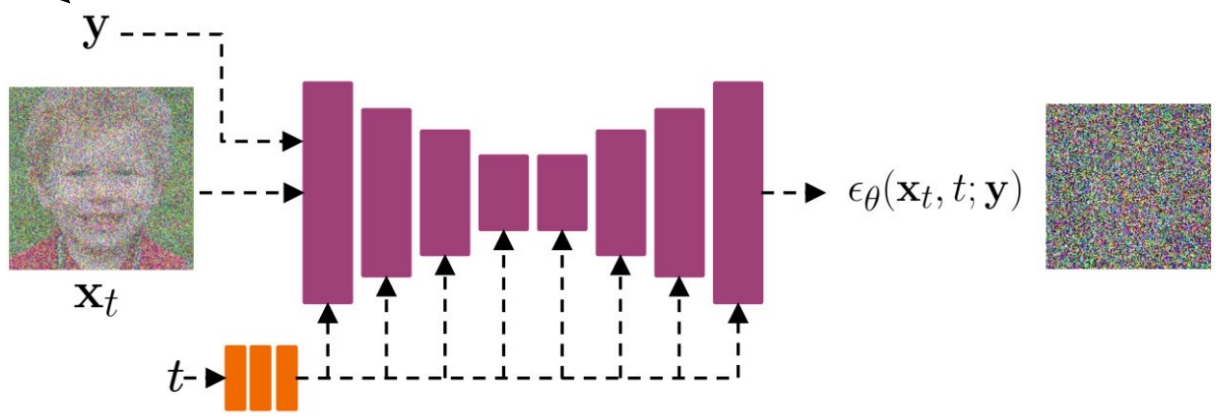
Classifier Guidance

Classifier-Free Guidance

How to Control Diffusion Models

Explicit Conditioning

"a young schoolboy in a red shirt"



Explicit Conditioning

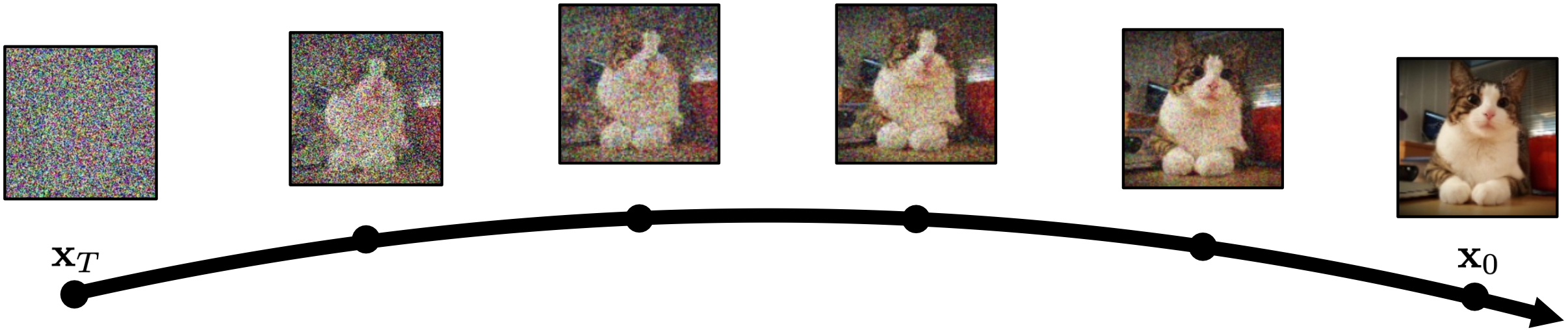
- How do we train this?
- Use an Image-Text dataset (for example, LAION 5B)
- Loss function:

$$\mathbb{E}_{(\mathbf{x},\mathbf{y})\sim p_{\text{data}}(\mathbf{x},\mathbf{y})}\mathbb{E}_{\epsilon\sim\mathcal{N}(\mathbf{0},\mathbf{I})}\mathbb{E}_{t\sim\mathcal{U}[0,T]}\ ||\epsilon_\theta(\mathbf{x}_t, t; \mathbf{y}) - \epsilon||_2^2$$

How to Control Diffusion Models

Classifier Guidance

Diffusion goes from noise to real images step-by-step



Idea: Perturb the Denoising Trajectory

Classifier Guidance: Bayes' Rule in Action

- When sampling from a conditional model $p(\boldsymbol{x}\,|\boldsymbol{y})$, we need to estimate $\nabla_{\mathbf{x_t}} \log p(\boldsymbol{x}_t|\boldsymbol{y})$
- Using Bayes' rule, we have:

Classifier gradient

Score model

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}) = \nabla_{\mathbf{x}_t} \log \frac{p(\mathbf{y}|\mathbf{x}_t)p(\mathbf{x}_t)}{p(\mathbf{y})} = \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) + \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$$

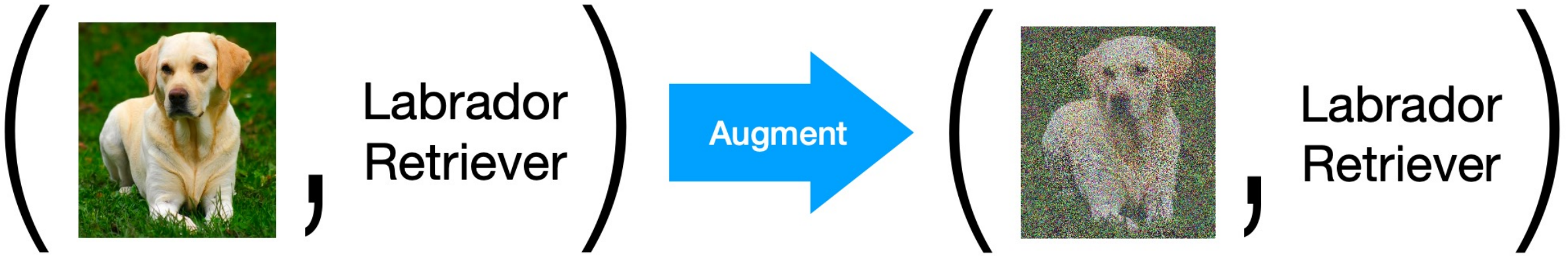
- Introduce a guidance scale (*w*):

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}) \approx w\nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) + \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$$

$$\left(\; p(\mathbf{x}_t|\mathbf{y}) \propto p(\mathbf{y}|\mathbf{x}_t)^w p(\mathbf{x}_t) \; \right)$$

Classifier Guidance

- **Problem:** Classifier isn't trained on noisy images!
- **Solution:** Finetune the classifier on noisy images



Classifier Guidance

Guidance Weight 1.0

Guidance Weight 10.0

Dhariwal and Nichol, "Diffusion Models Beat GANs on Image Synthesis"

Problems with Classifier Guidance

- Need to fine-tune or re-train a classifier on **noisy** data
- Need a pre-trained classification model
  - Classifier gradients are poor.
- What if we want to use *any* text prompt as input?

How to Control Diffusion Models

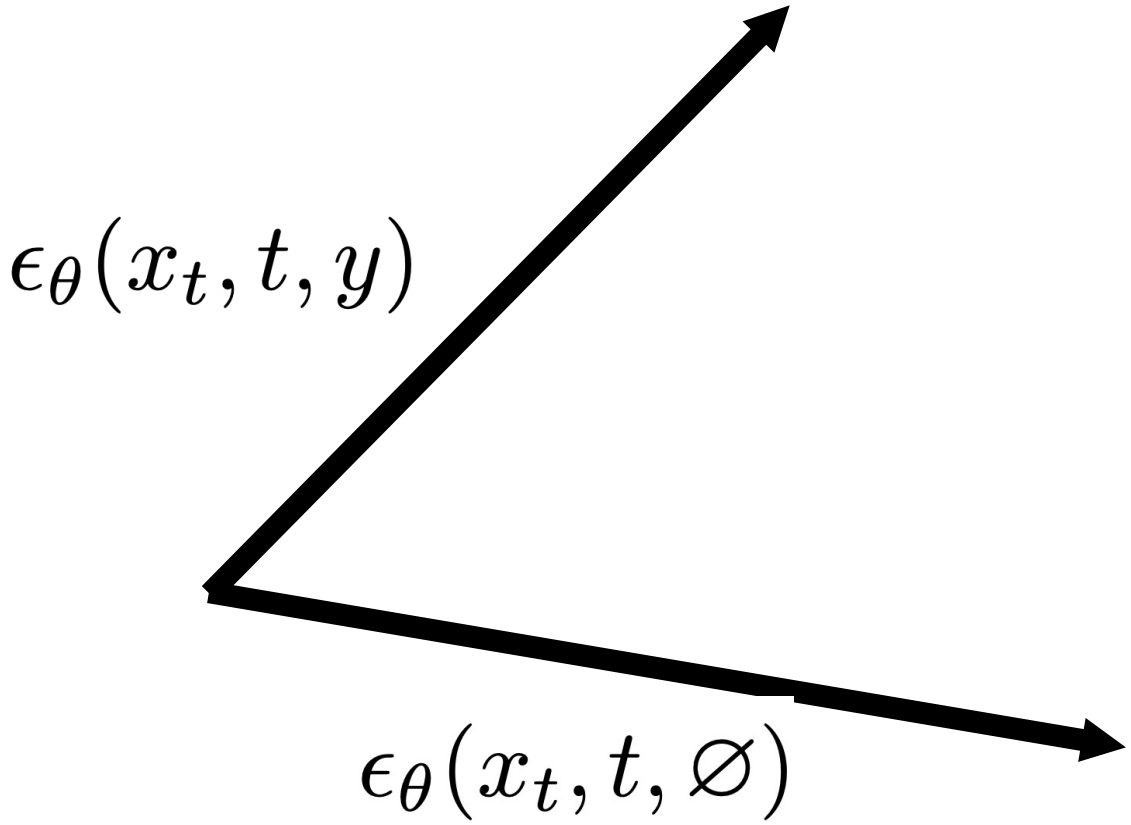
Classifier Free Guidance

- Idea: Use the diffusion model itself to get perturbations for guidance
- Train an explicitly conditioned diffusion model: $\epsilon_\theta(x_t, t, y)$

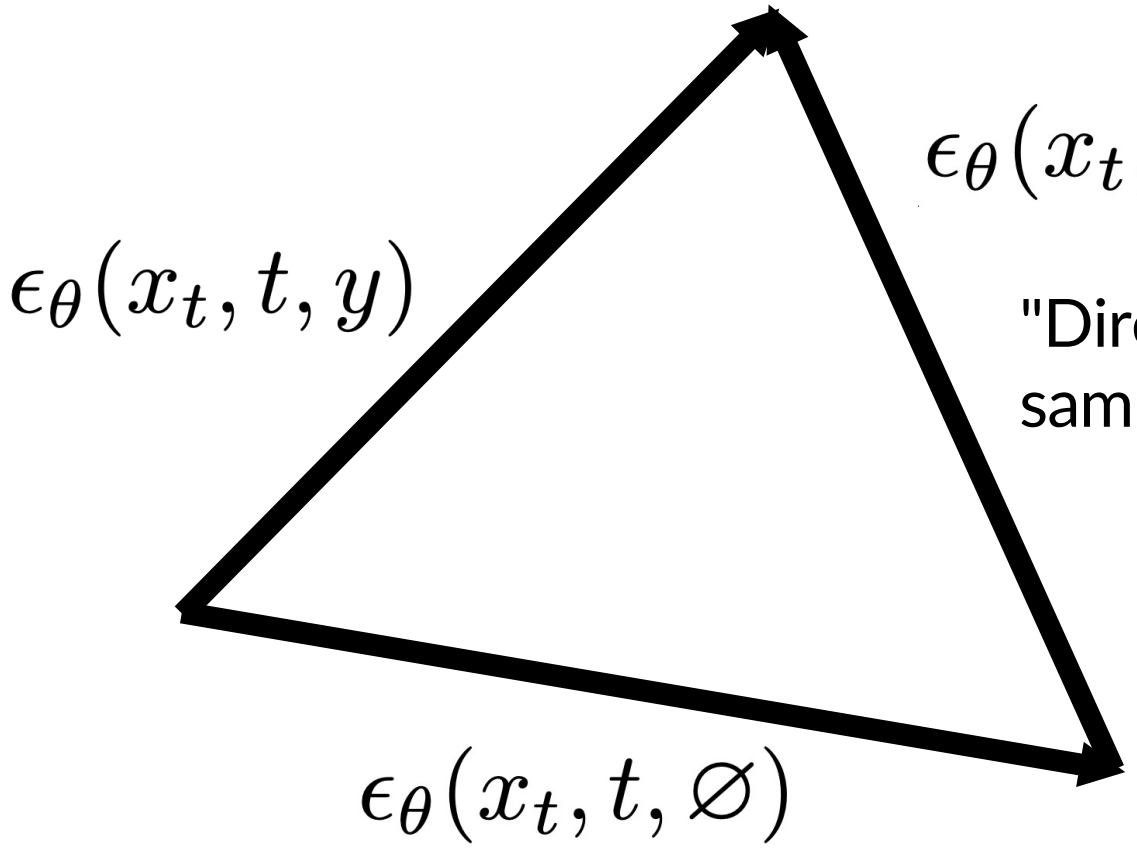
- But also train it to be **unconditional**

- We can do this with *conditioning dropout*: $\epsilon_\theta(x_t, t, \varnothing)$

Classifier Free Guidance



Classifier Free Guidance



$$\epsilon_\theta(x_t, t, y) - \epsilon_\theta(x_t, t, \varnothing)$$

"Direction" from unconditional sample to conditional sample

Use this as our guidance perturbation

Classifier Free Guidance

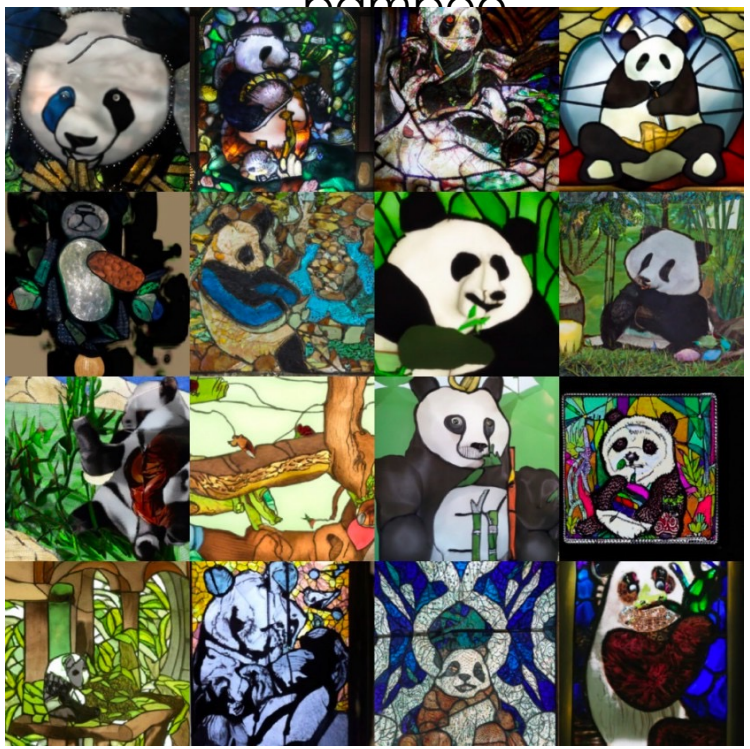
- Our new noise estimate will then be:

$$\tilde{\epsilon}(x_t, t, y) = \epsilon_\theta(x_t, t, \varnothing) + \gamma(\epsilon_\theta(x_t, t, y) - \epsilon_\theta(x_t, t, \varnothing))$$

"Direction" from unconditional to conditional

Classifier Free Guidance

"A stained glass window of a panda eating bamboo"



$\gamma = 1$

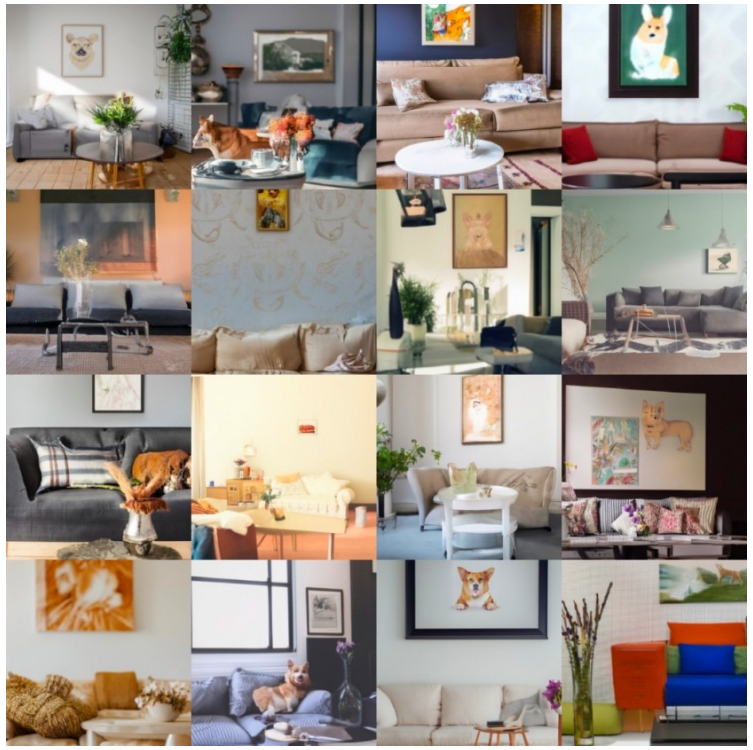
Equivalent to explicit conditioning.
No guidance

$\gamma = 3$

Nichol et al. "GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models"

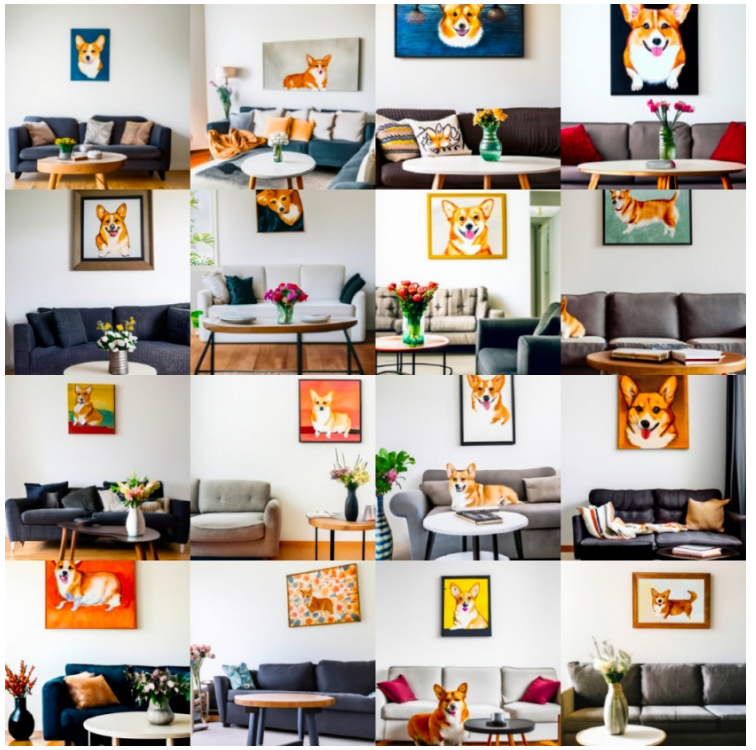
Classifier Free Guidance

"A cozy living room with a painting of a corgi on the wall above a couch and a round coffee table in front of a couch and a vase of flowers on a coffee table "



$\gamma = 1$

Equivalent to explicit conditioning.
No guidance



$\gamma = 3$

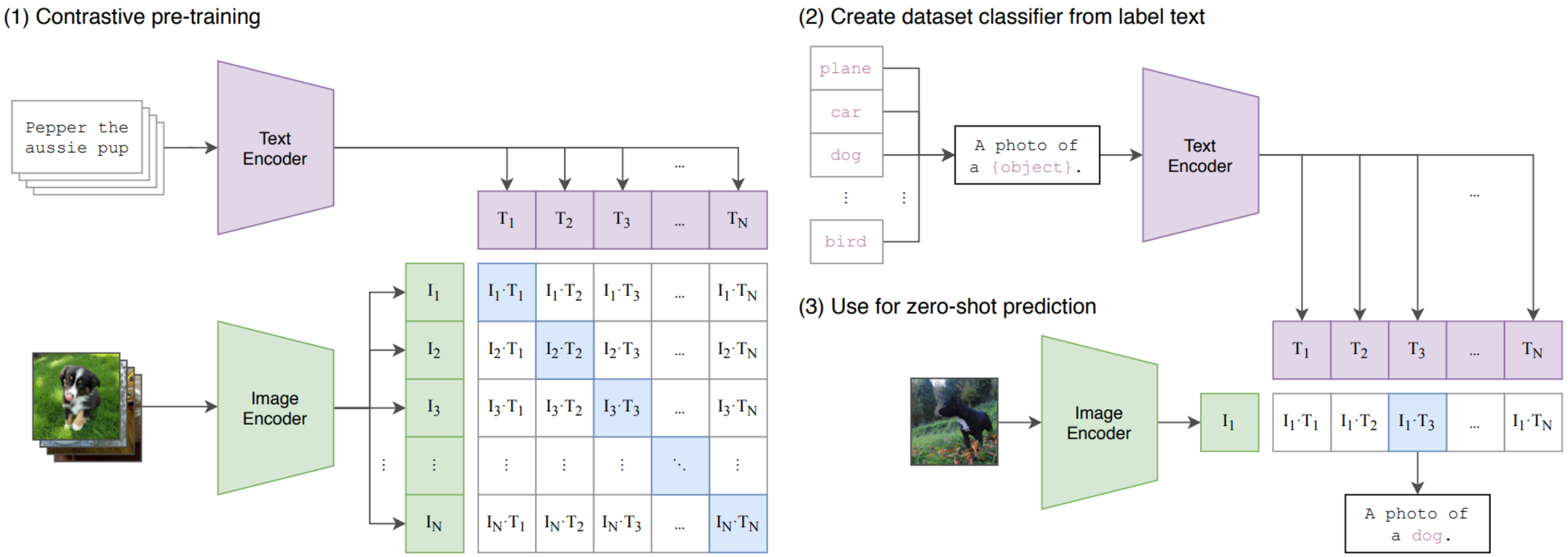
Nichol et al. "GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models"

More Resources

- Lilian Weng Tutorial: https://lilianweng.github.io/posts/2021-07-11-diffusion- models/
- Guidance Tutorial by Sander Dieleman: https://sander.ai/2022/05/26/ guidance.html

Part (3): Text-to-image Diffusion Models

CLIP Model

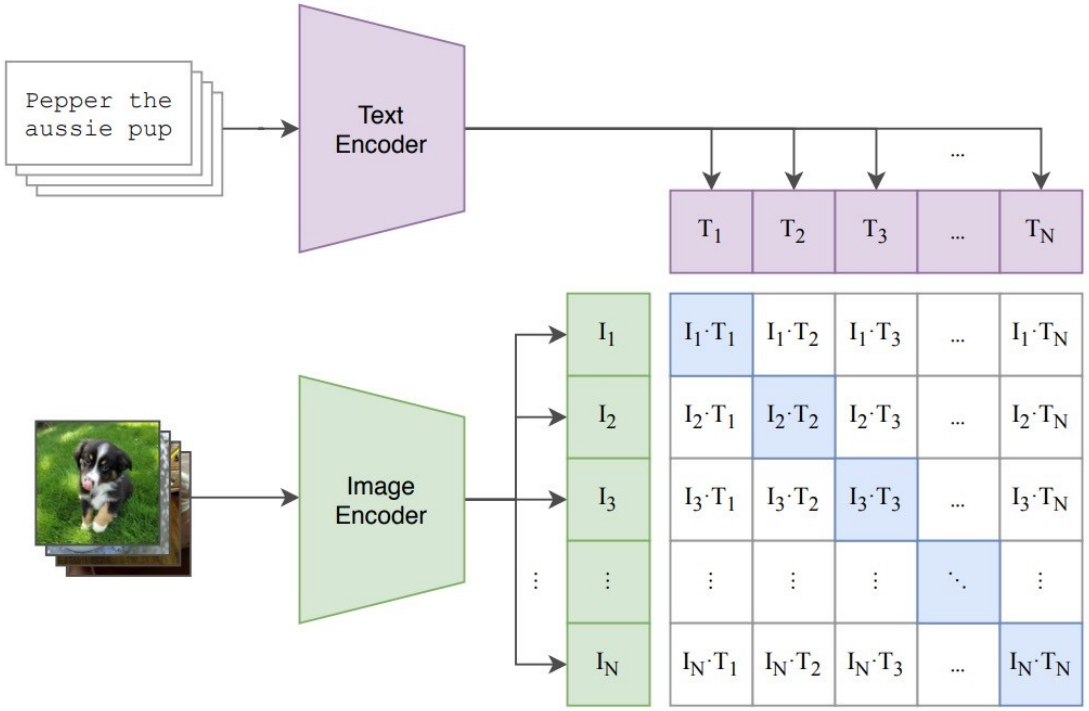


Radford et al., "Learning Transferable Visual Models From Natural Language Supervision", 2021.

CLIP guidance - What is a CLIP model?

- Trained by contrastive cross-entropy loss:

$$-\log \frac{\exp(f(\mathbf{x}_i)\cdot g(\mathbf{c}_j)/\tau)}{\sum_k \exp(f(\mathbf{x}_i)\cdot g(\mathbf{c}_k)/\tau)} - \log \frac{\exp(f(\mathbf{x}_i)\cdot g(\mathbf{c}_j)/\tau)}{\sum_k \exp(f(\mathbf{x}_k)\cdot g(\mathbf{c}_j)/\tau)}$$



- The optimal value of $f(\mathbf{x})\cdot g(\mathbf{c})$ is

$$\log \frac{p(\mathbf{x},\mathbf{c})}{p(\mathbf{x})p(\mathbf{c})} = \log p(\mathbf{c}|\mathbf{x}) - \log p(\mathbf{c})$$

Radford et al., “Learning Transferable Visual Models From Natural Language Supervision”, 2021.
Nichol et al., “GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models”, 2021.

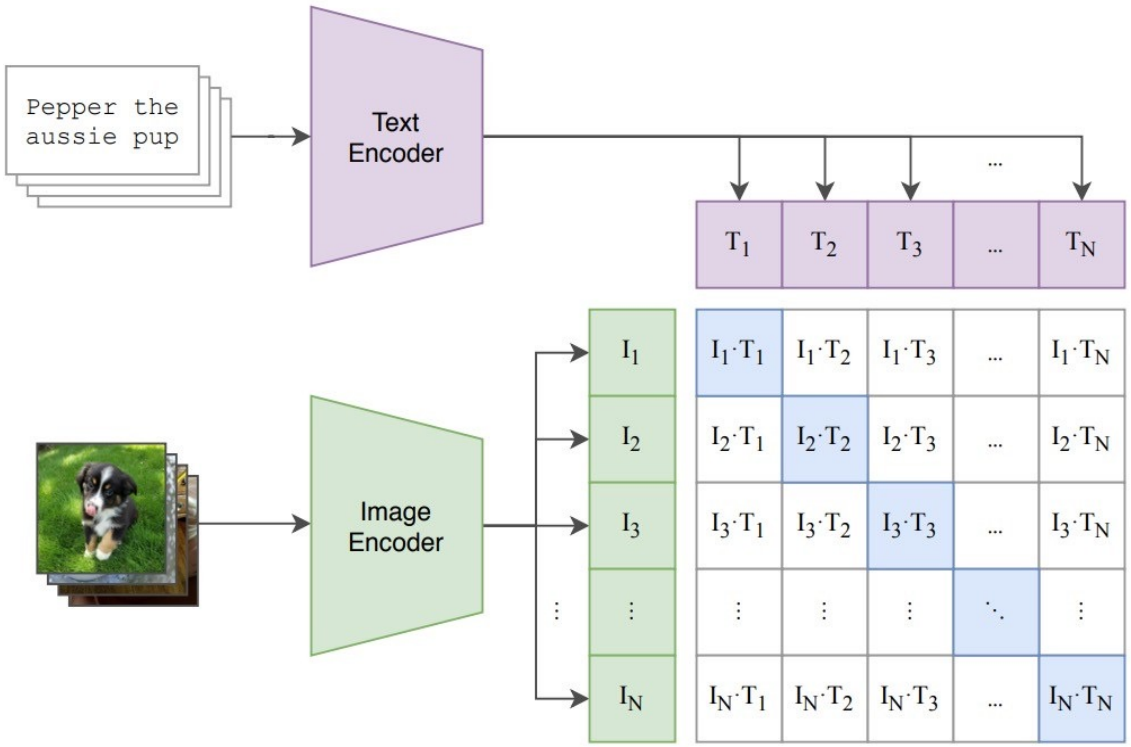
Replace the classifier with a CLIP model

- Sample with a modified score:

$$\nabla_{\mathbf{x}_t}[\log p(\mathbf{x}_t|\mathbf{c}) + \omega \log p(\mathbf{c}|\mathbf{x}_t)]$$

$$= \nabla_{\mathbf{x}_t}[\log p(\mathbf{x}_t|\mathbf{c}) + \omega(\underbrace{\log p(\mathbf{c}|\mathbf{x}_t) - \log p(\mathbf{c})}_{\text{CLIP model}})]$$

$$= \nabla_{\mathbf{x}_t}[\log p(\mathbf{x}_t|\mathbf{c}) + \omega(f(\mathbf{x}_t) \cdot g(\mathbf{c}))]$$



Radford et al., “Learning Transferable Visual Models From Natural Language Supervision”, 2021.
Nichol et al., “GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models”, 2021.

GLIDE - OpenAI

- A 64x64 base model + a 64x64 → 256x256 super-resolution model.
- Classifier-free guidance works better than CLIP guidance.

"a hedgehog using a calculator"

"a corgi wearing a red bowtie and a purple party hat"

"robots meditating in a vipassana retreat"

"a fall landscape with a small cottage next to a lake"

Samples generated with classifier-free guidance (256x256)

Nichol et al., "GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models", 2021.

GLIDE - OpenAI

- Fine-tune the model especially for inpainting: feed randomly occluded images with an additional mask channel as the input.

"an old car in a snowy forest"

"a man wearing a white hat"

Text-conditional image inpainting examples

Nichol et al., "GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models", 2021.

DALL·E 2 - OpenAI

a shiba inu wearing a beret and black turtleneck

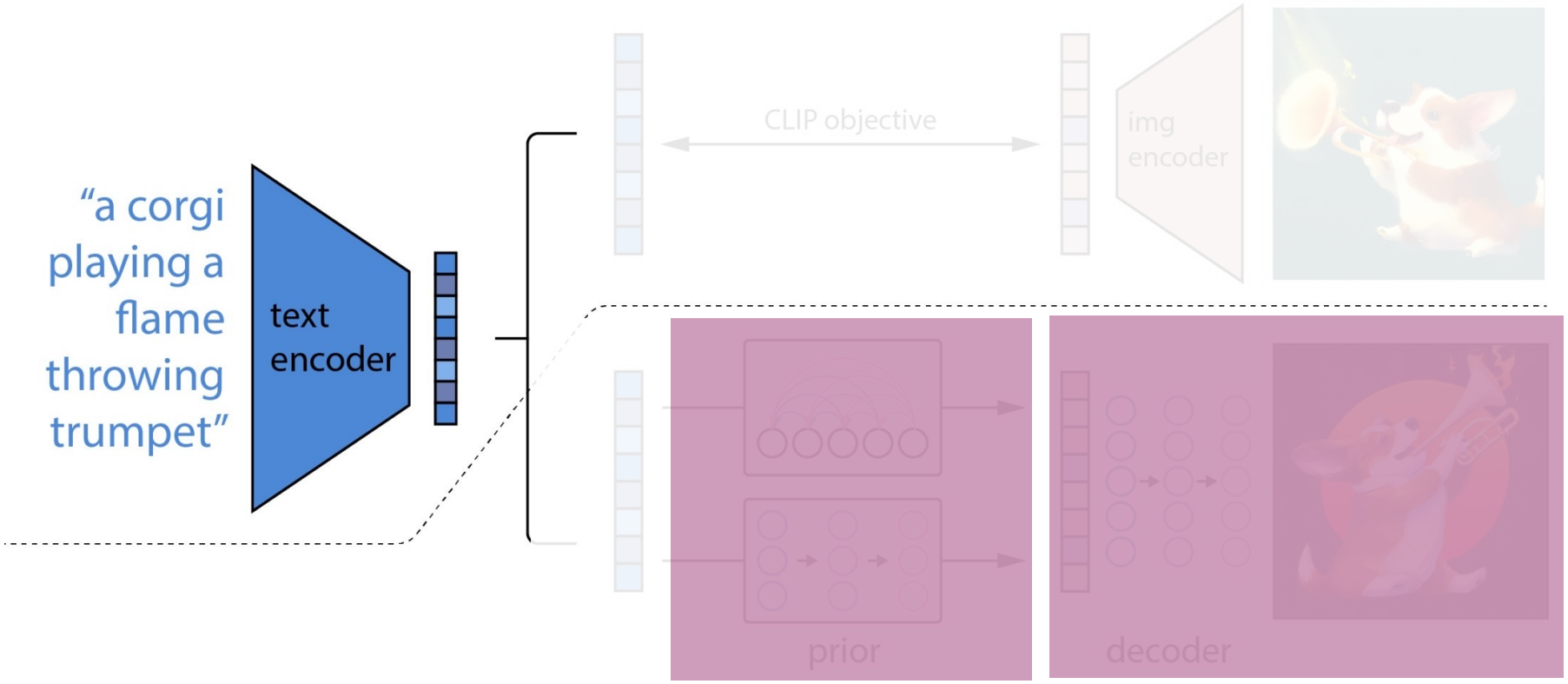
a close up of a handpalm with leaves growing from it

1kx1k Text-to-image generation.

Outperform DALL-E (autoregressive transformer).

Ramesh et al., “Hierarchical Text-Conditional Image Generation with CLIP Latents”, arXiv 2022.

DALL·E 2 - Model components



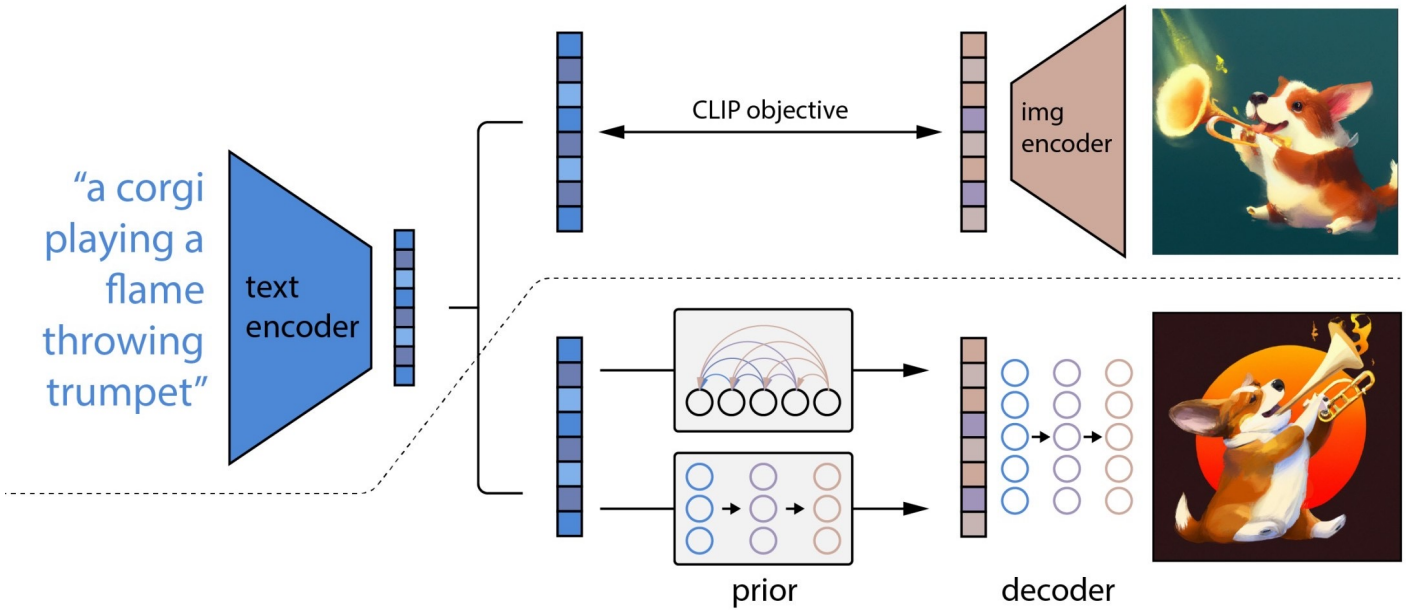
Prior: produces CLIP image embeddings conditioned on the caption.

Decoder: produces images conditioned on CLIP image embeddings and text.

Ramesh et al., "Hierarchical Text-Conditional Image Generation with CLIP Latents", arXiv 2022.

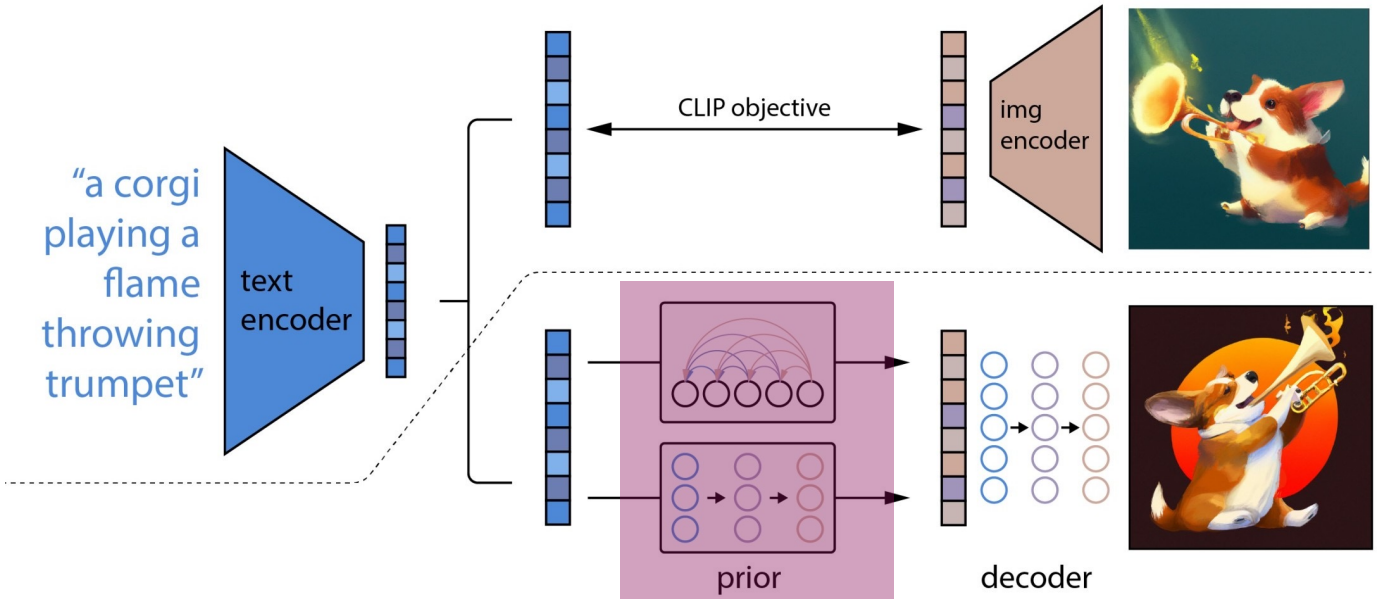
DALL·E 2 - Model components

- Why conditional on CLIP image embeddings?
- CLIP image embeddings capture high-level semantic meaning; latents in the decoder model take care of the rest.
- The bipartite latent representation enables several text-guided image manipulation tasks.



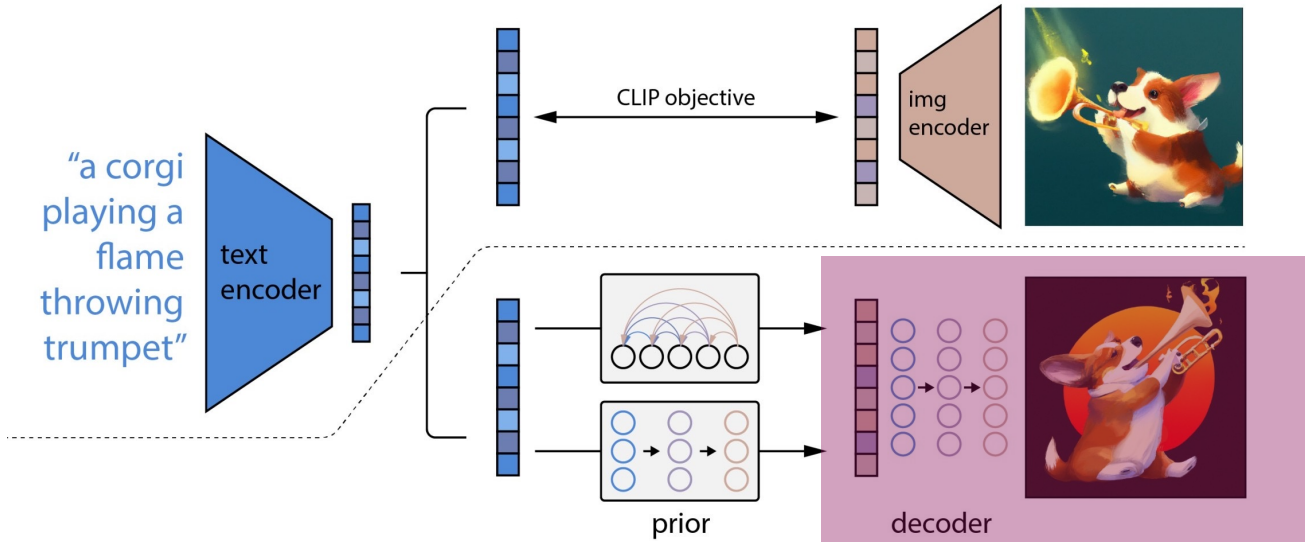
DALL·E 2 - Model components (1/2): prior model

- Prior: produces CLIP image embeddings conditioned on the caption.
- Option 1. autoregressive prior: quantize image embedding to a seq. of discrete codes and predict them autoregressively.
- Option 2. diffusion prior: model the continuous image embedding by diffusion models conditioned on caption.



DALL·E 2 - Model components (2/2): decoder model

- Decoder: produces images conditioned on CLIP image embeddings (and text).
- Cascaded diffusion models: 1 base model (64x64), 2 super-resolution models (64x64 → 256x256, 256x256 → 1024x1024).
- Largest super-resolution model is trained on patches and takes full-res inputs at inference time.
- Classifier-free guidance and noise conditioning augmentation are important.

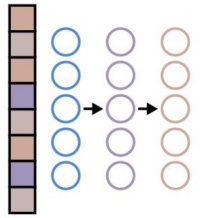


DALL·E 2 - Bipartite latent representations

Bipartite latent representations

z: CLIP image embeddings

$\mathbf{x}_T$: inversion of DDIM sampler (latents in the decoder model)



decoder

Near exact reconstruction

Ramesh et al., “Hierarchical Text-Conditional Image Generation with CLIP Latents”, arXiv 2022.

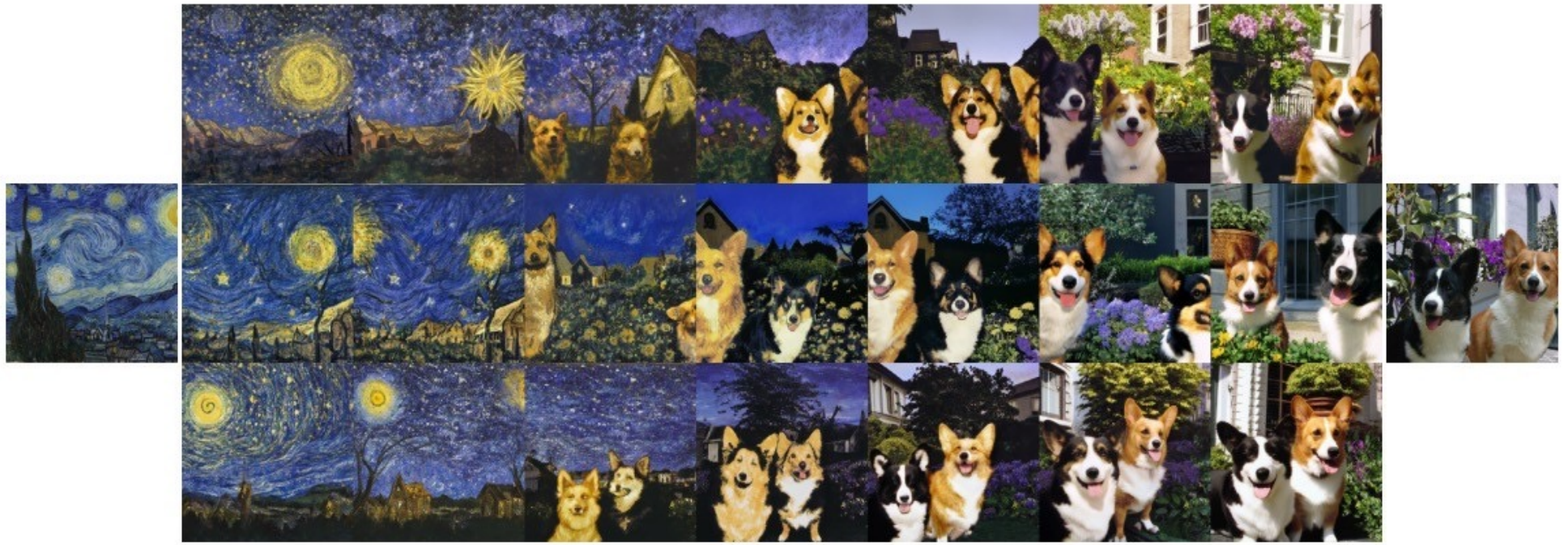
DALL·E 2 - Image variations

Fix the CLIP embedding $\mathbf{z}$.

Decode using different decoder latents $\mathbf{x}_T$

Ramesh et al., “Hierarchical Text-Conditional Image Generation with CLIP Latents”, arXiv 2022.

DALL·E 2 - Image interpolation



Interpolate image CLIP embeddings z.

Use different x_T to get different interpolation trajectories.

Ramesh et al., “Hierarchical Text-Conditional Image Generation with CLIP Latents”, arXiv 2022.

DALL·E 2 – Text Diffs

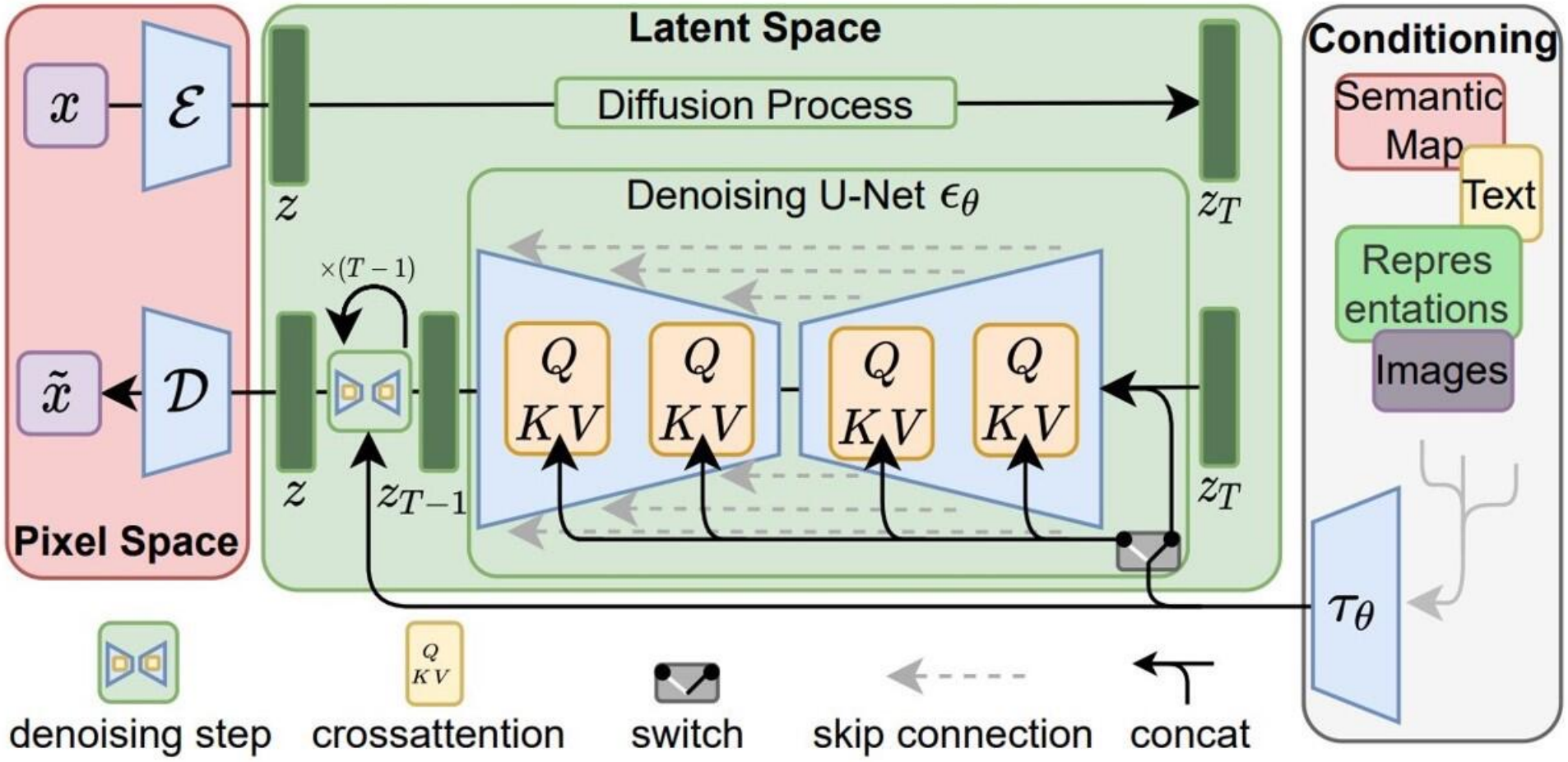
- Change the image CLIP embedding towards the difference of the text CLIP embeddings of two prompts.
- Decoder latent is kept as a constant.

a photo of a cat → an anime drawing of a super saiyan cat, artstation

a photo of a victorian house → a photo of a modern house

a photo of an adult lion → a photo of lion cub

Latent Diffusion Models



Rombach et al., "High-Resolution Image Synthesis with Latent Diffusion Models", CVPR 2022.

Imagen - Google Research, Brain team

- Input: text;
- Output: 1kx1k images
- An unprecedented degree of photorealism
- SOTA automatic scores and human ratings
- A deep level of language understanding
- Extremely simple
- no latent space, no quantization

A brain riding a rocketship heading towards the moon.

Saharia et al., “Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding”, arXiv 2022.

Imagen - Google Research, Brain team

A photo of a Shiba Inu dog with a backpack riding a bike. It is wearing sunglasses and a beach hat.

Saharia et al., “Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding”, arXiv 2022.

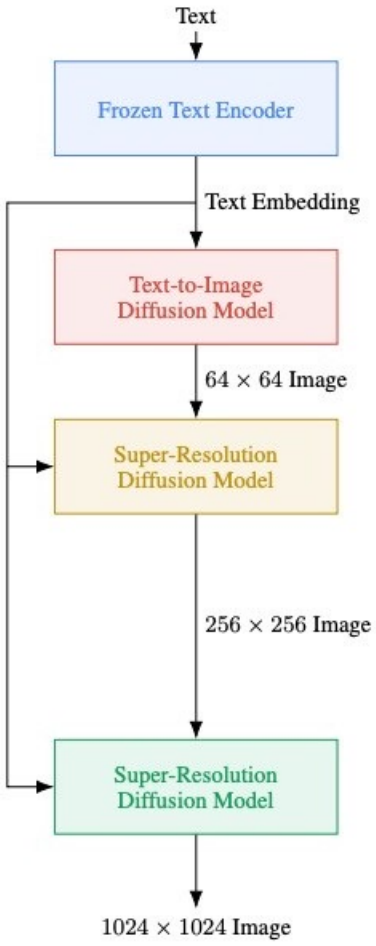
Imagen - Google Research, Brain team

A dragon fruit wearing karate belt in the snow.

Saharia et al., “Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding”, arXiv 2022.

Imagen - Google Research, Brain team

- Key modeling components:
  - Cascaded diffusion models
  - Classifier-free guidance and dynamic thresholding.
  - Frozen large pretrained language models as text encoders. (T5-XXL)



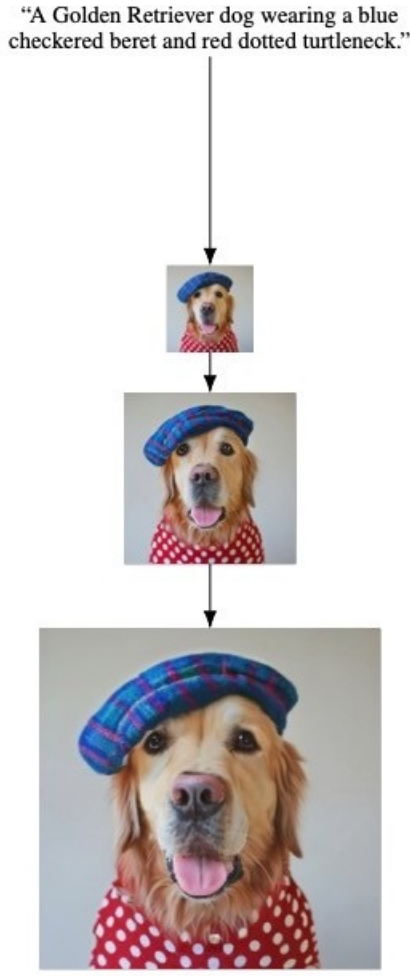
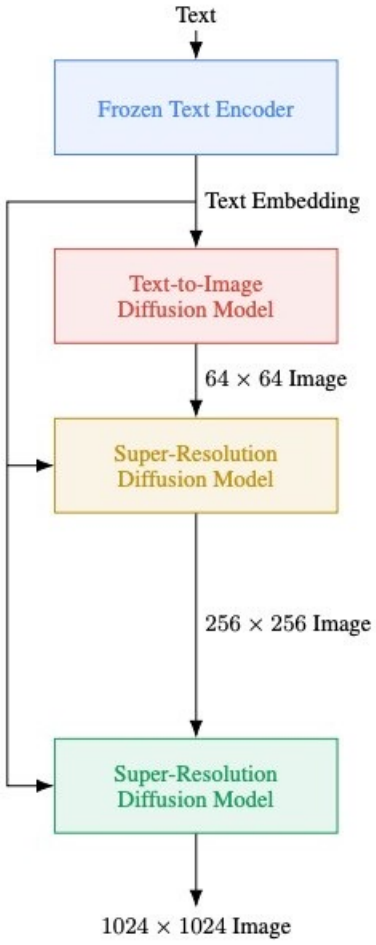


Imagen - Google Research, Brain team

- Key observations:
  - Beneficial to use text conditioning for all super-res models.
    - Noise conditioning augmentation weakens information from low-res models, thus needs text conditioning as extra information input.
  - Scaling text encoder is extremely efficient.
    - More important than scaling diffusion model size.
  - Human raters prefer T5-XXL as the text encoder over CLIP encoder on DrawBench.



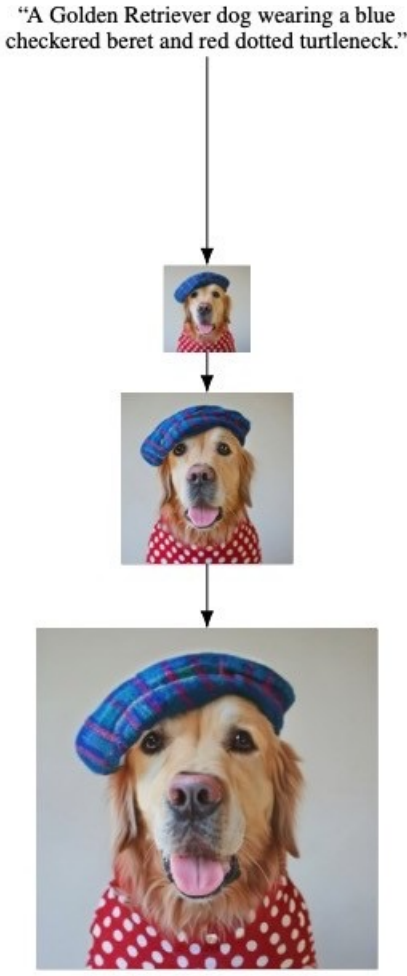
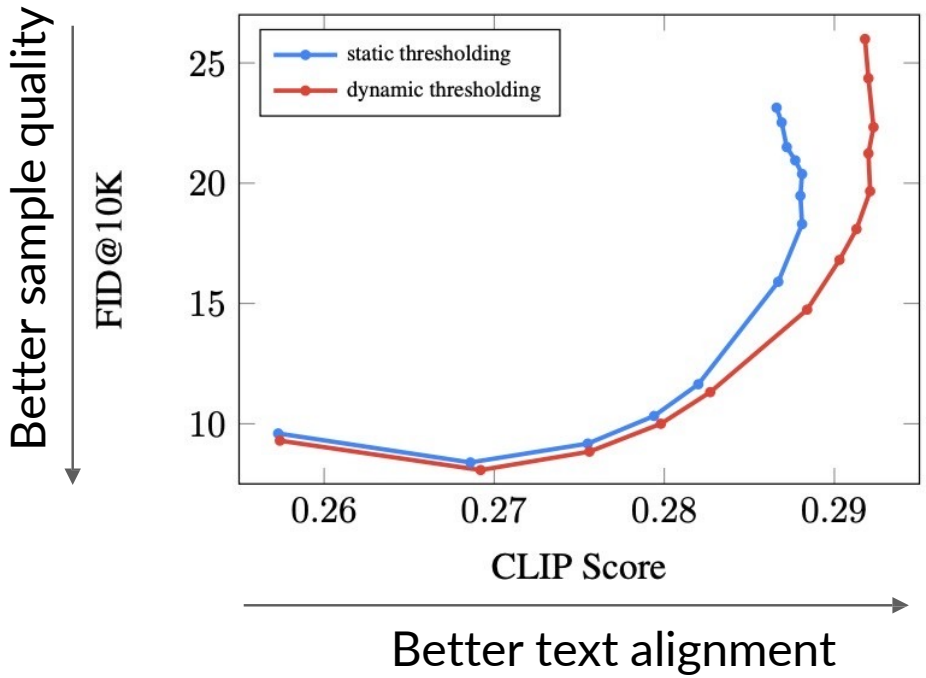


Imagen - Dynamic thresholding

- Large classifier-free guidance weights → better text alignment, worse image quality



Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

Imagen - Dynamic thresholding

- Large classifier-free guidance weights → better text alignment, worse image quality
- Hypothesis : at large guidance weight, the generated images are saturated due to the very large gradient updates during sampling
- Solution – dynamic thresholding: adjusts the pixel values of samples at each sampling step to be within a dynamic range computed over the statistics of the current samples.

Saharia et al., “Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding”, arXiv 2022.

Imagen - Dynamic thresholding

Saharia et al., “Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding”, arXiv 2022.

Reference

- Denoising Diffusion-based Generative Modeling CVPR2022 tutorial
- Denoising Diffusion Models: A Generative Learning Big Bang CVPR2023 tutorial