ITCS 6156/8156 Spring 2024
Machine Learning

Deep Generative Models

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Class Meeting: Mon & Wed, 4:00 PM – 5:15 PM, Denny 109

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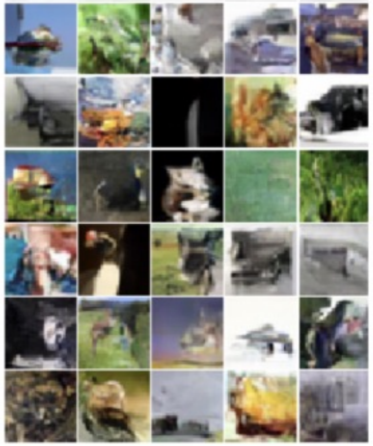
Some content in the slides is based on Dr. Ruohan Gao's lectures

Where We Came From

VAEs, 2013

GANs, 2014

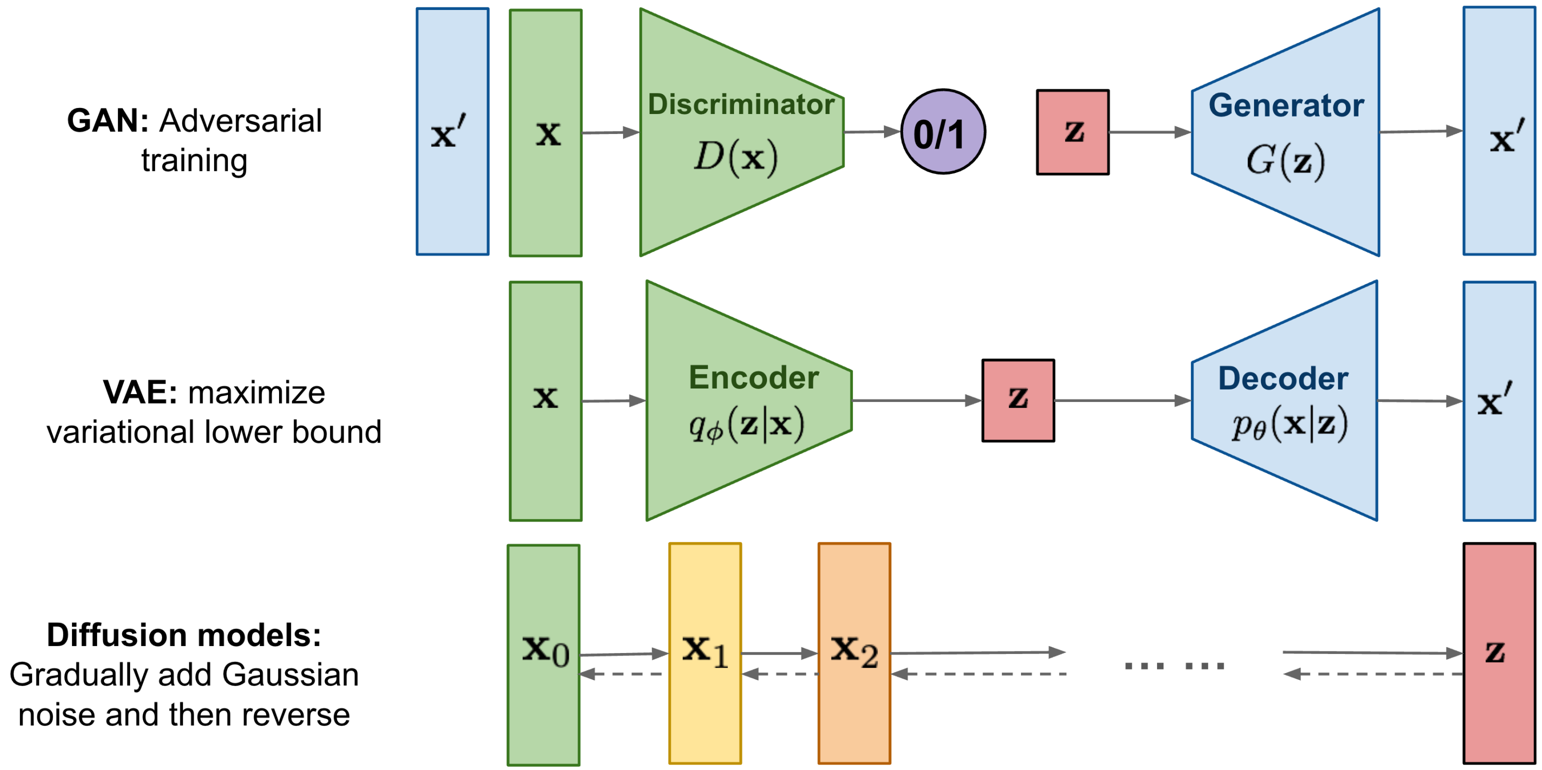
PixelCNN, 2016



BigGAN, 2019

Imagen, 2022

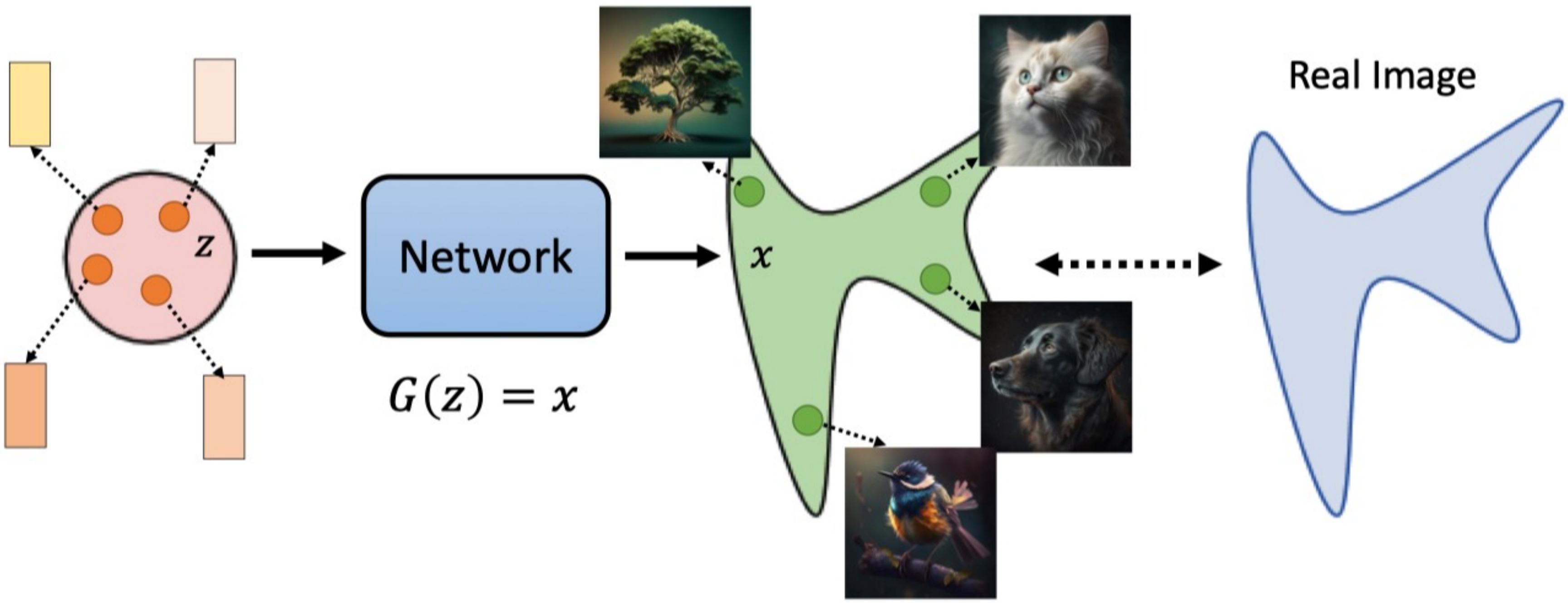
Generative Models



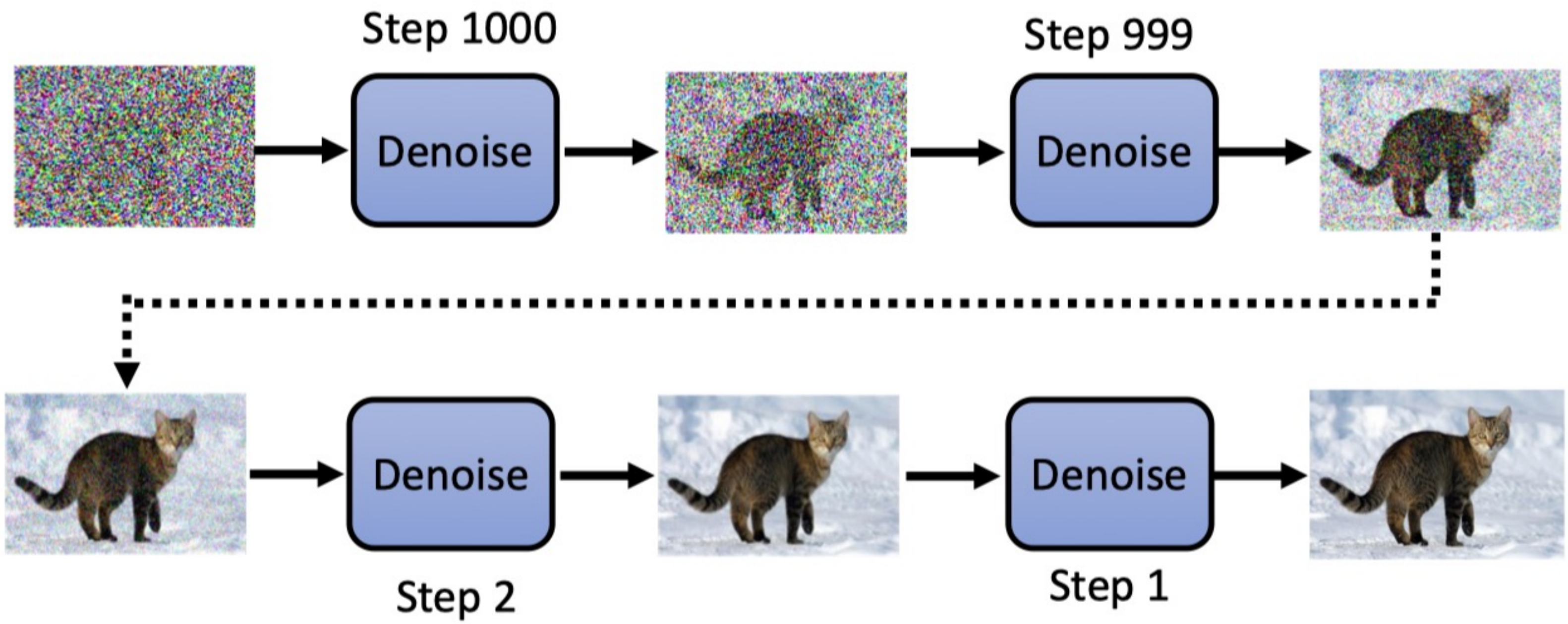
GAN: Hard to train two networks; hard to converge; biased discriminator

Denoising Diffusion Probabilistic Models (DDPM), 2020, https://arxiv.org/abs/2006.11239
Image source: https://lilianweng.github.io/posts/2021-07-11-diffusion-models/

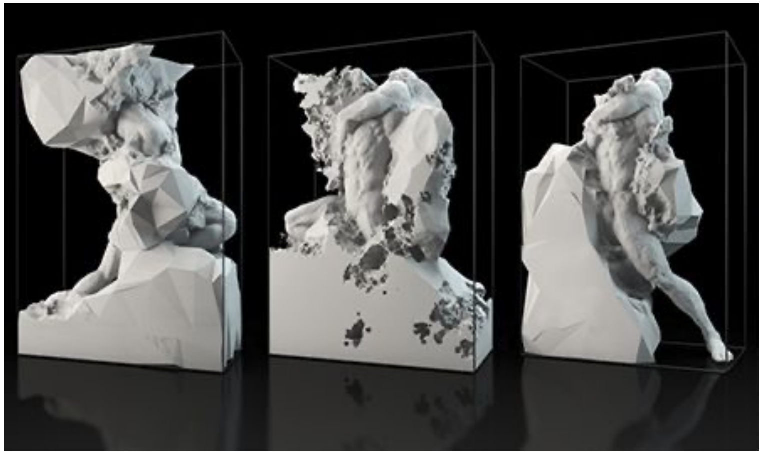
Goal of Generative Model



How the Diffusion Model Works?



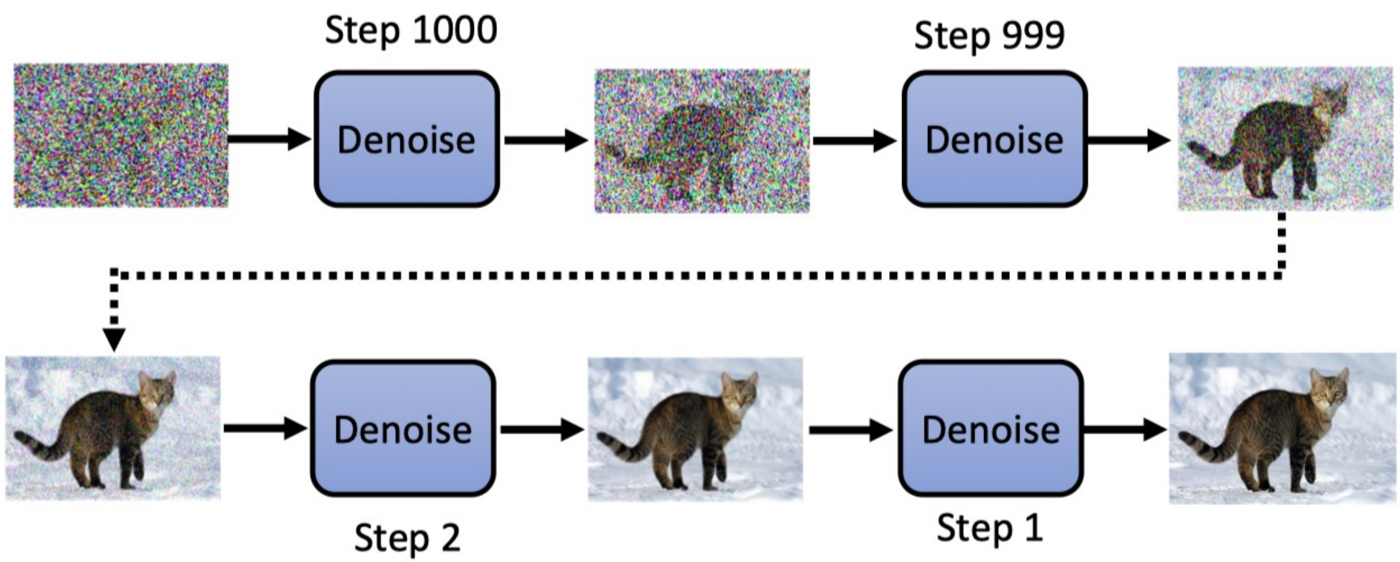
Reverse Process

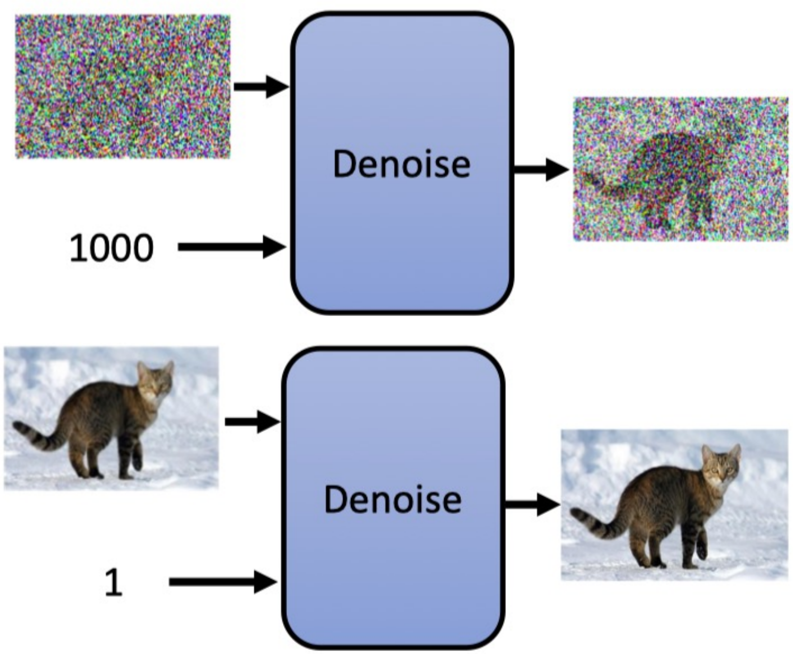


The sculpture is already complete within the marble block, before I start my work. It is already there, I just have to chisel away the superfluous material.

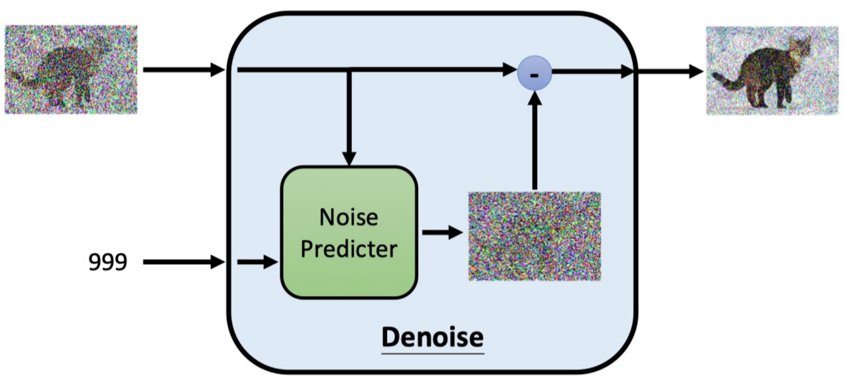
— **Michelangelo**

Denoising (Reverse) Process

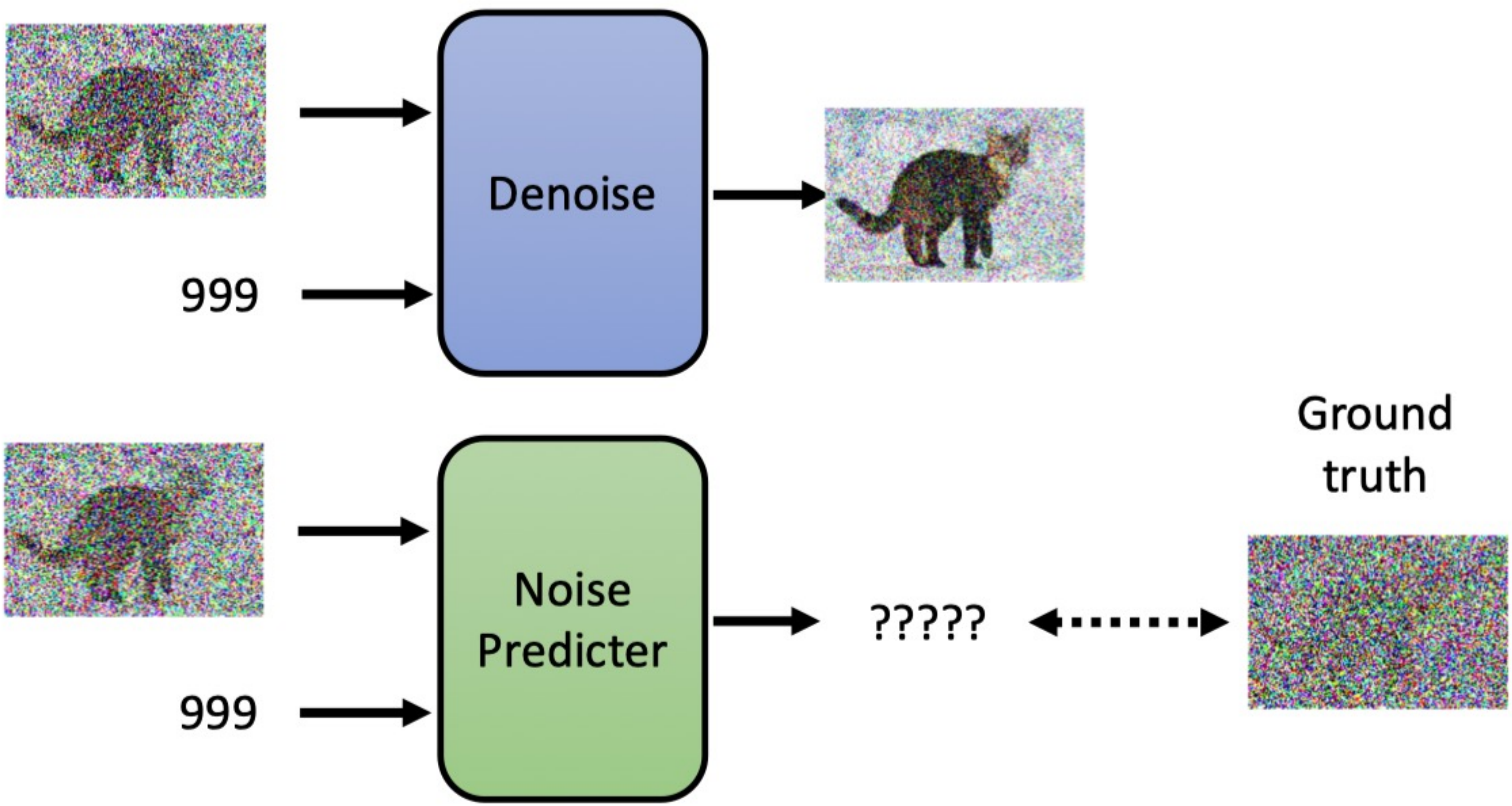




Denoise:

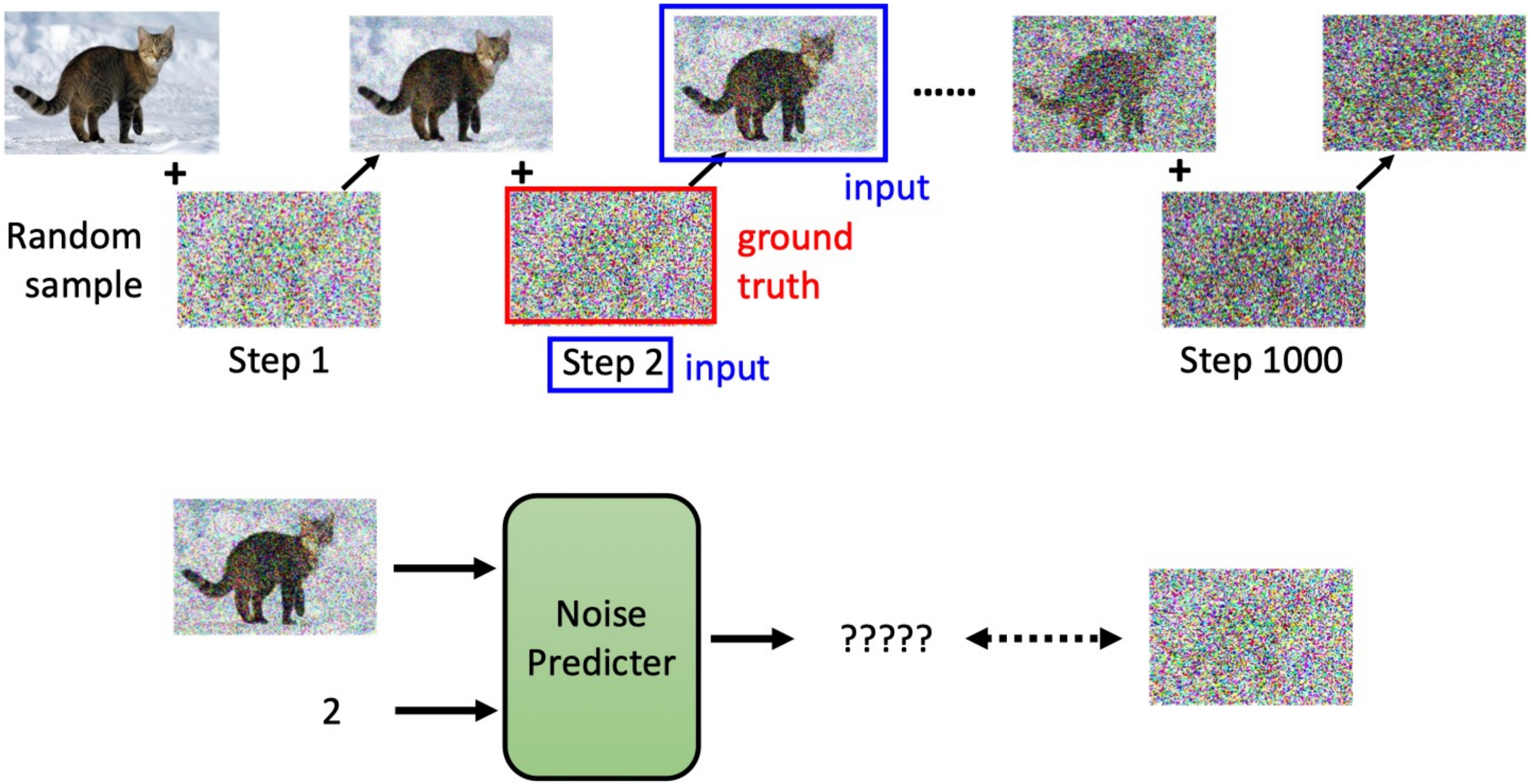


Train a Noise Predictor

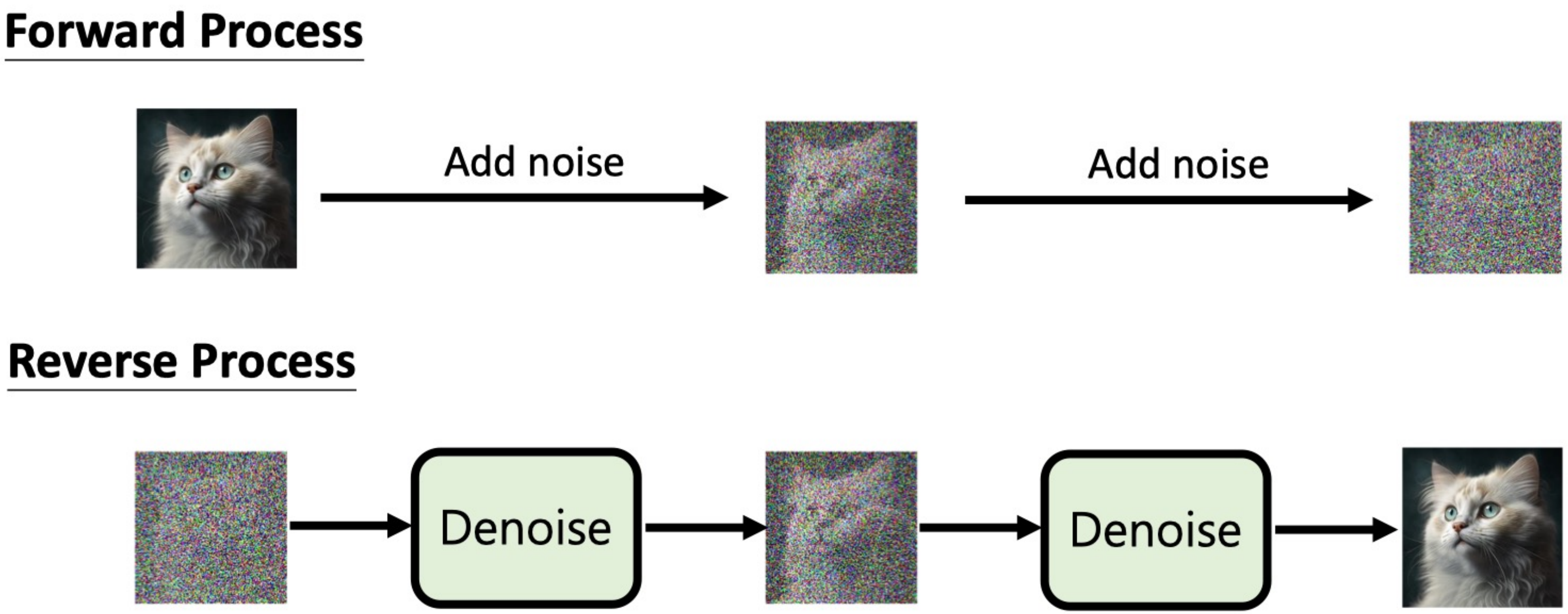


Forward/Diffusion Process

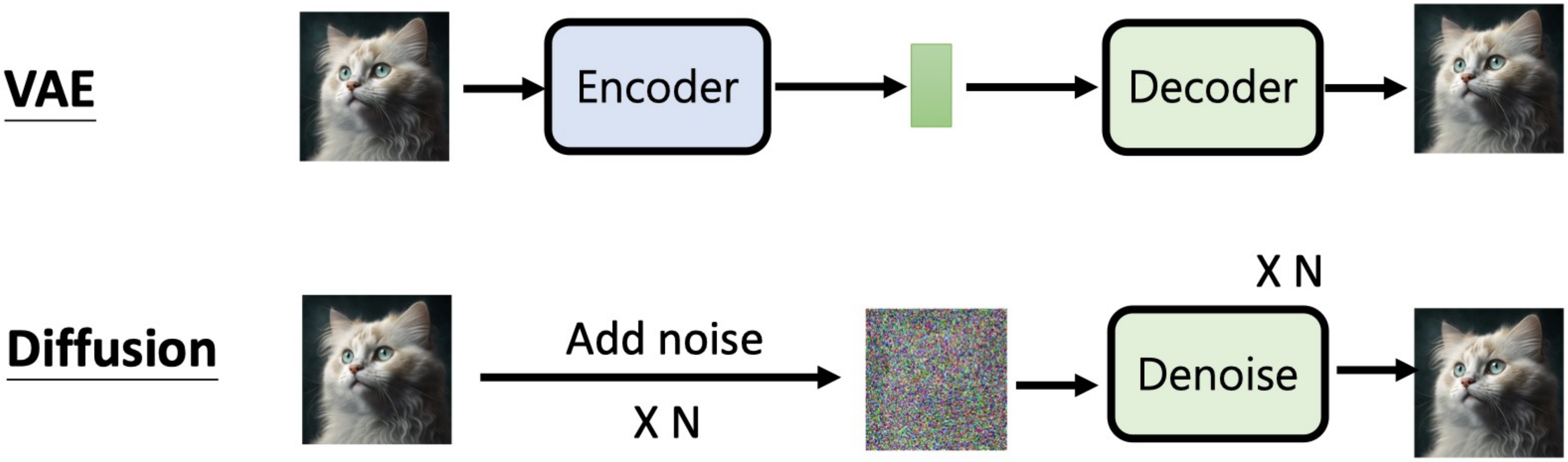
Forward/Diffusion Process:



Diffusion Model



VAE vs. Diffusion Model



Denoising Diffusion Probabilistic Models (DDPM)

Algorithm 1 Training

1: **repeat**
2: $\quad \mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $\quad t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
4: $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: $\quad$ 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

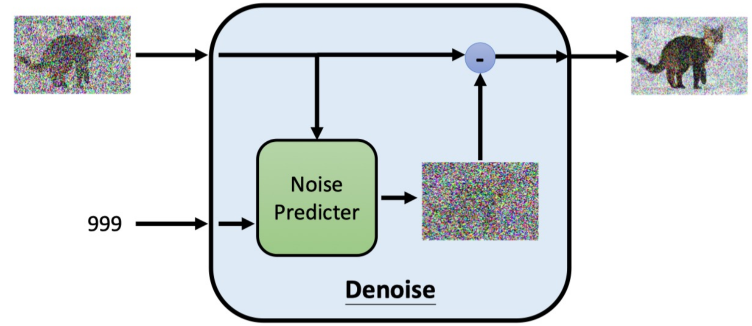
1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \ldots, 1$ **do**
3: $\quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\quad \mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t,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

Denoising Diffusion Probabilistic Models (DDPM)

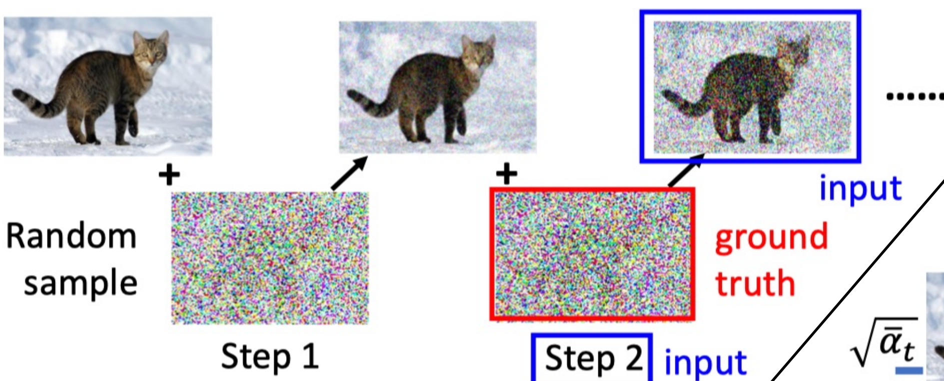
Algorithm 1 Training

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
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t} \boxed{\mathbf{x}_0} + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
6: **until** converged

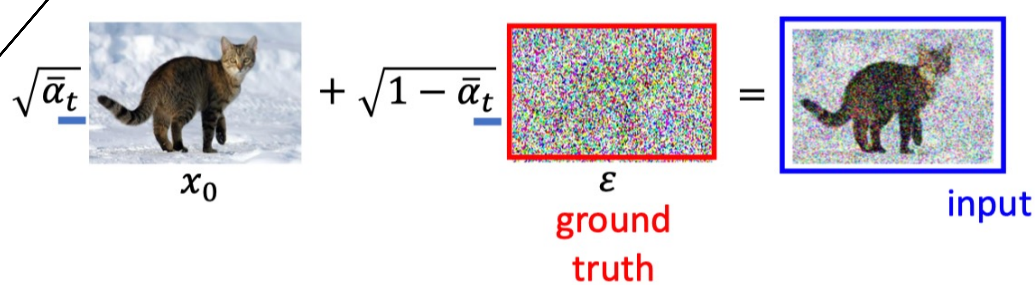
Why x_0 not x_{t-1}?



What I told you:



Real implementation:

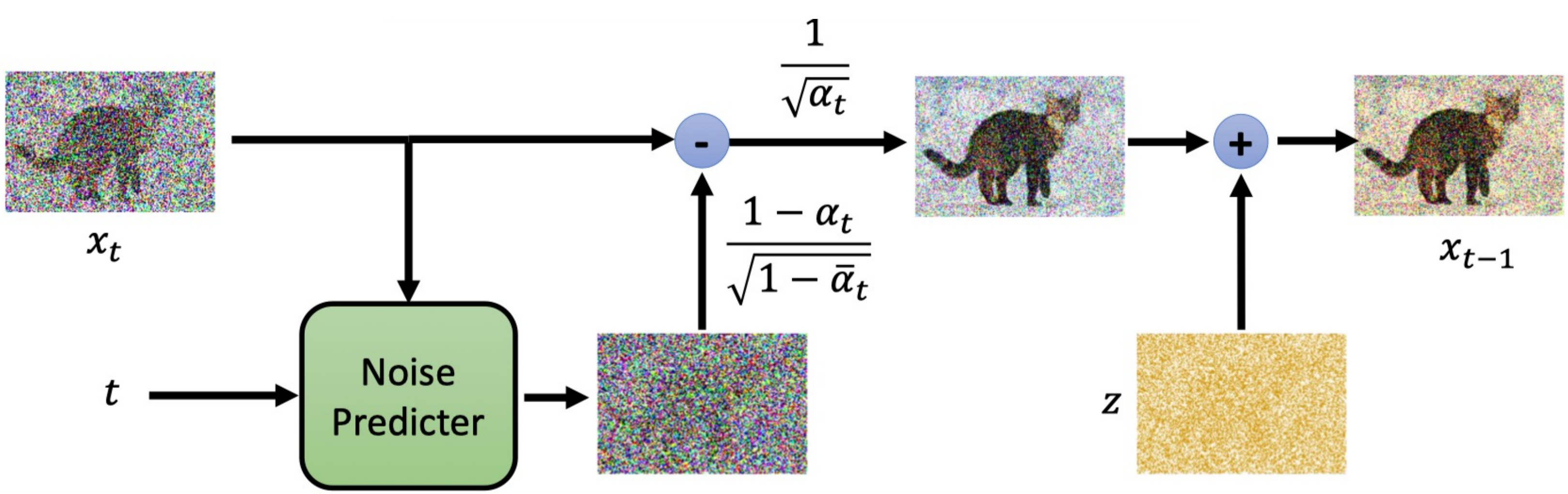


Denoising Diffusion Probabilistic Models (DDPM)

Algorithm 2 Sampling

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

Sample and add a noise during the denoising steps?!



Probabilistic Explanation

$$P_\theta(x_0) = \int_{x_1:x_T} P(x_T)P_\theta(x_{T-1}|x_T)\dots P_\theta(x_{t-1}|x_t)\dots P_\theta(x_0|x_1)dx_1{:}\,x_T$$

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

VAE Maximize $logP_\theta(x)$ $\longrightarrow$ Maximize $\mathbb{E}_{\boxed{q(z|x)}}\left[log\left(\frac{P(x,z)}{q(z|x)}\right)\right]$

Encoder

DDPM Maximize $logP_\theta(x_0)$ $\longrightarrow$ Maximize $\mathbb{E}_{\boxed{q(x_1:x_T|x_0)}}\left[log\left(\frac{P(x_0:x_T)}{q(x_1:x_T|x_0)}\right)\right]$

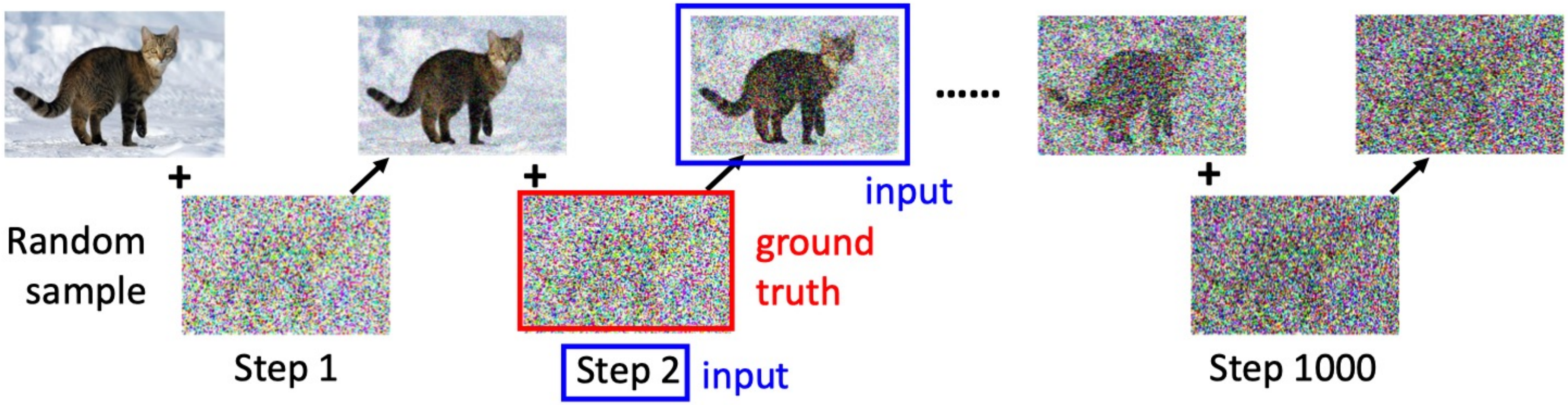
Forward Process
(Diffusion Process)

$$q(x_1:x_T|x_0) = q(x_1|x_0)q(x_2|x_1)\dots q(x_T|x_{T-1})$$

https://arxiv.org/pdf/2208.11970.pdf

Forward/Diffusion Process

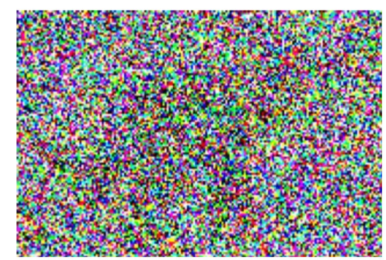
- We add noise step by step:



- We have α_t to control how much noise we want to add.

$= \sqrt{\alpha_t}$

$+\sqrt{1-\alpha_t}$



x_t x_{t-1} z_t

- Equation: $x_t = \sqrt{\alpha_t} x_{t-1} + \sqrt{1-\alpha_t} z_1$
- α_t decreases when t increases.

Forward/Diffusion Process

- We have α_t to control how much noise we want to add.

x_t

$= \sqrt{\alpha_t}$

x_{t-1}

$+\sqrt{1-\alpha_t}$

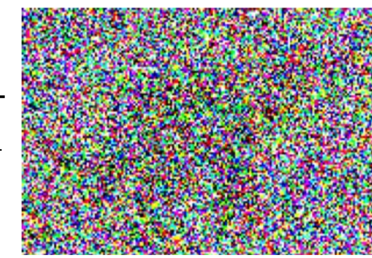
z_t

x_{t-1}

$= \sqrt{\alpha_{t-1}}$

x_{t-2}

$+\sqrt{1-\alpha_{t-1}}$



z_{t-1}

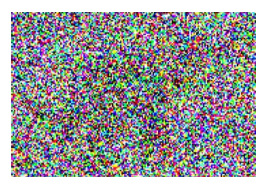
- Combine them, we have:

x_t

$=\sqrt{\alpha_t \alpha_{t-1}}$

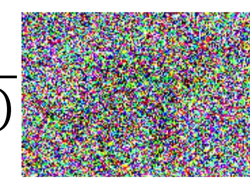
x_{t-2}

$+\sqrt{1-\alpha_t}$



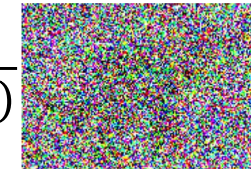
z_t

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



z_{t-1}

Forward/Diffusion Process

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

x_t x_{t-2} z_t z_{t-1}

- Let's formulate it:

$$\begin{aligned} x_t &= \sqrt{\alpha_t}\left(\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{1-\alpha_{t-1}}z_{t-1}\right) + \sqrt{1-\alpha_t}z_t \\ &= \sqrt{\alpha_t\alpha_{t-1}}x_{t-2} + \left(\sqrt{\alpha_t(1-\alpha_{t-1})}z_{t-1} + \sqrt{1-\alpha_t}z_t\right) \end{aligned}$$

- We know that $z_t, z_{t-1}, \ldots, \sim \mathcal{N}(0, I)$.
- So $\sqrt{\alpha_t(1-\alpha_{t-1})}z_{t-1} \sim \mathcal{N}\left(0, \alpha_t(1-\alpha_{t-1})\right)$, and $\sqrt{1-\alpha_t}z_t \sim \mathcal{N}(0, 1-\alpha_t)$
- We also know that $\mathcal{N}(0, {\sigma_1}^2 I) + \mathcal{N}(0, {\sigma_2}^2 I) = \mathcal{N}(0, ({\sigma_1}^2 + {\sigma_2}^2)I)$.

$$\begin{aligned} x_t &= \sqrt{\alpha_t\alpha_{t-1}}x_{t-2} + \left(\sqrt{\alpha_t(1-\alpha_{t-1})}z_{t-1} + \sqrt{1-\alpha_t}z_t\right) \\ &= \sqrt{\alpha_t\alpha_{t-1}}x_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\tilde{z}_{t-1} \\ &= \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\tilde{z}_1 \end{aligned}$$

Where $\bar{\alpha}_t = \alpha_t\alpha_{t-1}, \ldots, \alpha_1$

$z_t, z_{t-1}, \ldots, \sim \mathcal{N}(0, I)$

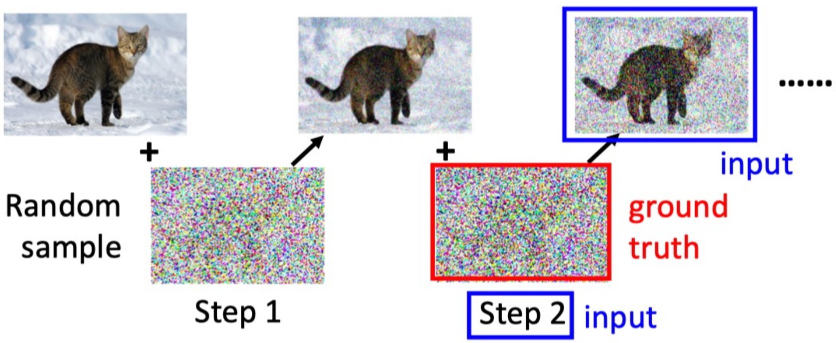
$\tilde{z}_t, \tilde{z}_{t-1}, \ldots, \sim \mathcal{N}(0, I)$

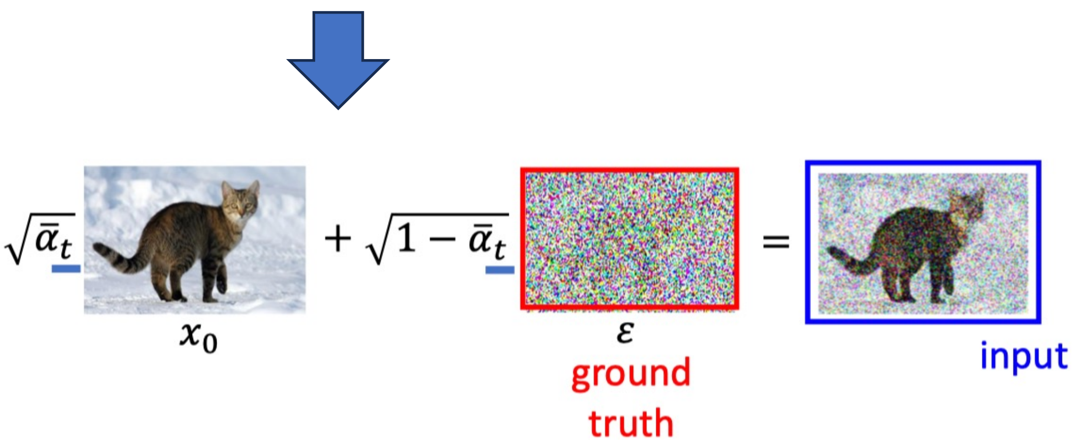
Forward/Diffusion Process

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\tilde{z}_1$$

Where $\bar{\alpha}_t = \alpha_t\alpha_{t-1}, \dots, \alpha_1$

$$\tilde{z}_t, \tilde{z}_{t-1}, \dots, \sim \mathcal{N}(0, I)$$





Algorithm 1 Training

1: **repeat**

2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$

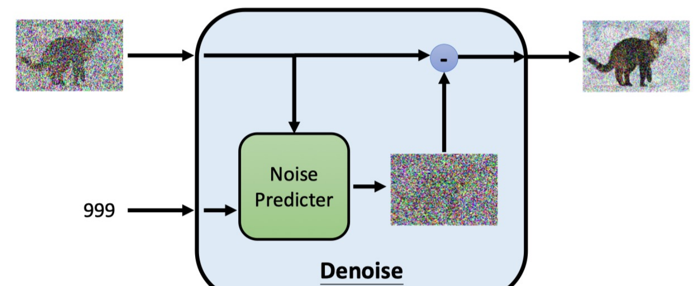
3: $t \sim \mathrm{Uniform}(\{1, \dots, T\})$

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



Denoising/Reverse Process

- Goal: $q(x_{t-1}|x_t)$, but we don't know how to calculate it. We only know $q(x_t|x_{t-1})$.
- Using Bayes Rule we have:

$$q(x_{t-1}|x_t) = q(x_t|x_{t-1})\frac{\boxed{q(x_{t-1})}}{\boxed{q(x_t)}}$$

Hard to model directly.

- Instead, we can model $q(x_{t-1}|x_t, x_0)$
- Using Bayes Rule we have:

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

- For each term, we have:

$$\boxed{x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\tilde{z}_1}$$

$$q(x_{t-1}|x_0) = \sqrt{\bar{\alpha}_{t-1}}x_0 + \sqrt{1-\bar{\alpha}_{t-1}}z \sim \mathcal{N}\left(\sqrt{\bar{\alpha}_{t-1}}x_0, 1-\bar{\alpha}_{t-1}\right)$$
$$q(x_t|x_0) = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}z \sim \mathcal{N}\left(\sqrt{\bar{\alpha}_t}x_0, 1-\bar{\alpha}_t\right)$$
$$q(x_t|x_{t-1}, x_0) = \sqrt{\alpha_t}x_{t-1} + \sqrt{1-\alpha_t}z \sim \mathcal{N}\left(\sqrt{\alpha_t}x_{t-1}, 1-\alpha_t\right)$$

- So, we have:

$$q(x_{t-1}|x_t, x_0) \propto \exp\left(-\frac{1}{2}\left(\frac{(x_t-\sqrt{\alpha_t}x_{t-1})^2}{\beta_t} + \frac{\left(x_{t-1}-\sqrt{\bar{\alpha}_{t-1}}x_0\right)^2}{1-\bar{\alpha}_{t-1}} - \frac{\left(x_t-\sqrt{\bar{\alpha}_t}x_0\right)^2}{1-\bar{\alpha}_t}\right)\right), \text{ let } 1-\alpha_t = \beta_t$$

$$= \exp\left(-\frac{1}{2}\left(\left(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}\right){x_{t-1}}^2 - \left(\frac{2\sqrt{\alpha_t}}{\beta_t}x_t + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}x_0\right)x_{t-1} + C(x_t, x_0)\right)\right), \text{ C is a constant}$$

Denoising/Reverse Process

$$q(x_{t-1}|x_t,x_0) \propto \exp(-\frac{1}{2}(\frac{(x_t-\sqrt{\alpha_t}x_{t-1})^2}{\beta_t}+\frac{\left(x_{t-1}-\sqrt{\bar{\alpha}_{t-1}}x_0\right)^2}{1-\bar{\alpha}_{t-1}}-\frac{\left(x_t-\sqrt{\bar{\alpha}_t}x_0\right)^2}{1-\bar{\alpha}_t})),\text{ let } 1-\alpha_t=\beta_t$$

$$=\exp\left(-\frac{1}{2}\left(\left(\frac{\alpha_t}{\beta_t}+\frac{1}{1-\bar{\alpha}_{t-1}}\right){x_{t-1}}^2-\left(\frac{2\sqrt{\alpha_t}}{\beta_t}x_t+\frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}x_0\right)x_{t-1}+C(x_t,x_0)\right)\right),\text{ C is a constant}$$

- For normal distribution we have: $\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)=\exp(-\frac{1}{2}(\frac{1}{\sigma^2}x^2-\frac{2\mu}{\sigma^2}x+\frac{\mu^2}{\sigma^2}))$
- So, we have:

$$\sigma^2=\frac{1}{\left(\frac{\alpha_t}{\beta_t}+\frac{1}{1-\bar{\alpha}_{t-1}}\right)}$$ is a constant

$$\frac{2\mu}{\sigma^2}=\left(\frac{2\sqrt{\alpha_t}}{\beta_t}x_t+\frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}x_0\right)$$

We can estimate x_{t-1} from x_t, x_0

We don't know this in reverse process

$$\boxed{\tilde{\mu}_t(x_t,x_0)}=\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}x_t+\frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\boxed{x_0}$$

Actually, we even don't need the reverse process if we know this. LOL.

Denoising/Reverse Process

$$\sigma^2 = \frac{1}{\left(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}\right)} \qquad \tilde{\mu}_t(x_t, x_0) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t} x_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t} x_0$$

- But we have: $x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t} z_t$
- So, $x_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1-\bar{\alpha}_t} z_t)$

Estimated by the neural network

- Finally, we have: $$\tilde{\mu}_t = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \boxed{z_t}\right)$$

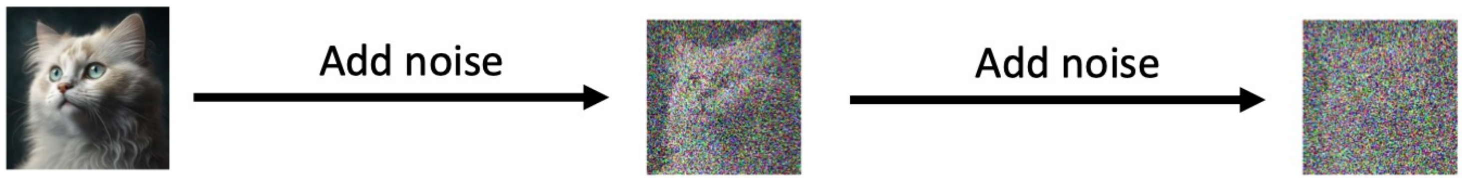
Algorithm 2 Sampling

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: $\quad \mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \boxed{\sigma_t \mathbf{z}}$
5: **end for**
6: **return** $\mathbf{x}_0$

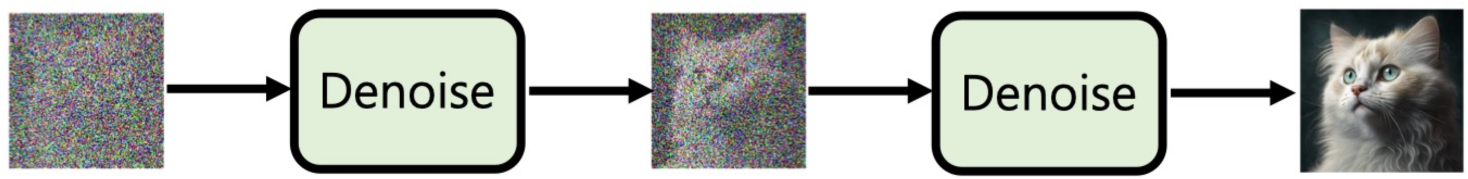
Sampling from the data distribution

Diffusion Model

Forward Process



Reverse Process



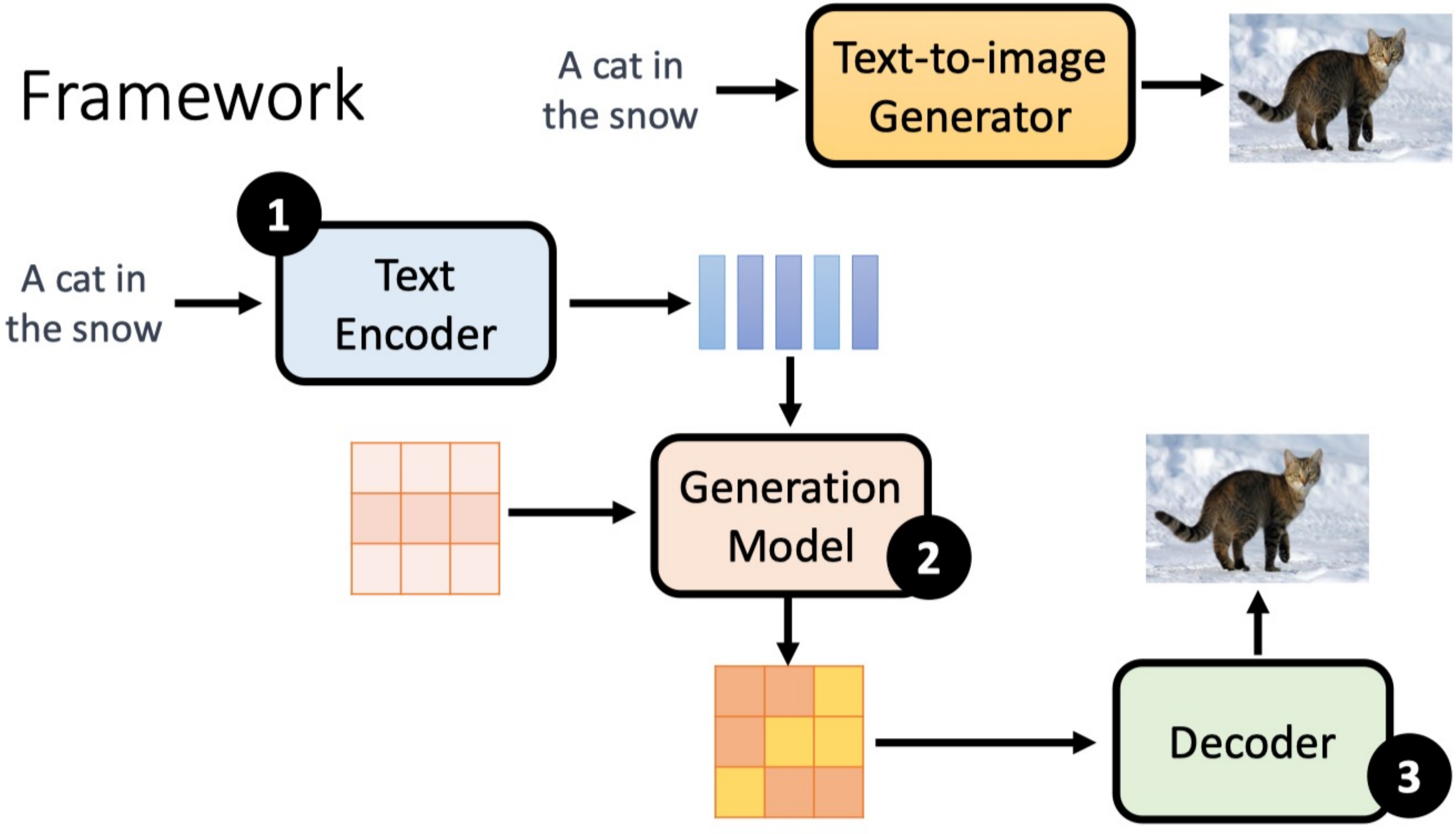
Algorithm 1 Training

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

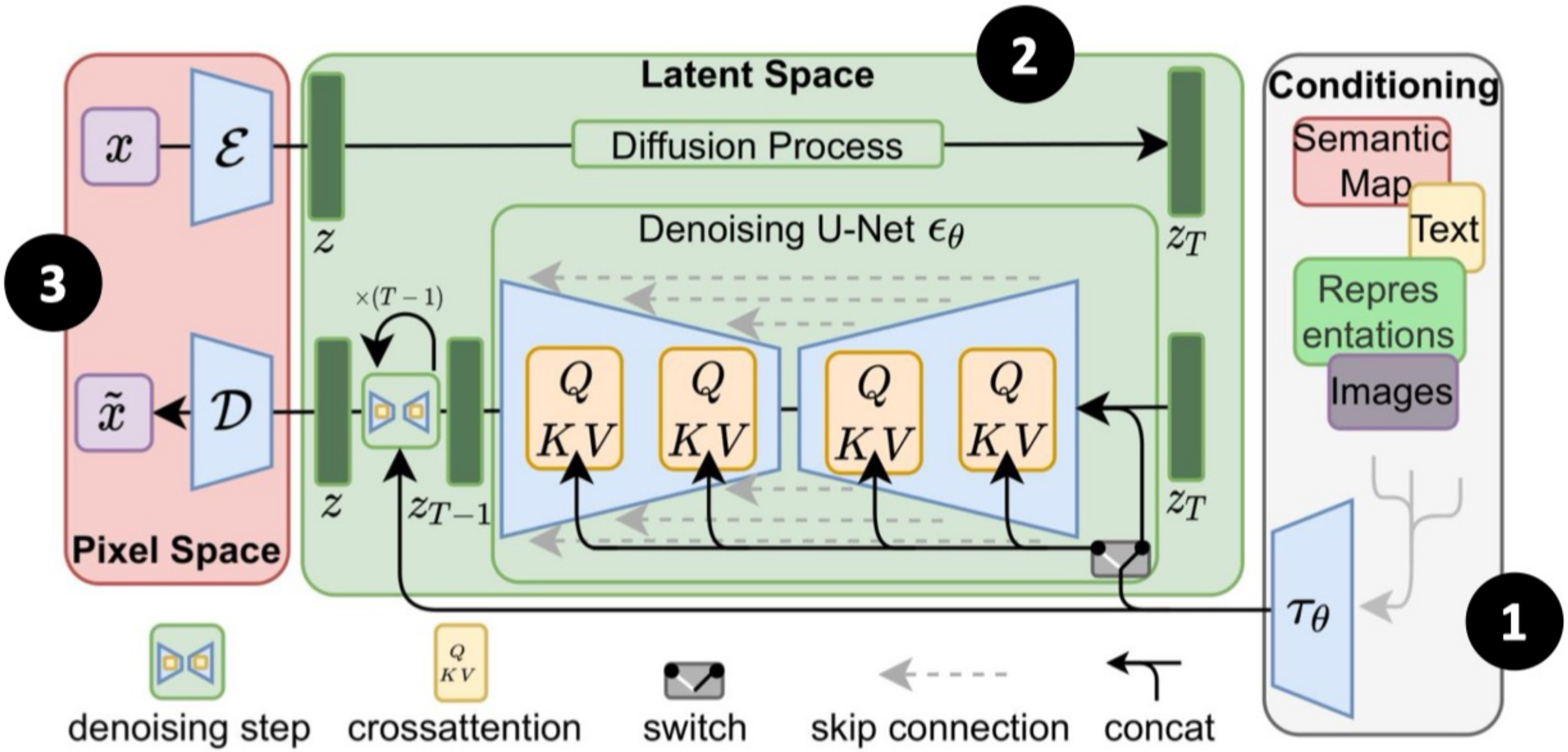
Algorithm 2 Sampling

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

Stable Diffusion

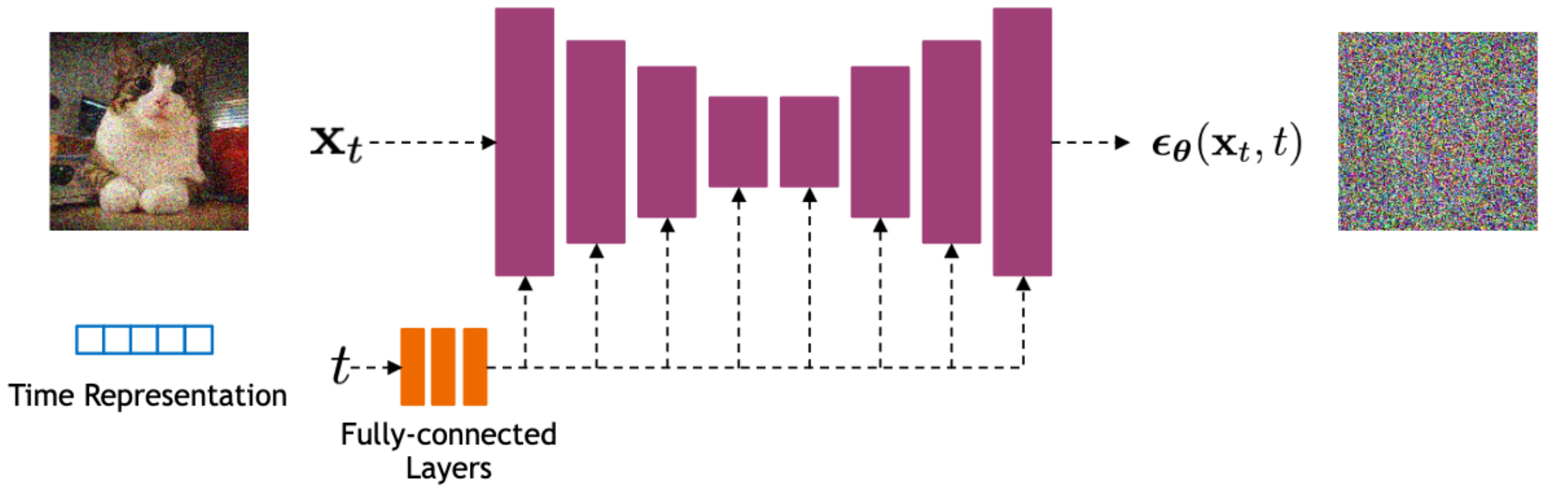


Stable Diffusion



Network Architectures

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



Time representation: sinusoidal positional embeddings or random Fourier features.

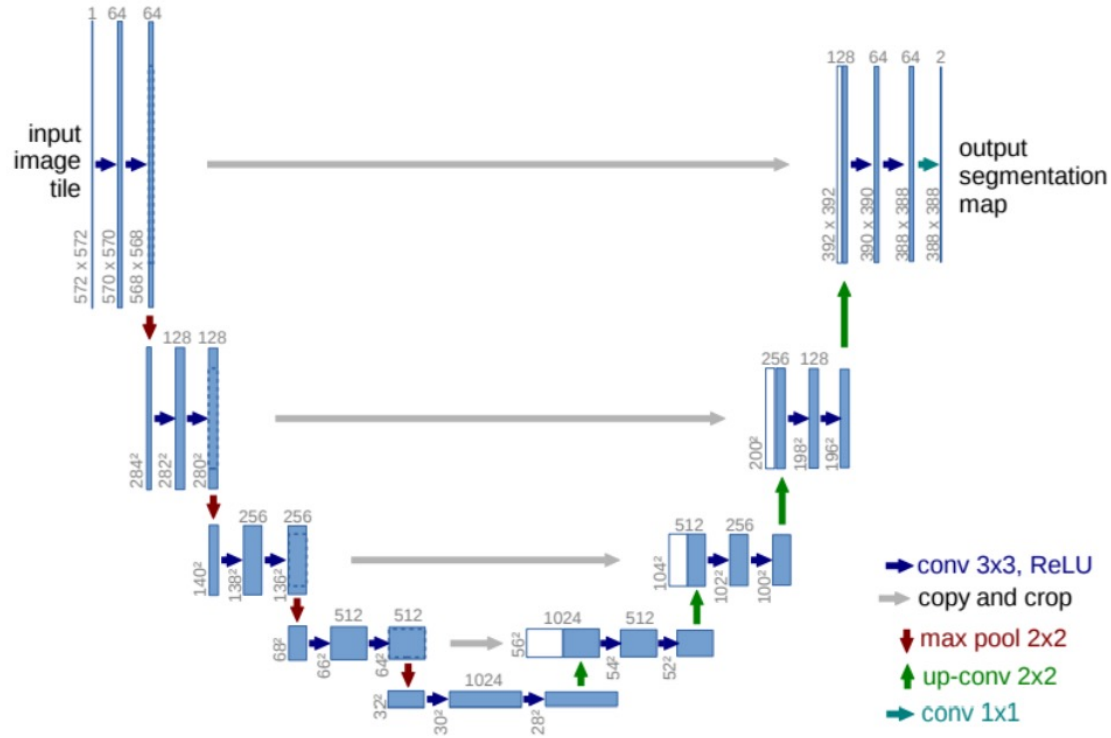
U-Net

Contracting path

- block consists of:
  - 3x3 convolution
  - 3x3 convolution
  - ReLU
  - max-pooling with stride of 2 (downsample)
- repeat the block N times, doubling number of channels

Expanding path

- block consists of:
  - 2x2 convolution (upsampling)
  - concatenation with contracting path features
  - 3x3 convolution
  - 3x3 convolution
  - ReLU
- repeat the block N times, halving the number of channels



U-Net

- Originally designed for applications to biomedical segmentation
- Key observation is that the output layer has the **same** dimensions as the input image (possibly with different number of channels)

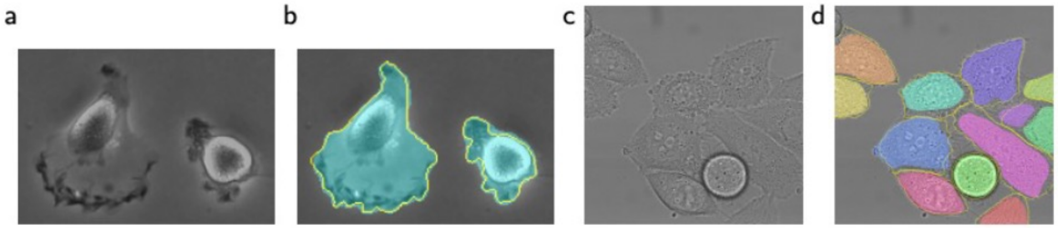
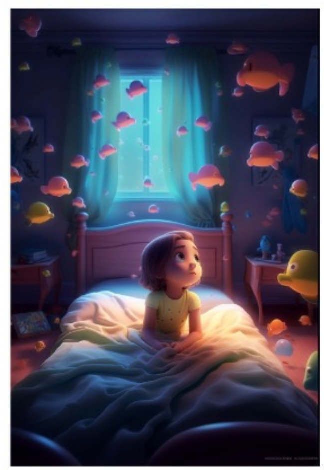
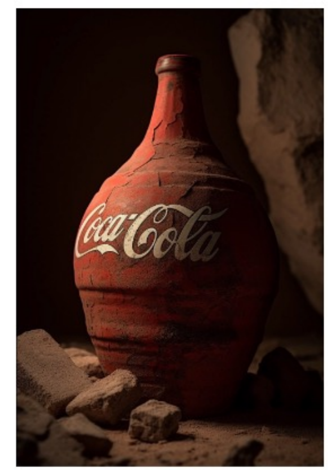


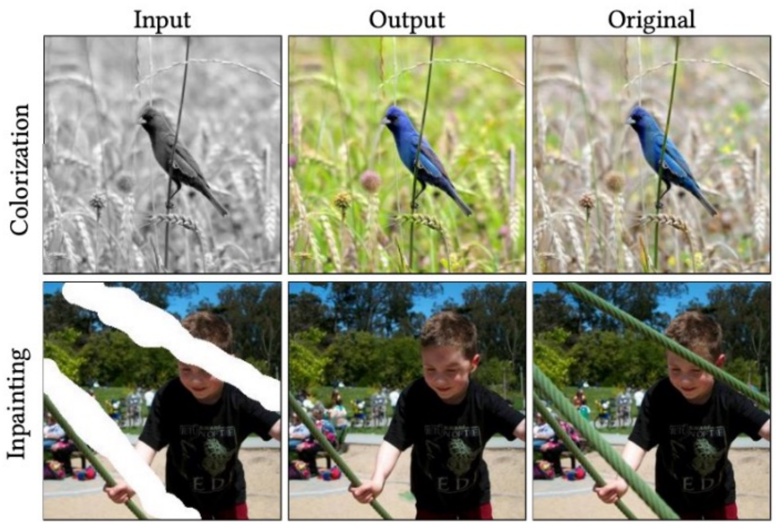
Fig. 4. Result on the ISBI cell tracking challenge. (**a**) part of an input image of the "PhC-U373" data set. (**b**) Segmentation result (cyan mask) with manual ground truth (yellow border) (**c**) input image of the "DIC-HeLa" data set. (**d**) Segmentation result (random colored masks) with manual ground truth (yellow border).

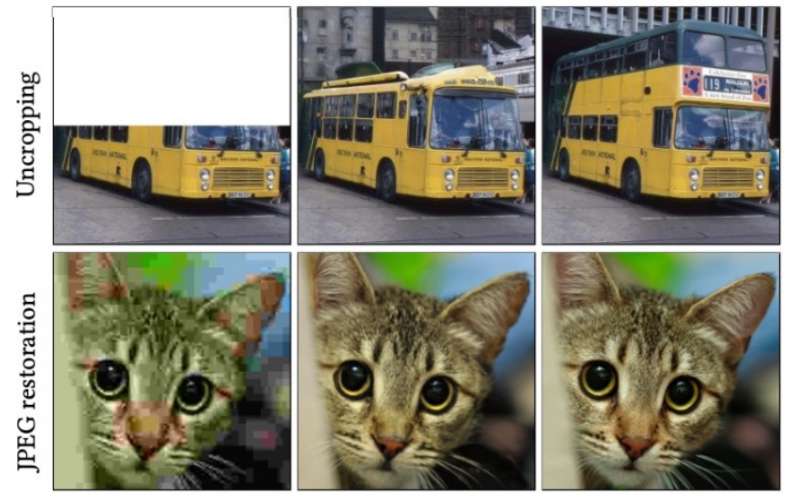
Applications: AI Art

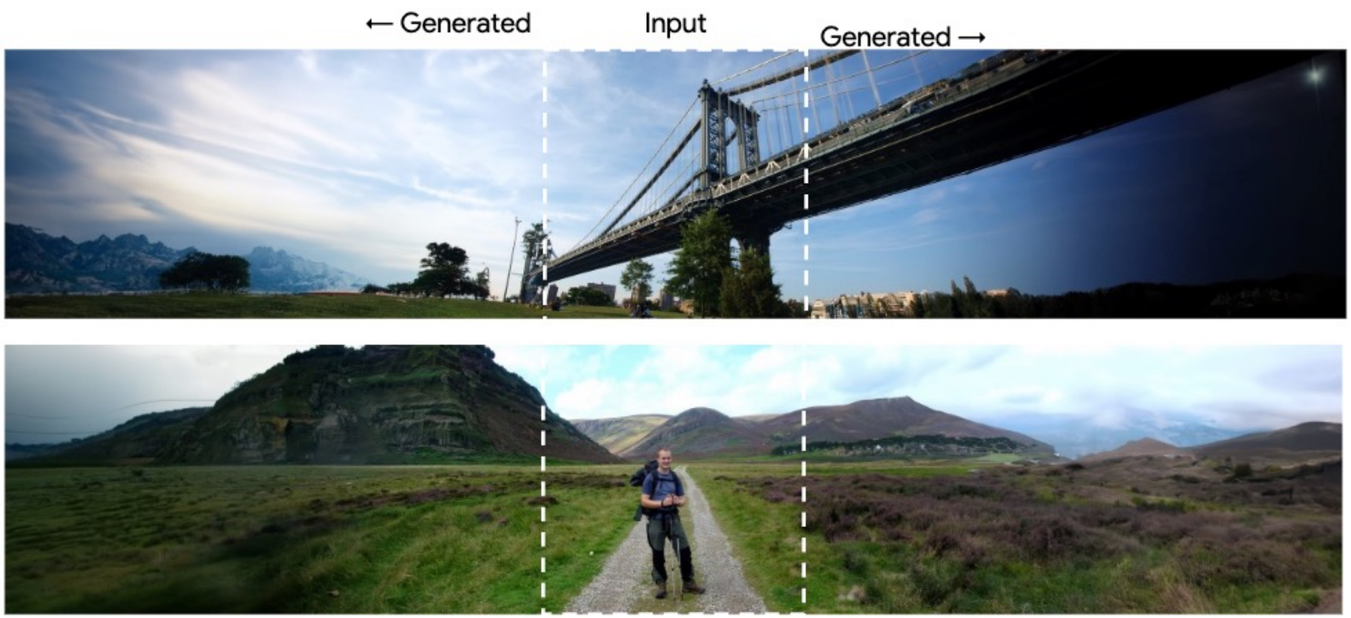




Applications: Colorization, Inpainting, Restoration, Outfilling







Questions?

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