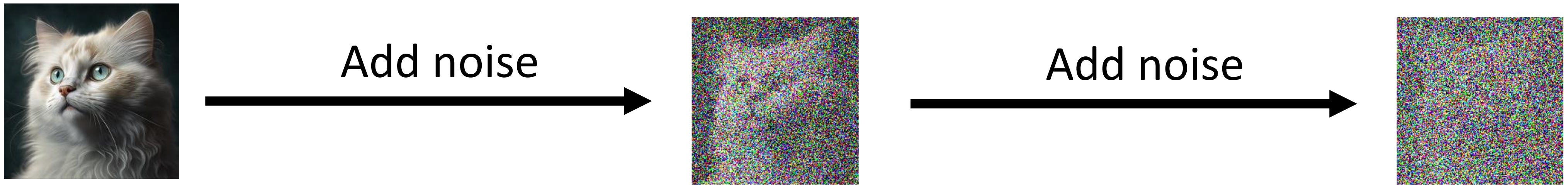
Diffusion Model 背後的數學原理

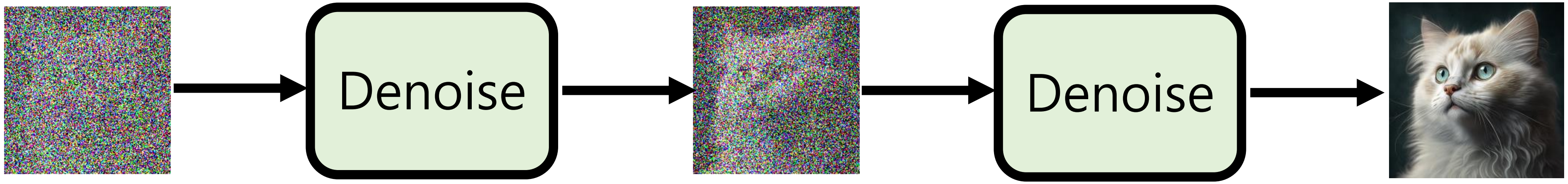
感謝姜成翰同學大力協助

基本概念

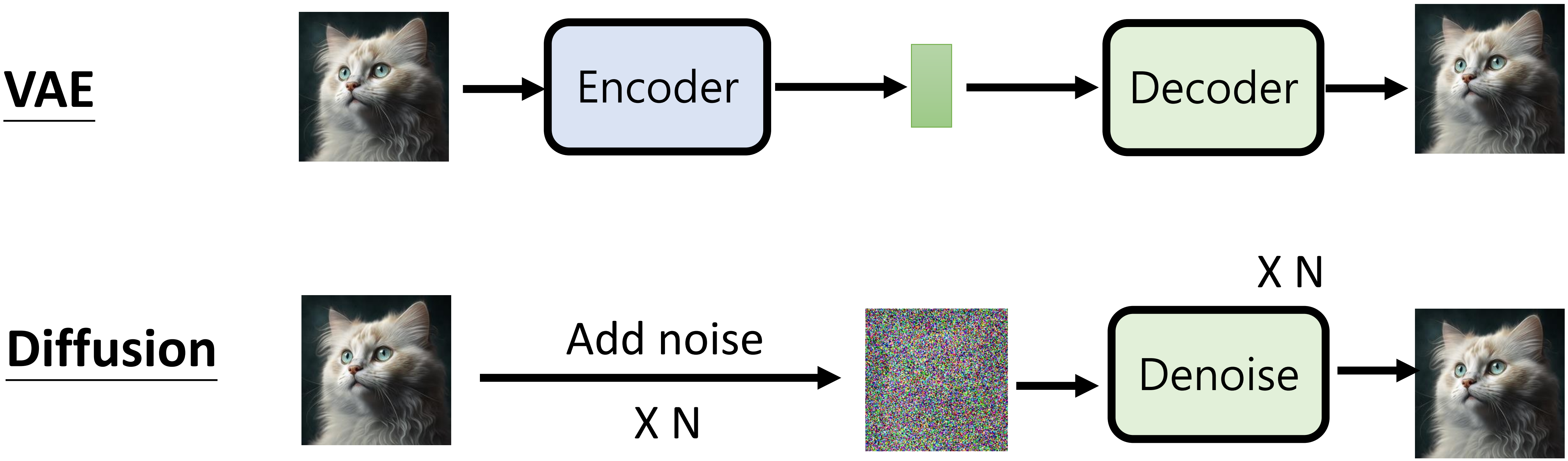
Forward Process



Reverse Process



VAE vs. Diffusion Model



Denoising Diffusion Probabilistic Models

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** $\mathbf{x}_0$

暗藏玄機!

Training

x_0: clean image

ε: noise

Algorithm 1 Training

repeat

$\mathbf{x}_0 \sim q(\mathbf{x}_0)$ sample clean image

$t \sim \mathrm{Uniform}(\{1, \ldots, T\})$

$\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ sample a noise

Take gradient descent step on

$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \underbrace{\boldsymbol{\epsilon}_\theta(\boxed{\sqrt{\bar\alpha_t}\mathbf{x}_0 + \sqrt{1-\bar\alpha_t}\boldsymbol{\epsilon}}, t)}_{\text{Noise predictor}} \right\|^2$$

until converged

Noisy image

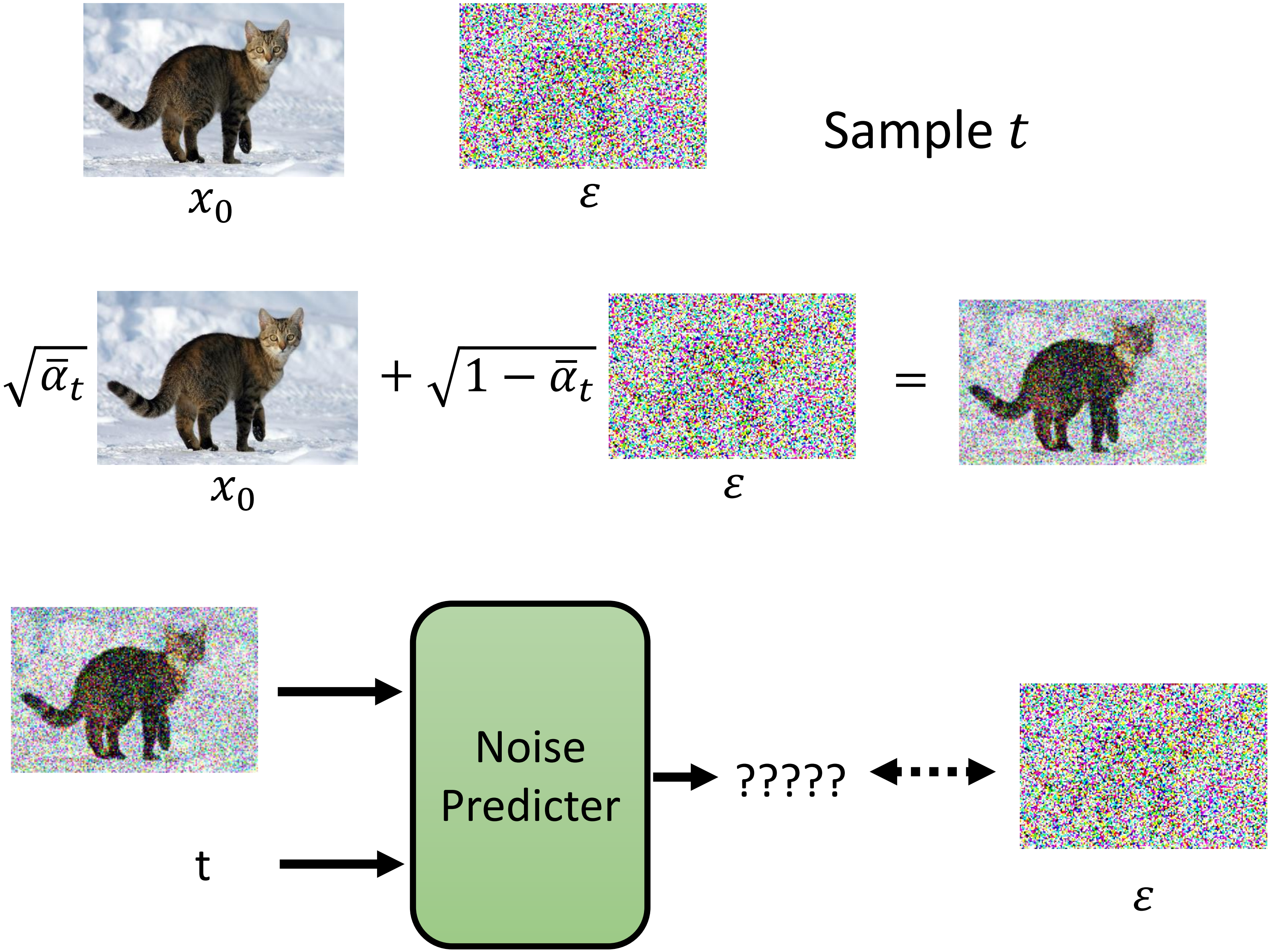
Target Noise

$\bar\alpha_1, \bar\alpha_2, \ldots \bar\alpha_T$

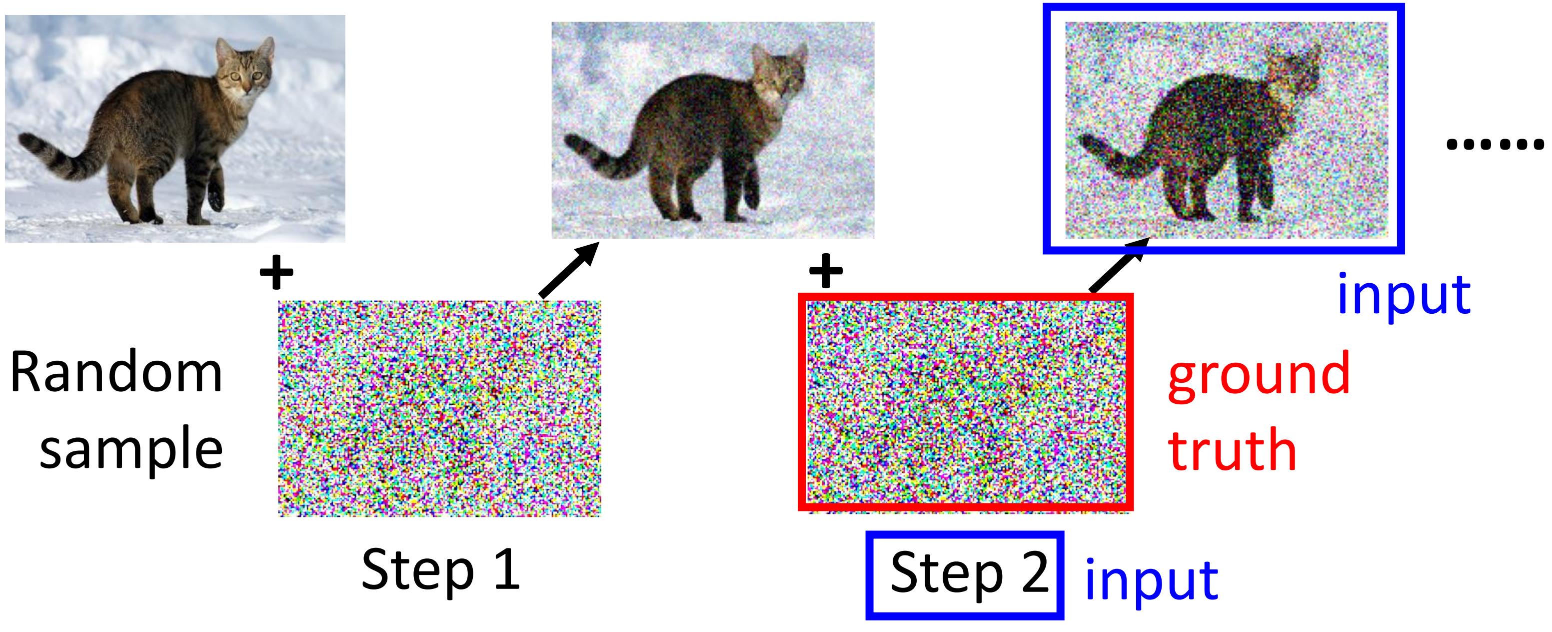
smaller

Training

$\bar{\alpha}_1, \bar{\alpha}_2, \ldots \bar{\alpha}_T$

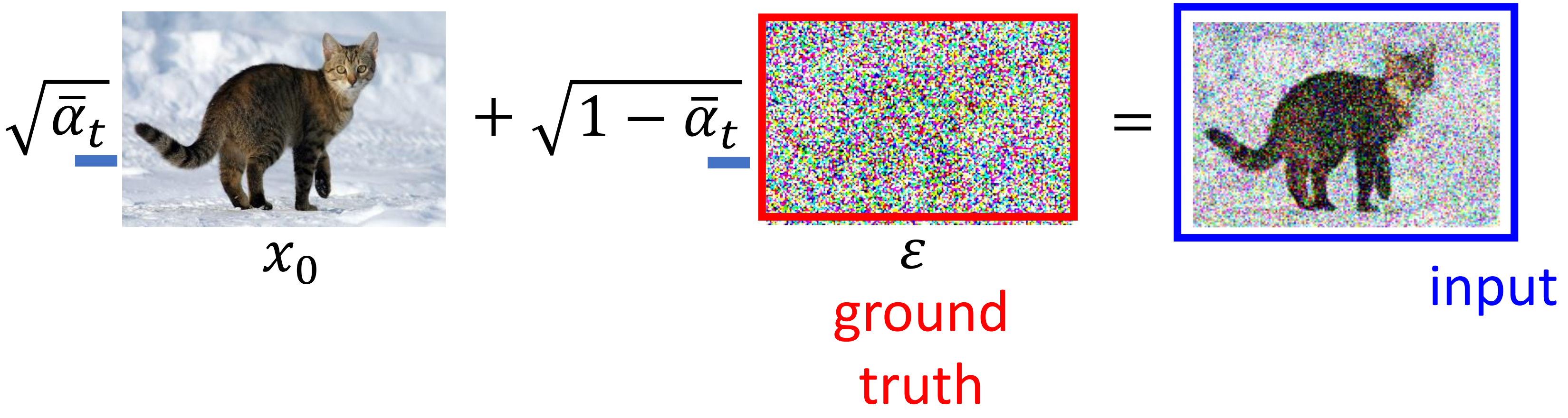


想像中 ...



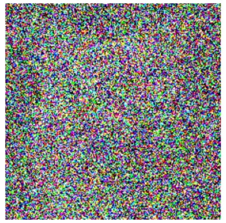
Random sample
Step 1
Step 2
input
ground truth
input
......

實際上 ...



$\sqrt{\bar{\alpha}_t}\,x_0 + \sqrt{1-\bar{\alpha}_t}\,\varepsilon =$
x_0
ε
ground truth
input

Inference



x_T

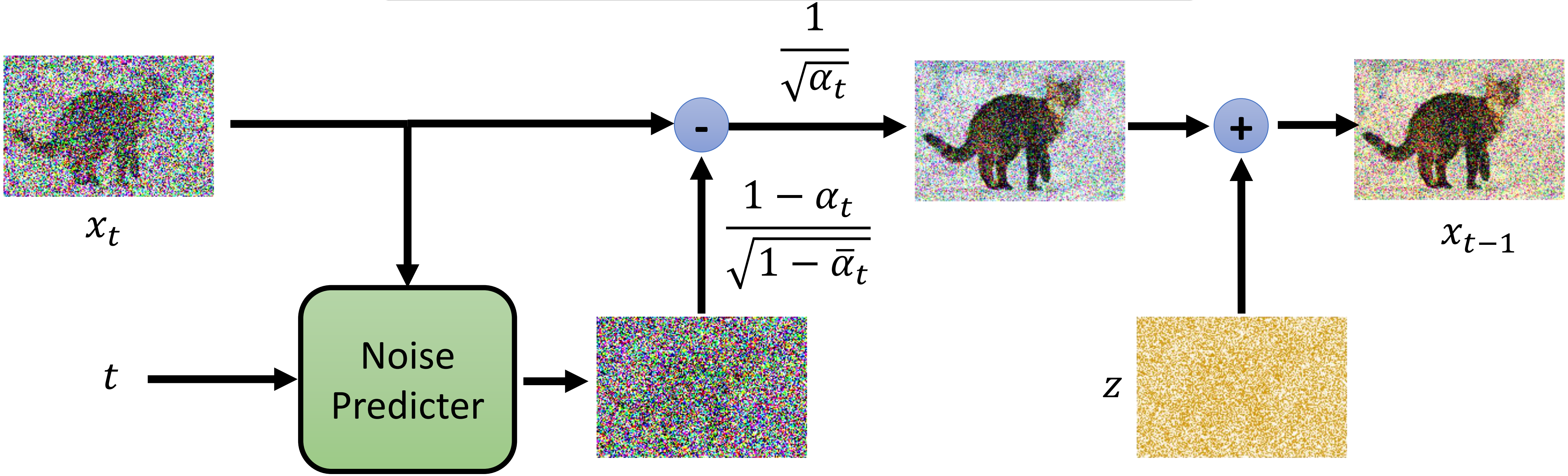
Algorithm 2 Sampling

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

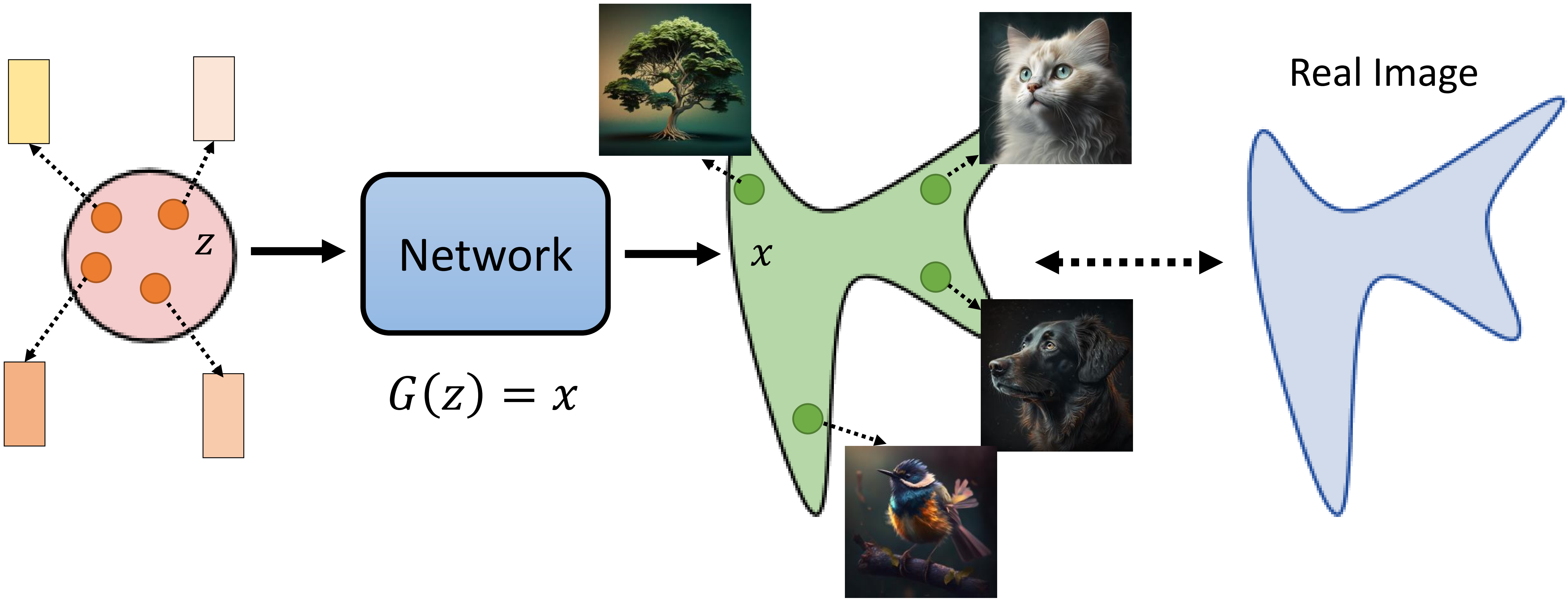
sample a noise?!

$\bar{\alpha}_1, \bar{\alpha}_2, \ldots \bar{\alpha}_T$

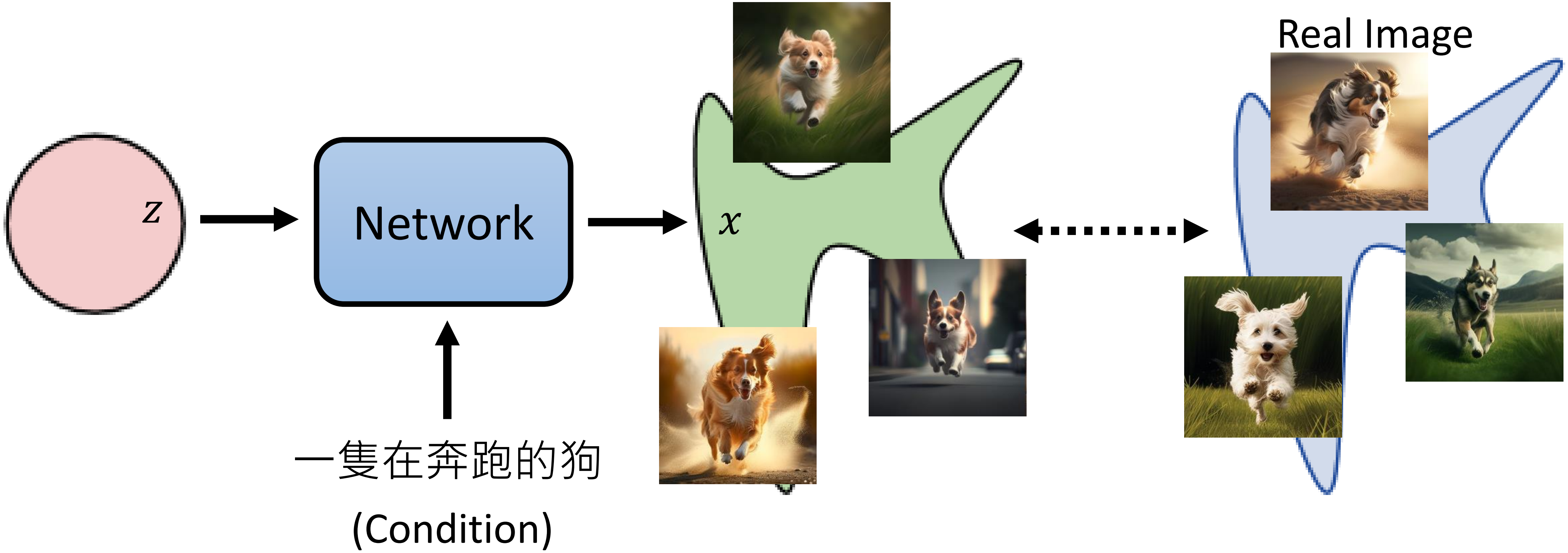
$\alpha_1, \alpha_2, \ldots \alpha_T$



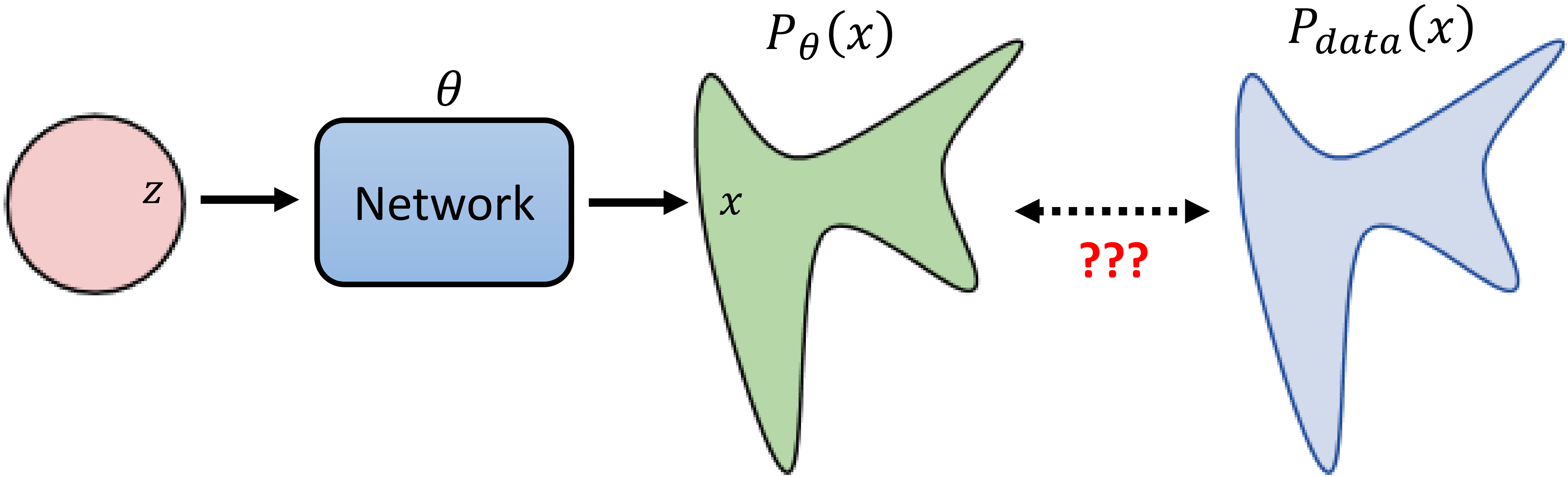
影像生成模型本質上的共同目標



影像生成模型本質上的共同目標



Maximum Likelihood Estimation



Sample $\{x^1, x^2, \dots, x^m\}$ from $P_{data}(x)$

We can compute $P_\theta(x^i)$

???

$$\theta^* = arg \max_\theta \prod_{i=1}^{m} P_\theta(x^i)$$

Sample $\{x^1, x^2, \dots, x^m\}$ from $P_{data}(x)$

$$\theta^* = arg\max_{\theta} \prod_{i=1}^{m} P_\theta(x^i) \quad = arg\max_{\theta} log \prod_{i=1}^{m} P_\theta(x^i)$$

$$= arg\max_{\theta} \sum_{i=1}^{m} logP_\theta(x^i) \quad \approx arg\max_{\theta} E_{x\sim P_{data}}[logP_\theta(x)]$$

(not related to θ)

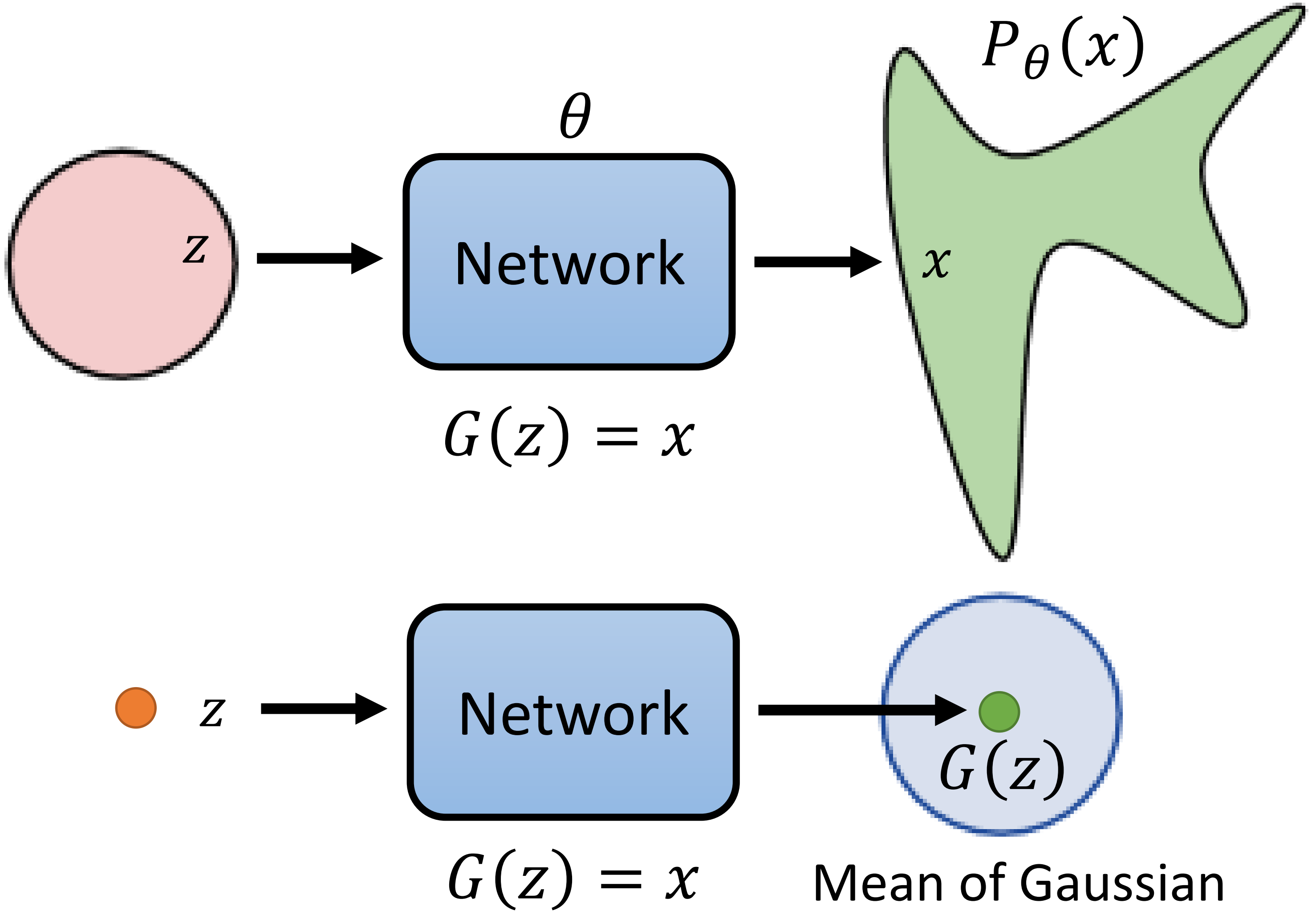
$$= arg\max_{\theta} \int_x P_{data}(x)logP_\theta(x)dx \quad - \int_x P_{data}(x)logP_{data}(x)dx$$

Difference between P_{data} and P_θ

$$= arg\max_{\theta} \int_x P_{data}(x)log\frac{P_\theta(x)}{P_{data}(x)}dx \quad = arg\min_{\theta} KL(P_{data}||P_\theta)$$

Maximum Likelihood = Minimize KL Divergence

VAE: Compute $P_\theta(x)$



$$P_\theta(x) = \int_z P(z) P_\theta(x|z) dz$$

$$P_\theta(x|z) = \begin{cases} 1, & G(z) = x \\ 0, & G(z) \neq x \end{cases}$$

可能會幾乎都是 0 ☹

$$P_\theta(x|z)$$
$$\propto exp(-\|G(z) - x\|_2)$$

VAE: Lower bound of $logP(x)$

$$logP_\theta(x) = \int_z q(z|x) logP(x) dz$$

$q(z|x)$ can be any distribution

$$= \int_z q(z|x) log\left(\frac{P(z,x)}{P(z|x)}\right) dz = \int_z q(z|x) log\left(\frac{P(z,x)}{q(z|x)} \frac{q(z|x)}{P(z|x)}\right) dz$$

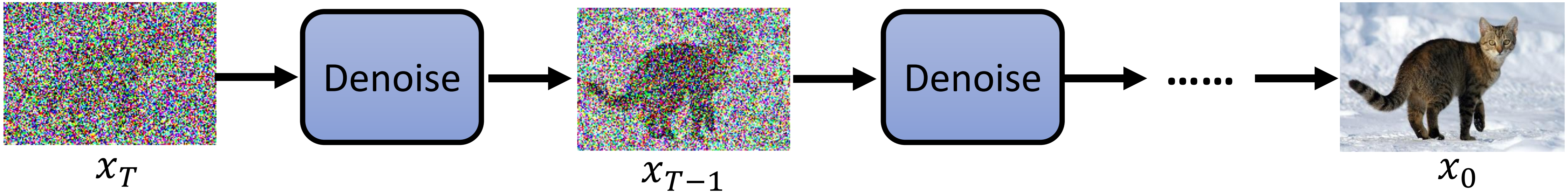
$$= \int_z q(z|x) log\left(\frac{P(z,x)}{q(z|x)}\right) dz + \underbrace{\int_z q(z|x) log\left(\frac{q(z|x)}{P(z|x)}\right) dz}_{KL(q(z|x)||P(z|x))}$$

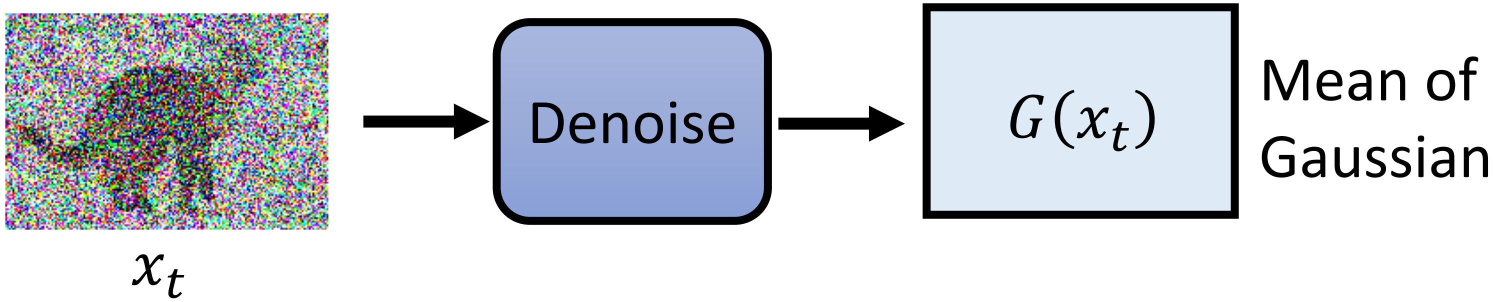
≥ 0

$$\geq \int_z q(z|x) log\left(\frac{P(z,x)}{q(z|x)}\right) dz = \underbrace{E_{q(z|x)}}_{\text{Encoder}}[log\left(\frac{P(x,z)}{q(z|x)}\right)]$$

lower bound

DDPM: Compute $P_\theta(x)$





$$P_\theta(x_{t-1}|x_t) \propto \exp(-\|G(x_t) - x_{t-1}\|_2)$$

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

DDPM: Lower bound of $logP(x)$

VAE

Maximize $logP_\theta(\underline{x})$ $\longrightarrow$ Maximize $E_{\boxed{q(\underline{z}|x)}}[log\left(\frac{P(x,\underline{z})}{q(\underline{z}|x)}\right)]$

Encoder

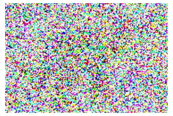
DDPM

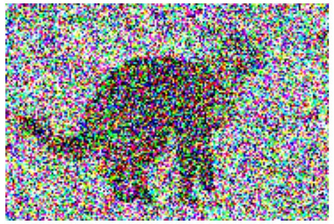
Maximize $logP_\theta(\underline{x_0})$ $\longrightarrow$ Maximize $E_{\boxed{q(\underline{x_1:x_T}|x_0)}}[log\left(\frac{P(x_0:\underline{x_T})}{q(\underline{x_1:x_T}|x_0)}\right)]$

Forward Process
(Diffusion Process)

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

$q(x_t|x_{t-1})$

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

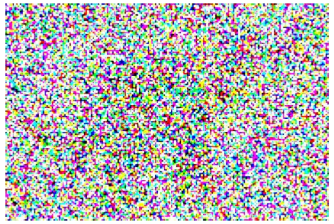


x_{t-1}

$=\sqrt{1-\beta_t}$

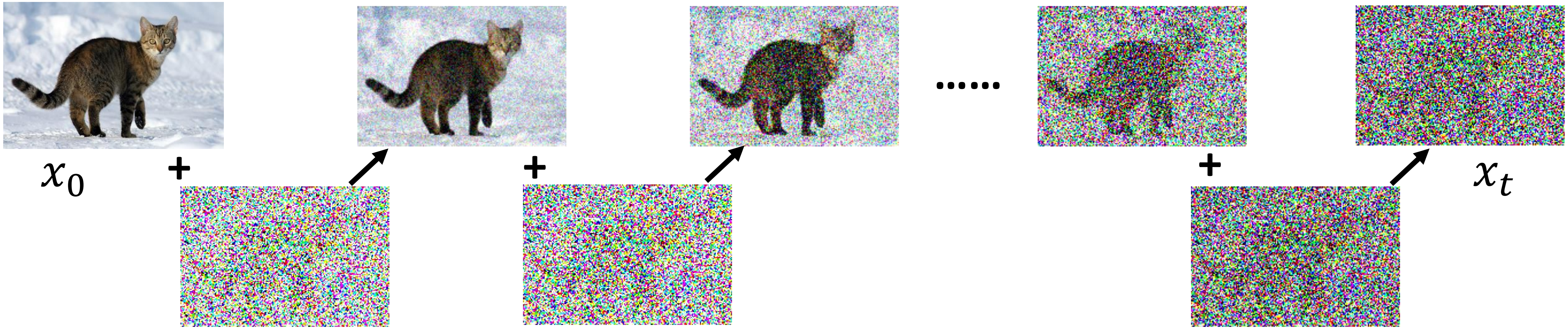
x_t

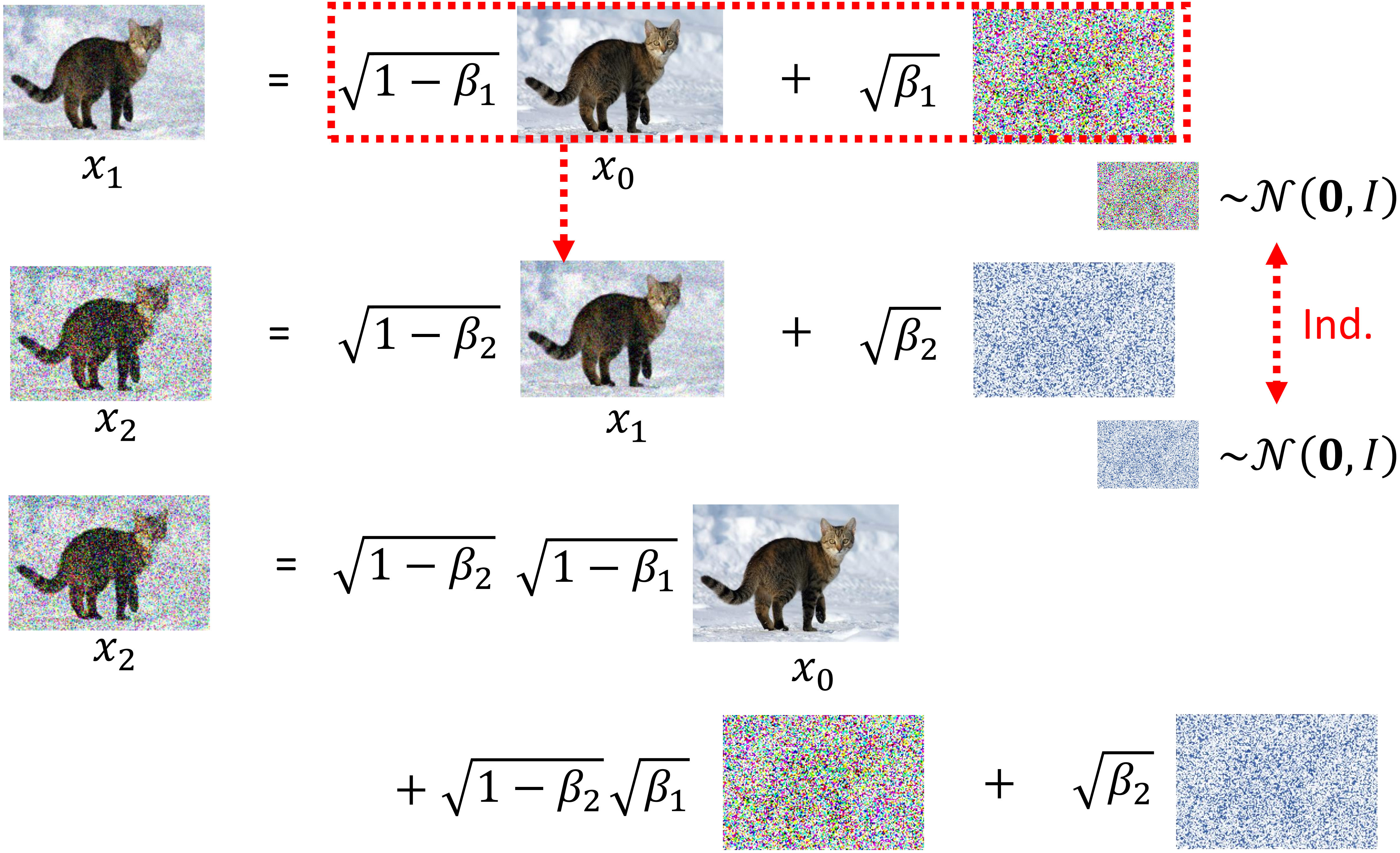
$+\sqrt{\beta_t}$



$\beta_1, \beta_2, \ldots, \beta_T$

$q(x_t|x_0)$

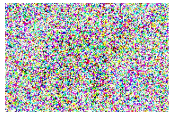


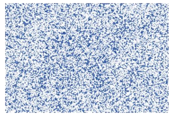


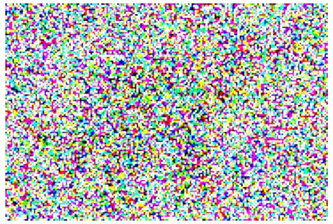
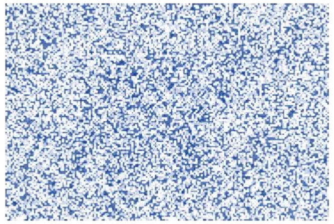
$x_1 = \sqrt{1-\beta_1}\, x_0 + \sqrt{\beta_1}$
$\sim\mathcal{N}(\mathbf{0}, I)$
Ind.
$x_2 = \sqrt{1-\beta_2}\, x_1 + \sqrt{\beta_2}$
$\sim\mathcal{N}(\mathbf{0}, I)$
$x_2 = \sqrt{1-\beta_2}\sqrt{1-\beta_1}\, x_0$
$+\sqrt{1-\beta_2}\sqrt{\beta_1} + \sqrt{\beta_2}$

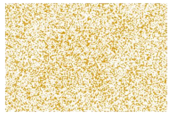
x_2

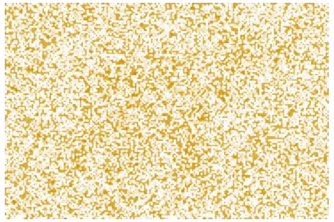
$= \sqrt{1-\beta_2}\,\sqrt{1-\beta_1}$  x_0

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

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

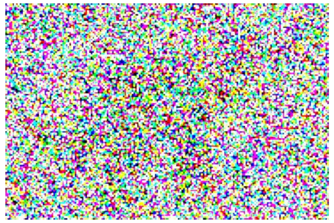
$+\sqrt{1-\beta_2}\sqrt{\beta_1}$  $+\sqrt{\beta_2}$ 

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

$+\sqrt{1-(1-\beta_2)(1-\beta_1)}$ 

$q(x_t|x_0)$

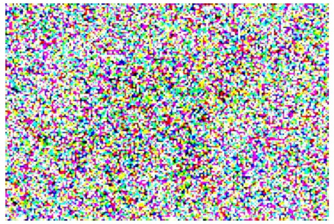
$\beta_1, \beta_2, \dots, \beta_T$

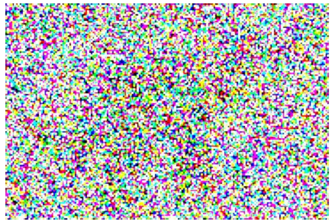


$\sim\mathcal{N}(\mathbf{0}, I)$

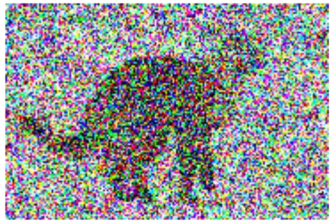
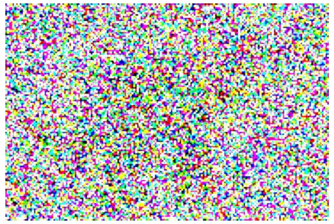
$\alpha_t = 1 - \beta_t$

$\bar{\alpha}_t = \alpha_1 \alpha_2 \dots \alpha_t$

 $=$ $\sqrt{1-\beta_1}$  $+$ $\sqrt{\beta_1}$ 

 $=$ $\sqrt{1-\beta_2}$  $+$ $\sqrt{\beta_2}$ 

⋮ ⋮ ⋮

 $=$ $\sqrt{1-\beta_t}$  $+$ $\sqrt{\beta_t}$ 

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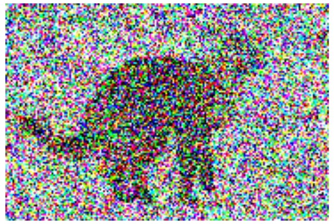
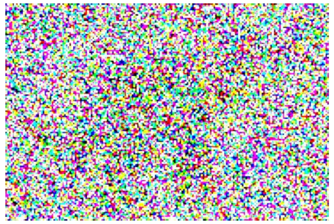
 $=$ $\underset{\sqrt{\bar{\alpha}_t}}{\boxed{\sqrt{1-\beta_1}\dots\sqrt{1-\beta_t}}}$  $+$ $\underset{\sqrt{1-\bar{\alpha}_t}}{\boxed{\sqrt{1-(1-\beta_1)\dots(1-\beta_t)}}}$ 

$$
\begin{aligned}
\log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right] && (47)\\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)\prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\prod_{t=1}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)\prod_{t=2}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)\prod_{t=2}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)}\right] && (50)\\
&= \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] && (51)\\
&= \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] && (52)\\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\cancel{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}}{\cancel{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}}\right] && (53)\\
&= \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] && (54)\\
&= \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] && (55)\\
&= \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] && (56)\\
&= \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] && (57)\\
&= \boxed{\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}} \quad (58)}
\end{aligned}
$$

$$\boxed{\text{Maximize } \mathrm{E}_{q(x_1:x_T|x_0)}\left[log\left(\frac{P(x_0:x_T)}{q(x_1:x_T|x_0)}\right)\right]}$$

Understanding Diffusion Models:
A Unified Perspective

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

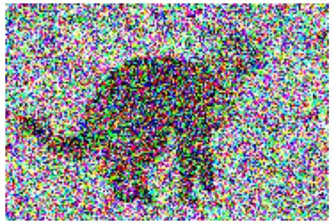
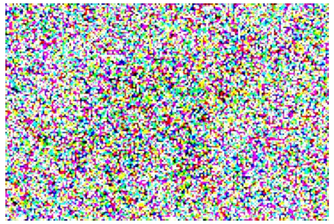
DDPM: Lower bound of $logP(x)$

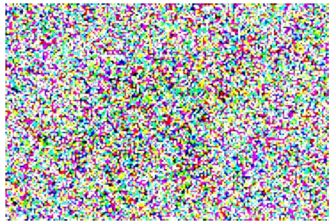
$$\mathrm{E}_{q(x_1|x_0)}[logP(x_0|x_1)] - KL\big(q(x_T|x_0)||P(x_T)\big)$$

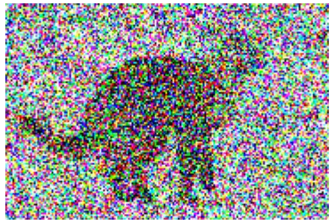
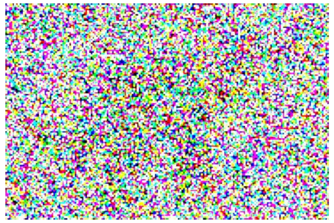
$$-\sum_{t=2}^{T} \mathrm{E}_{q(x_t|x_0)}\Big[KL\big(q(x_{t-1}|x_t, x_0)||P(x_{t-1}|x_t)\big)\Big]$$

$$E_{q(x_1|x_0)}[\log P(x_0|x_1)] - KL\left(q(x_T|x_0)||P(x_T)\right)$$

$$\boxed{-\sum_{t=2}^{T} E_{q(x_t|x_0)}\left[KL\left(\boxed{q(x_{t-1}|x_t, x_0)}||P(x_{t-1}|x_t)\right)\right]}$$

$q(x_t|x_0)$  $= \sqrt{\bar{\alpha}_t}$  $+ \sqrt{1-\bar{\alpha}_t}$ 

$q(x_{t-1}|x_0)$  $= \sqrt{\bar{\alpha}_{t-1}}$  $+ \sqrt{1-\bar{\alpha}_{t-1}}$ 

$q(x_t|x_{t-1})$  $= \sqrt{1-\beta_t}$  $+ \sqrt{\beta_t}$ 

$$\mathrm{E}_{q(x_1|x_0)}[\log P(x_0|x_1)] - KL\big(q(x_T|x_0)||P(x_T)\big)$$

$$-\sum_{t=2}^{T} \boxed{\mathrm{E}_{q(x_t|x_0)}\Big[KL\big(\boxed{q(x_{t-1}|x_t,x_0)}||P(x_{t-1}|x_t)\big)\Big]}$$

x_0

$q(x_t|x_0)$

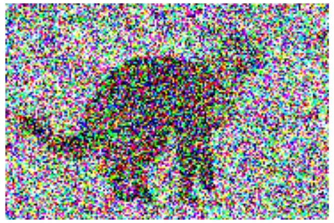
$q(x_{t-1}|x_0)$

$q(x_t|x_{t-1})$

x_{t-1}

已知

Gaussian



x_t

已知

Gaussian

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

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

已知

Gaussian

$$
\begin{aligned}
q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0) &= \frac{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}{q(\boldsymbol{x}_t|\boldsymbol{x}_0)} && (71)\\
&= \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})} && (72)\\
&\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\} && (73)\\
&= \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\} && (74)\\
&= \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\} && (75)\\
&\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\} && (76)\\
&= \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\} && (77)\\
&= \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\} && (78)\\
&= \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\} && (79)\\
&= \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\} && (80)\\
&= \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\} && (81)\\
&= \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\} && (82)\\
&= \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\} && (83)\\
&\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)}) && (84)
\end{aligned}
$$

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

$$\mathrm{E}_{q(x_1|x_0)}[\log P(x_0|x_1)] - KL\big(q(x_T|x_0)||P(x_T)\big)$$

$$-\sum_{t=2}^{T} \boxed{\mathrm{E}_{q(x_t|x_0)}\Big[KL\big(\boxed{q(x_{t-1}|x_t, x_0)}||P(x_{t-1}|x_t)\big)\Big]}$$

Mean

Variance

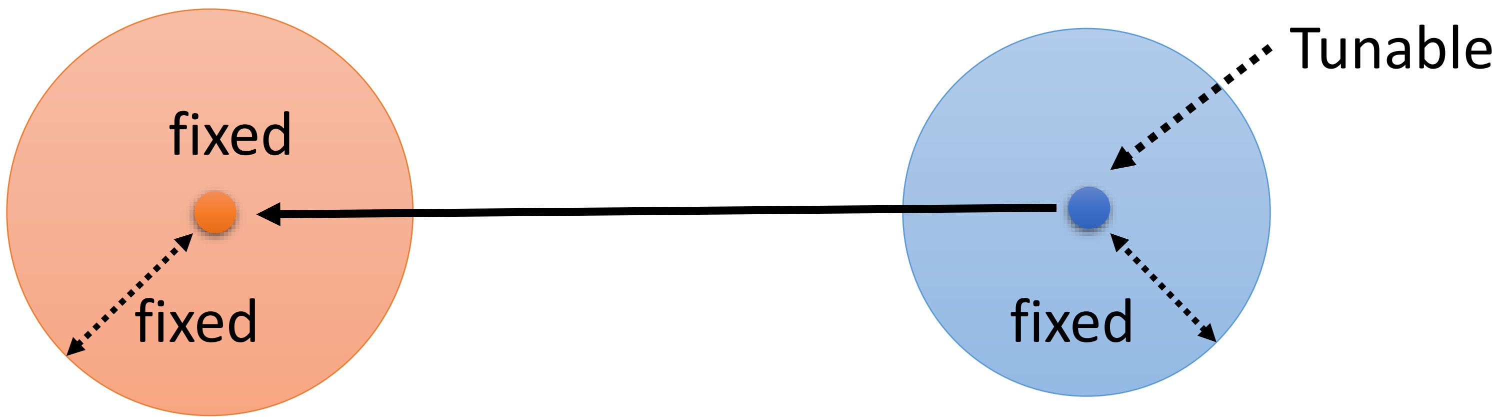
$$\frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t x_0 + \sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t}{1-\bar{\alpha}_t}$$

$$\frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t I$$

$$\mathrm{E}_{q(x_1|x_0)}[logP(x_0|x_1)] - KL(q(x_T|x_0)||P(x_T))$$

$$-\sum_{t=2}^{T} \boxed{\mathrm{E}_{q(x_t|x_0)}[KL(q(x_{t-1}|x_t, x_0)||P(x_{t-1}|x_t))]}$$

How to minimize KL divergence?



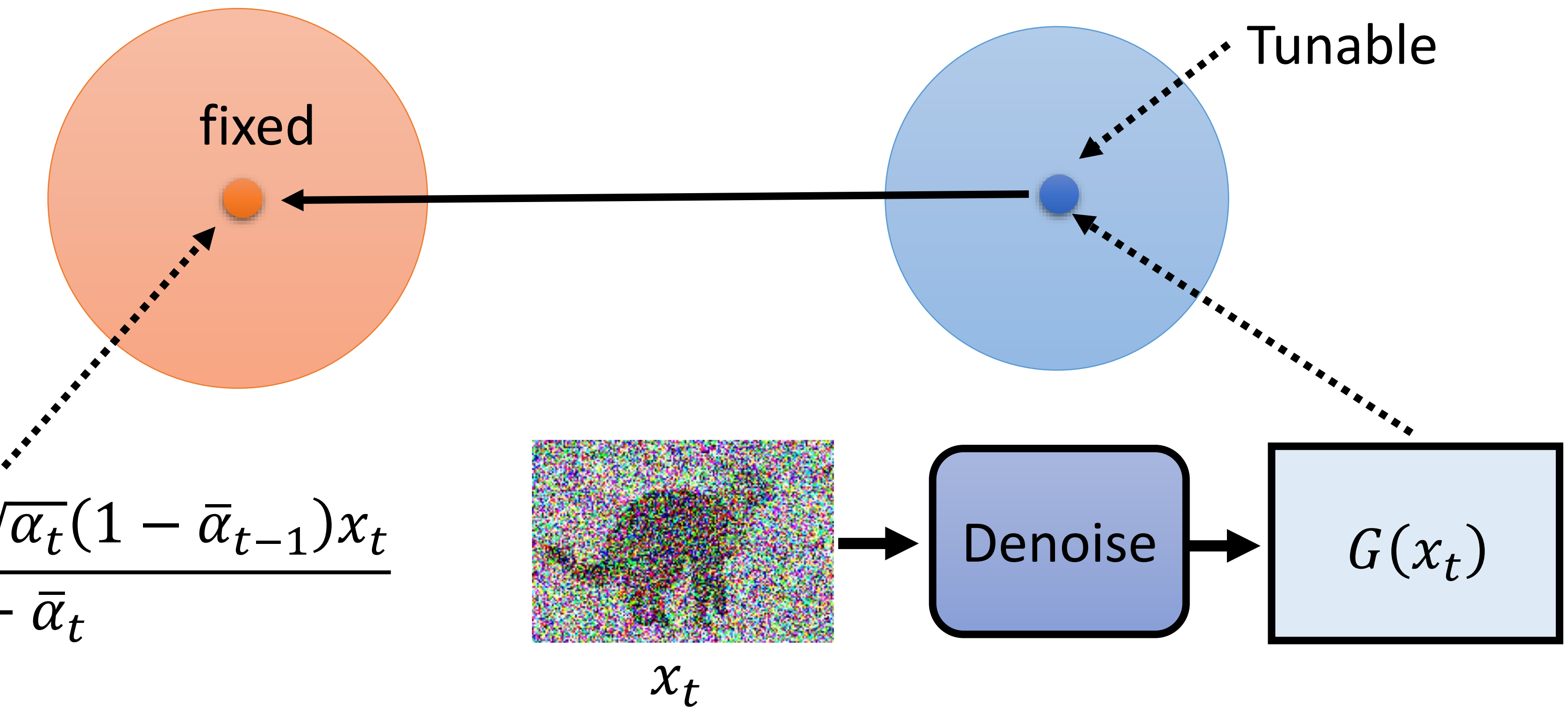
Recall that the KL Divergence between two Gaussian distributions is:

$$D_{\mathrm{KL}}(\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_x, \boldsymbol{\Sigma}_x) \parallel \mathcal{N}(\boldsymbol{y}; \boldsymbol{\mu}_y, \boldsymbol{\Sigma}_y)) = \frac{1}{2}\left[\log \frac{|\boldsymbol{\Sigma}_y|}{|\boldsymbol{\Sigma}_x|} - d + \mathrm{tr}(\boldsymbol{\Sigma}_y^{-1}\boldsymbol{\Sigma}_x) + (\boldsymbol{\mu}_y - \boldsymbol{\mu}_x)^T \boldsymbol{\Sigma}_y^{-1}(\boldsymbol{\mu}_y - \boldsymbol{\mu}_x)\right]$$

$$\mathrm{E}_{q(x_1|x_0)}[logP(x_0|x_1)] - KL\big(q(x_T|x_0)||P(x_T)\big)$$

$$-\sum_{t=2}^{T} \boxed{\mathrm{E}_{q(x_t|x_0)}\big[KL\big(q(x_{t-1}|x_t, x_0)||P(x_{t-1}|x_t)\big)\big]}$$

How to minimize KL divergence?

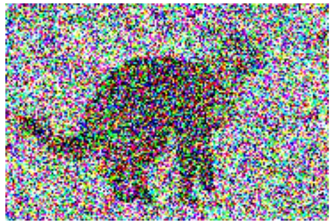


$$\frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t x_0 + \sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t}{1-\bar{\alpha}_t}$$

$$\mathrm{E}_{q(x_1|x_0)}[logP(x_0|x_1)] - KL\big(q(x_T|x_0)||P(x_T)\big)$$

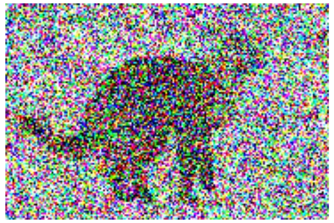
$$-\sum_{t=2}^{T} \boxed{\mathrm{E}_{q(x_t|x_0)}\Big[KL\big(q(x_{t-1}|x_t,x_0)||P(x_{t-1}|x_t)\big)\Big]}$$

Sample x_0



Sample x_t

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\varepsilon$$

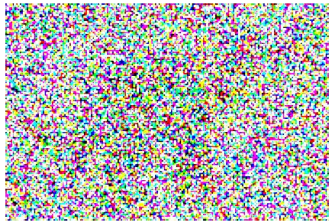


x_t

$= \sqrt{\bar{\alpha}_t}$

x_0

$+\sqrt{1-\bar{\alpha}_t}$

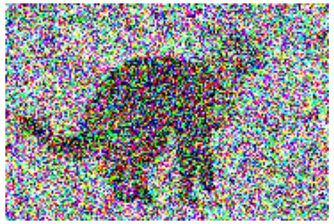


ε

$$\mathrm{E}_{q(x_1|x_0)}[logP(x_0|x_1)] - KL\big(q(x_T|x_0)||P(x_T)\big)$$

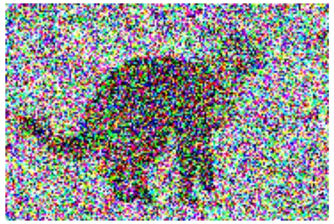
$$-\sum_{t=2}^{T} \boxed{\mathrm{E}_{q(x_t|x_0)}\big[KL\big(q(x_{t-1}|x_t, x_0)||P(x_{t-1}|x_t)\big)\big]}$$

x_0



Sample x_t

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} \varepsilon$$

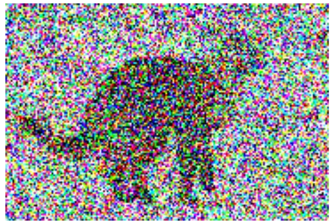


x_t

t

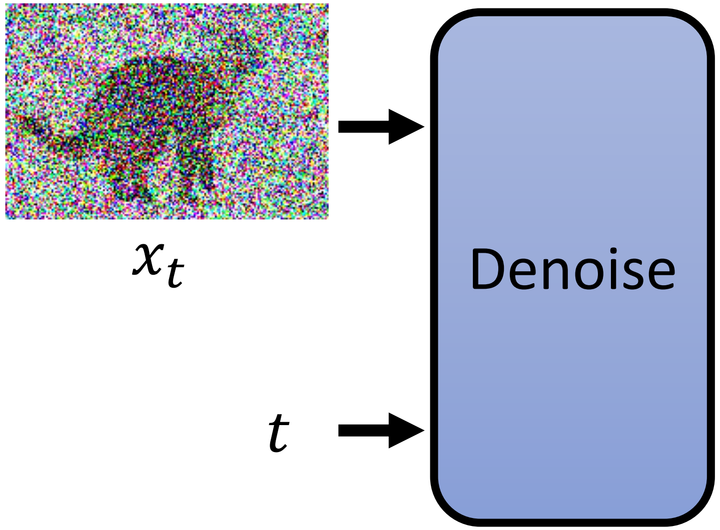
Denoise

?

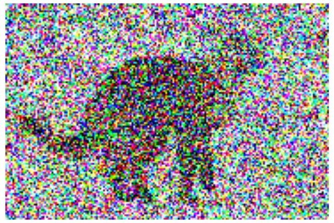


$$\frac{\sqrt{\bar{\alpha}_{t-1}} \beta_t x_0 + \sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1}) x_t}{1 - \bar{\alpha}_t}$$

x_0



$$? \longleftrightarrow \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t \boxed{x_0} + \sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t}{1-\bar{\alpha}_t}$$



Sample x_t

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\varepsilon$$

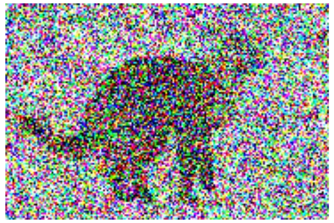
$$x_t - \sqrt{1-\bar{\alpha}_t}\varepsilon = \sqrt{\bar{\alpha}_t}x_0$$

$$\frac{x_t - \sqrt{1-\bar{\alpha}_t}\varepsilon}{\sqrt{\bar{\alpha}_t}} = x_0$$

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

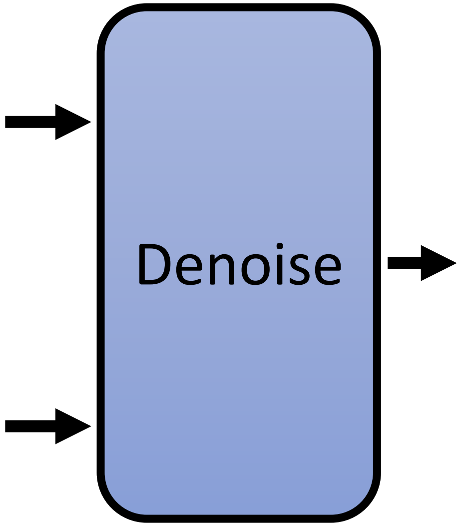
$$= \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon\right)$$

x_0



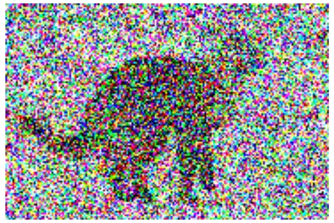
x_t

t



$$\frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boxed{\varepsilon}\right)$$

實際需要 network predict 的部分



Sample x_t

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\varepsilon$$

$$x_t - \sqrt{1-\bar{\alpha}_t}\varepsilon = \sqrt{\bar{\alpha}_t}x_0$$

$$\frac{x_t - \sqrt{1-\bar{\alpha}_t}\varepsilon}{\sqrt{\bar{\alpha}_t}} = x_0$$

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

Algorithm 2 Sampling

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

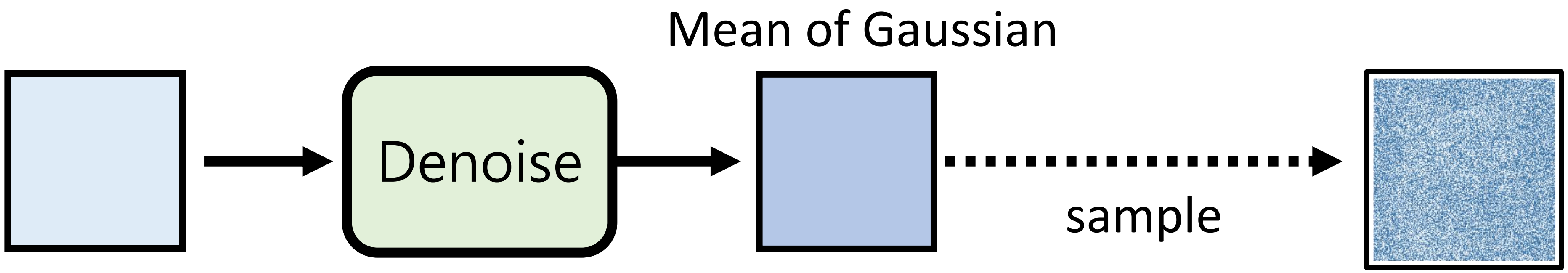
for $t = T, \dots, 1$ **do**

  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$

  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \underline{\sigma_t \mathbf{z}}$

end for

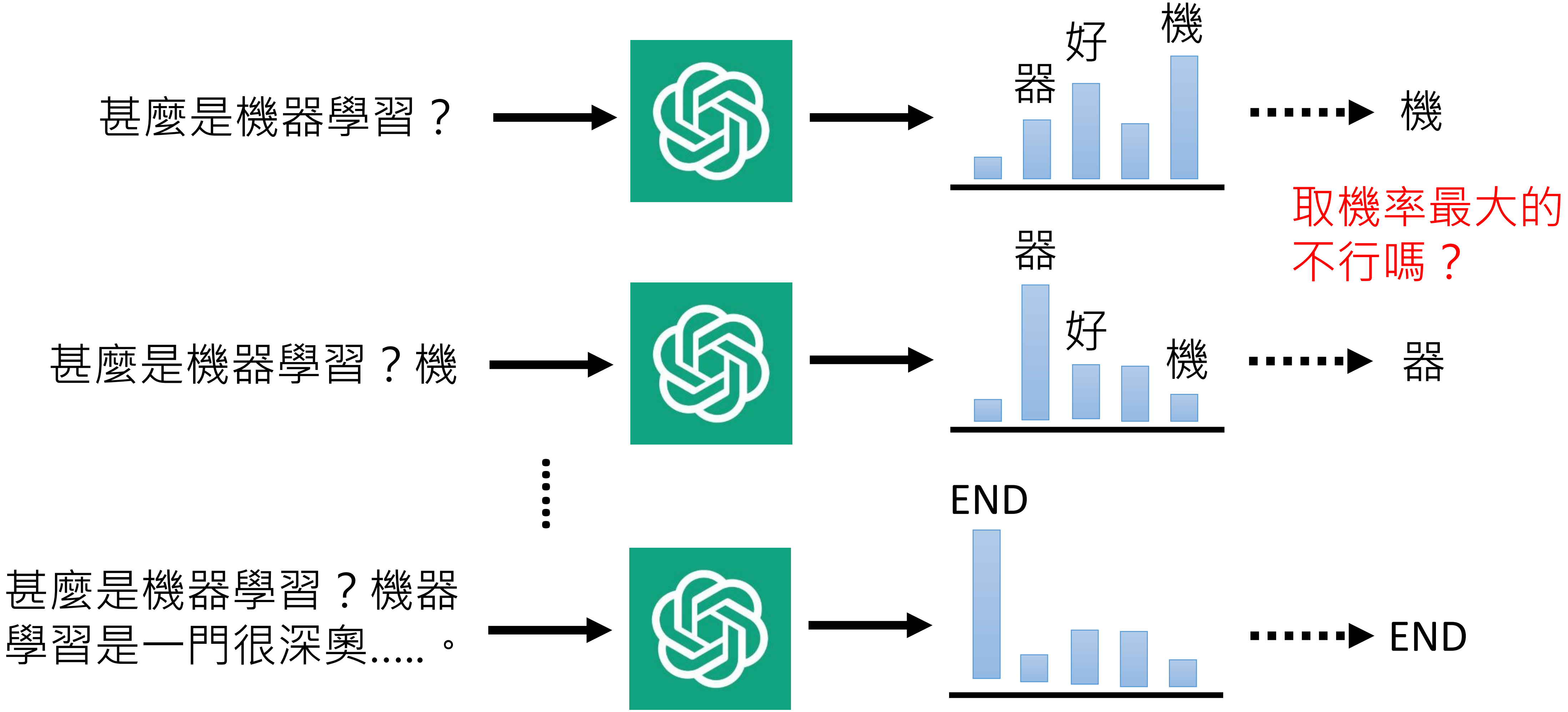
return $\mathbf{x}_0$



為什麼不直接取 Mean ?

免責聲明：以下只是猜測

為什麼生成文句時需要 Sample？



為什麼生成文句時需要 Sample？

- The Curious Case of Neural Text Degeneration

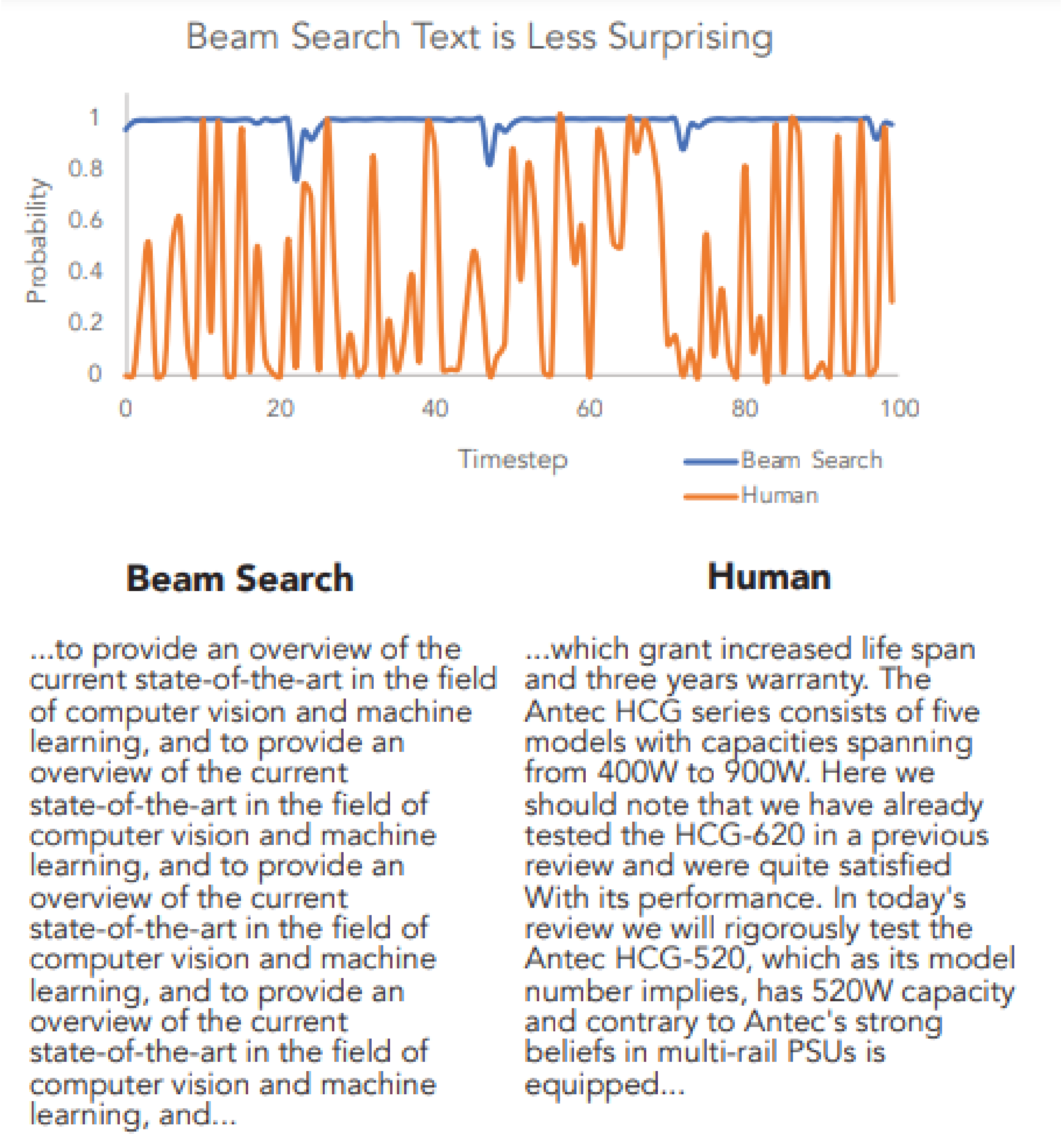
  https://arxiv.org/abs/1904.09751

Context: In a shocking finding, scientist discovered a herd of unicorns living in a remote, previously unexplored valley, in the Andes Mountains. Even more surprising to the researchers was the fact that the unicorns spoke perfect English.

Beam Search, *b*=32:
"The study, published in the Proceedings of the National Academy of Sciences of the United States of America (PNAS), was conducted by researchers from the Universidad Nacional Autónoma de México (UNAM) and the Universidad Nacional Autónoma de México (UNAM/Universidad Nacional Autónoma de México/Universidad Nacional Autónoma de México/Universidad Nacional Autónoma de México/Universidad Nacional Autónoma de ..."

Pure Sampling:
They were cattle called Bolivian Cavalleros; they live in a remote desert uninterrupted by town, and they speak huge, beautiful, paradisiacal Bolivian linguistic thing. They say, 'Lunch, marge.' They don't tell what the lunch is," director Professor Chuperas Omwell told Sky News. "They've only been talking to scientists, like we're being interviewed by TV reporters. We don't even stick around to be interviewed by TV reporters. Maybe that's how they figured out that they're cosplaying as the Bolivian Cavalleros."

https://arxiv.org/abs/1904.09751



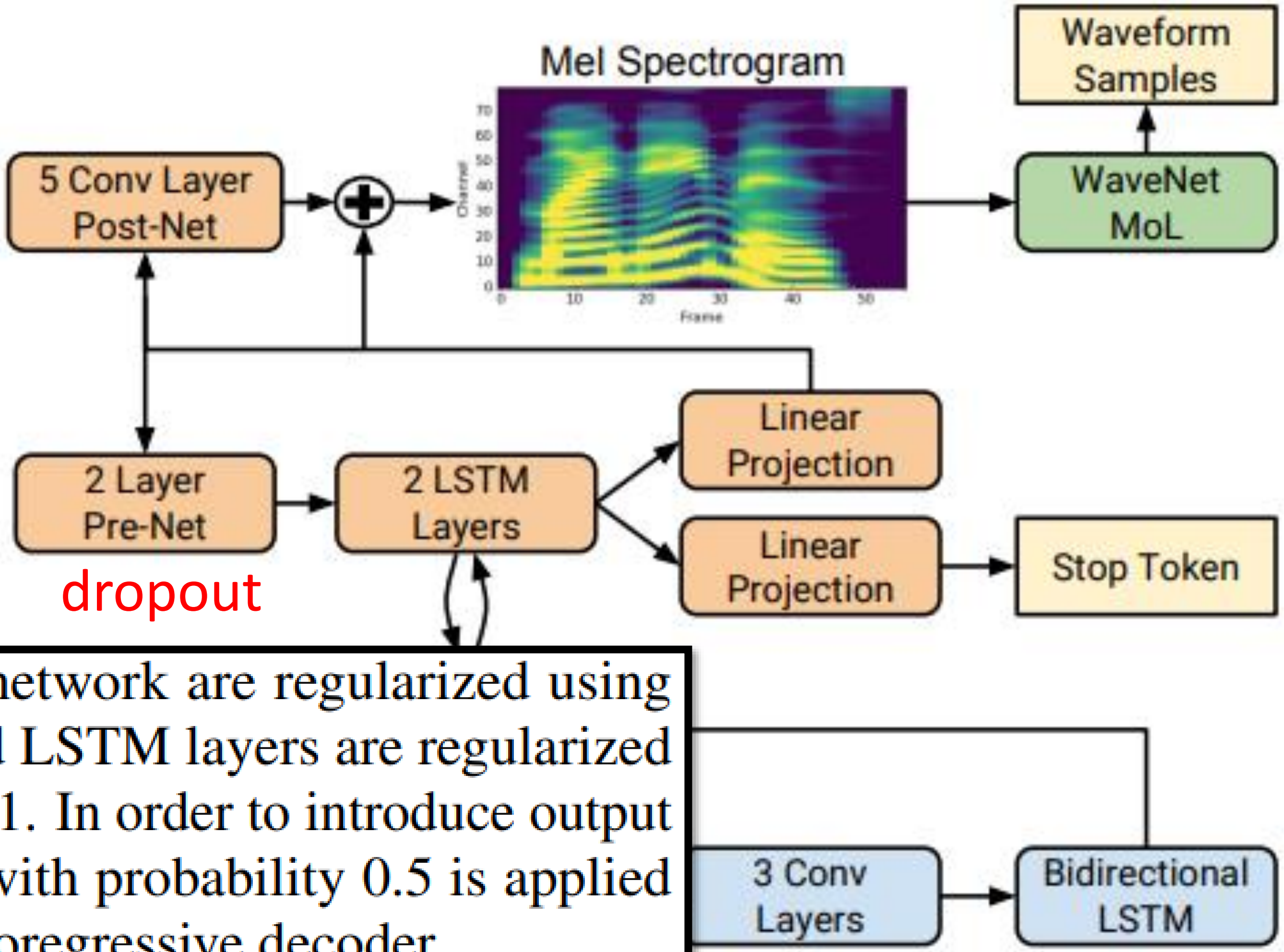
語音合成也需要 Sampling !

https://arxiv.org/abs/1712.05884

with dropout

without dropout

感謝杜濤同學提供實驗結果

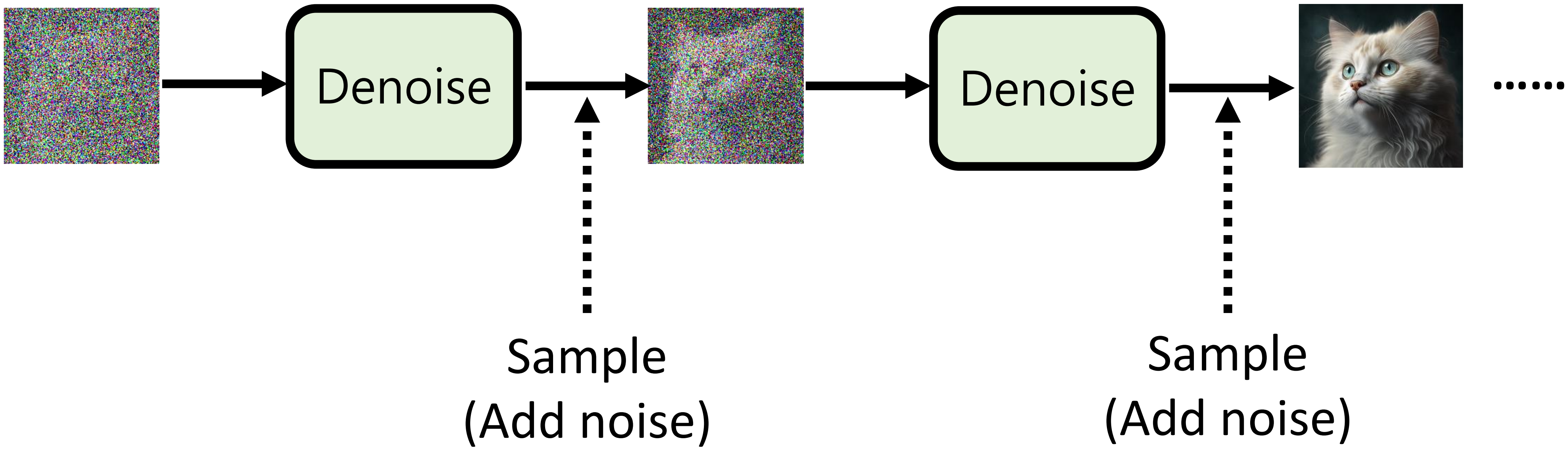


dropout

The convolutional layers in the network are regularized using dropout [25] with probability 0.5, and LSTM layers are regularized using zoneout [26] with probability 0.1. In order to introduce output variation at inference time, dropout with probability 0.5 is applied only to layers in the pre-net of the autoregressive decoder.

Diffusion Model 是一種 Autoregressive

「一次到位」改成「 N次到位」

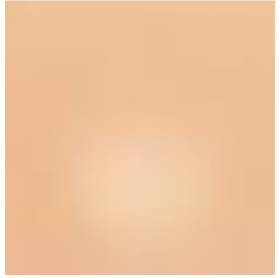


Algorithm 2 Sampling

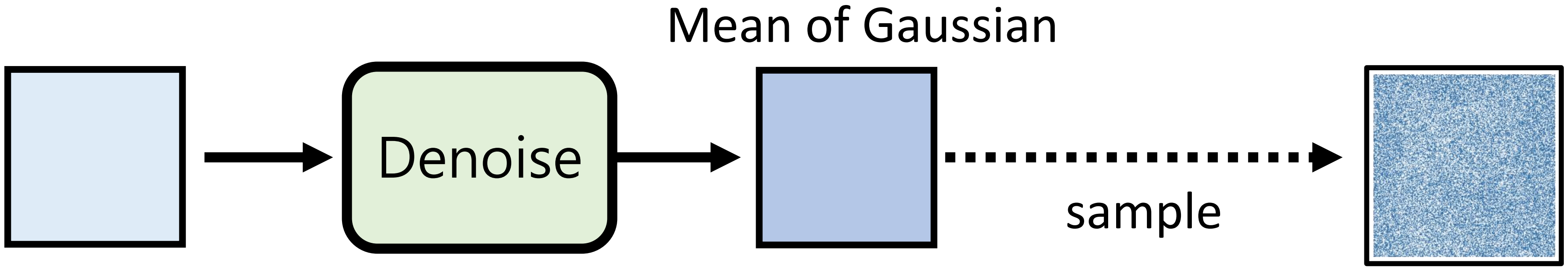
1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \ldots, 1$ **do**
3: $\quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\quad \mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t,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

σ_t as paper

$\sigma_t = 0$



感謝伏宇寬助
教提供結果



為什麼不直接取 Mean？

Denoising Diffusion Probabilistic Models

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

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

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 $\mathbf{z} = \mathbf{0}$

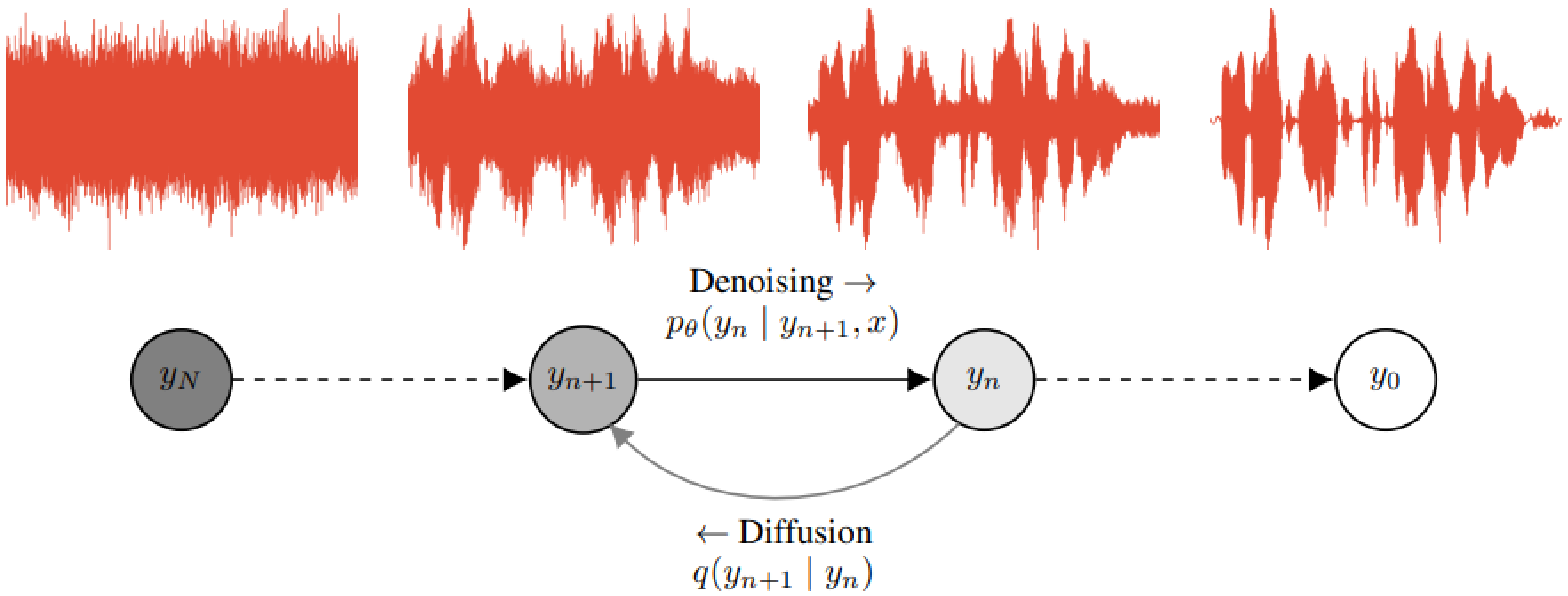
$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \boxed{\sigma_t \mathbf{z}}$$

end for

return $\mathbf{x}_0$

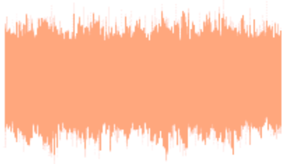
Diffusion Model for Speech

- WaveGrad



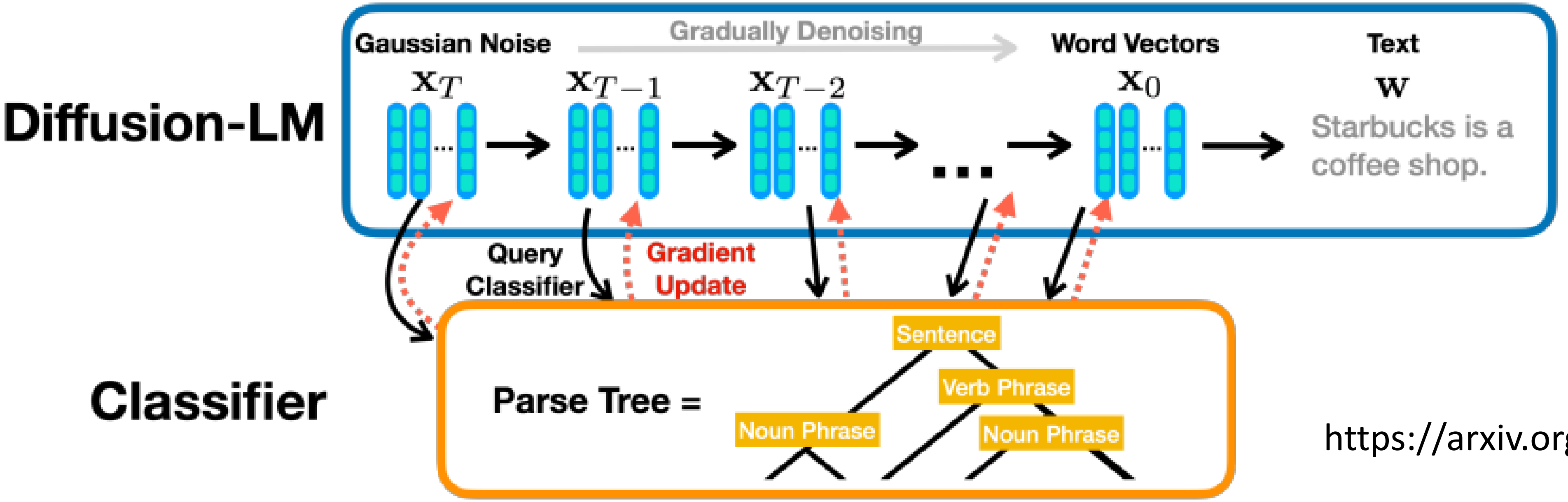
https://arxiv.org/abs/2009.00713

Diffusion Model for Text

- Difficulty: 你 好 嗎 ? → … → … → 

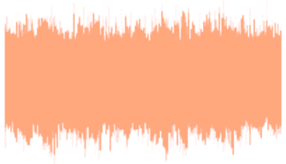
  Add noise

- Solution: Noise on latent space



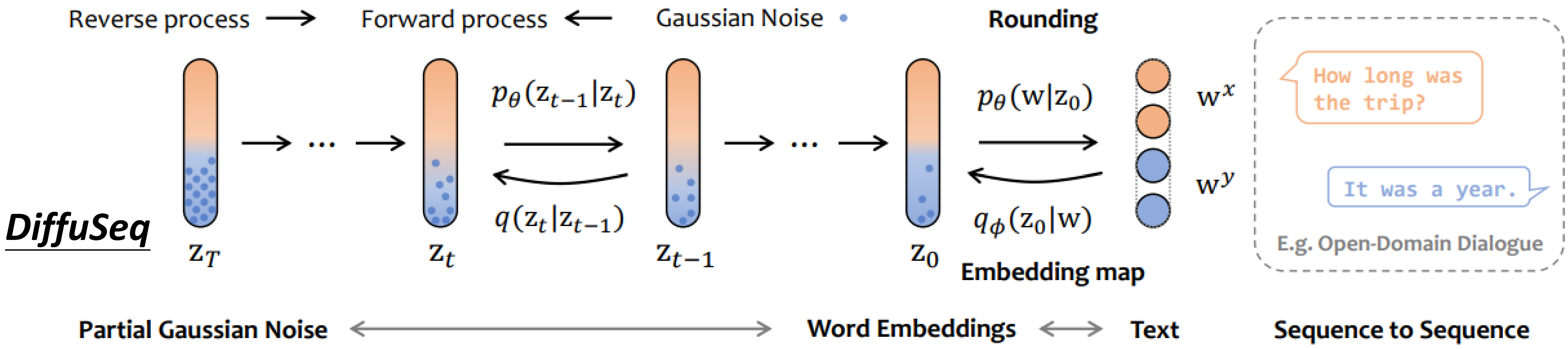
https://arxiv.org/abs/2205.14217

Diffusion Model for Text

- Difficulty: 你 好 嗎？ → … → … → 

  Add noise

- Solution: Noise on latent space



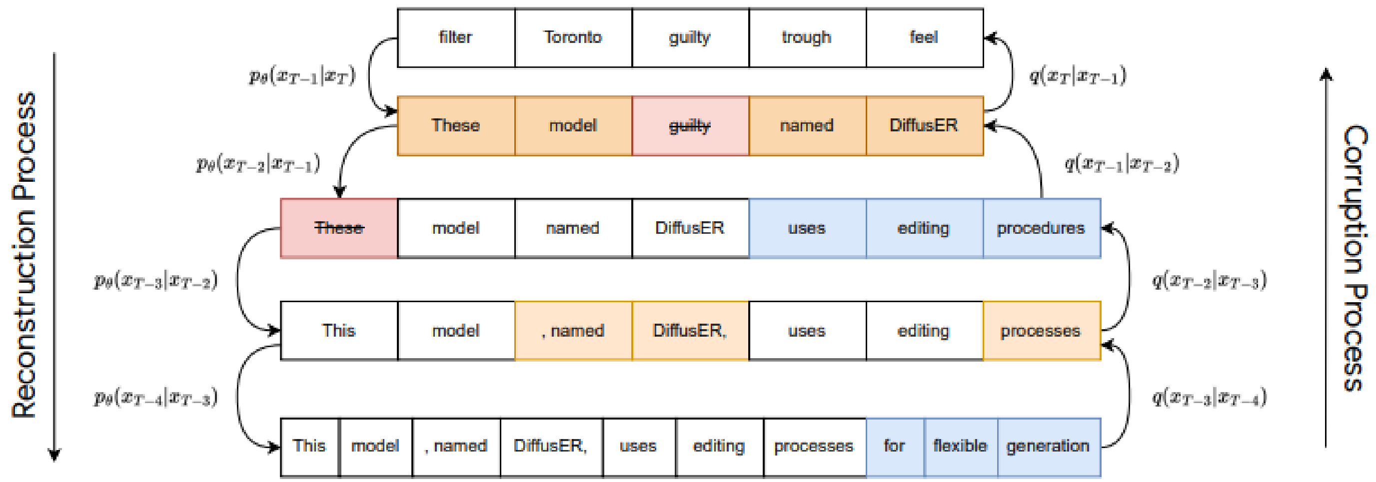
https://arxiv.org/abs/2210.08933

Diffusion Model for Text

- Solution: Don’t add Gaussian noise

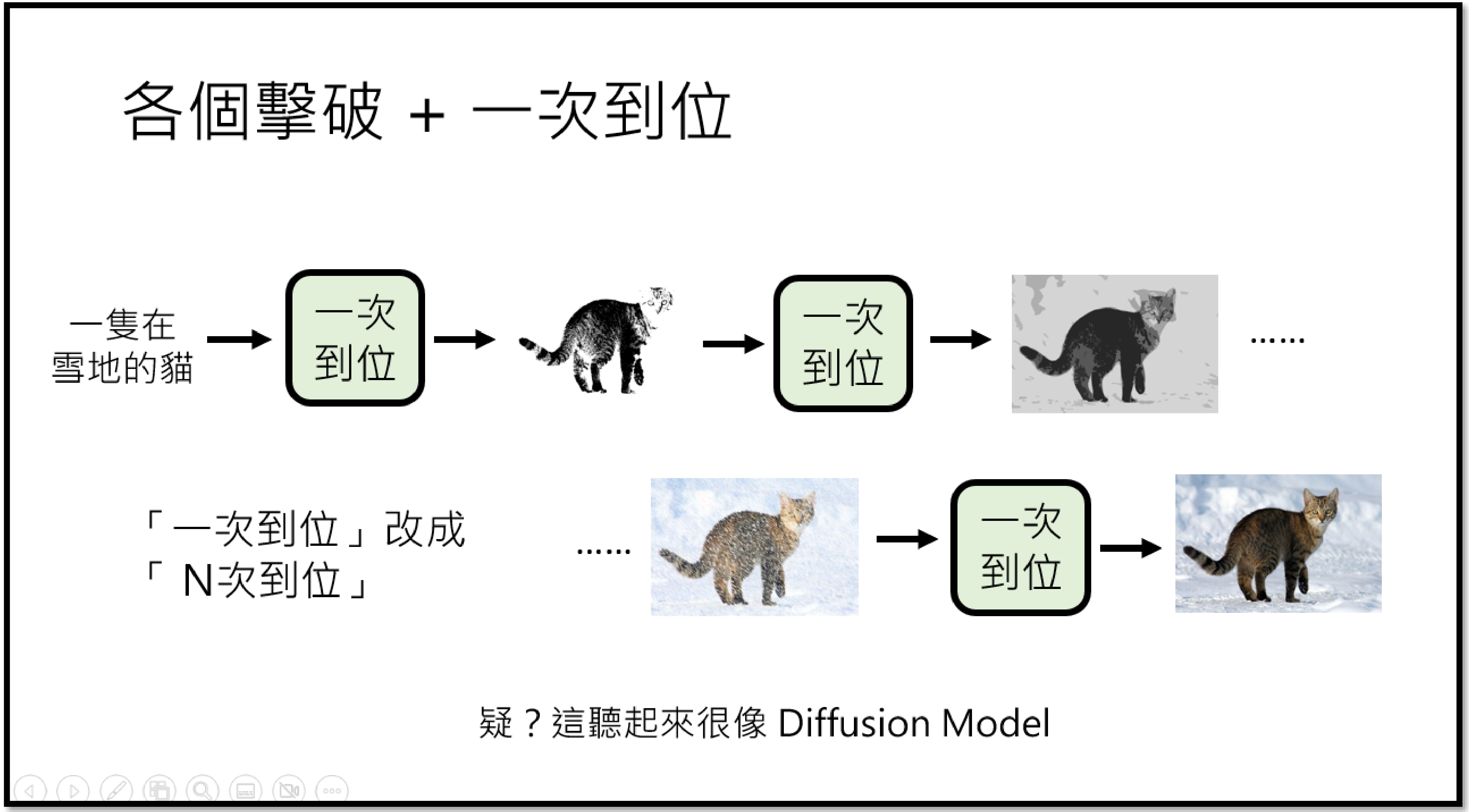
https://arxiv.org/abs/2210.16886

Diffusion via Edit-based Reconstruction (DiffusER)



t = 128 **[MASK] [MASK] [MASK] [MASK] [MASK] [MASK]**...
t = 25 In response **[MASK]** the demands , **[MASK] [MASK]**y Workers union said **[MASK]** backflow fund **[MASK]**s would face further investigation and a fine.
t = 0 In response to the demands , the Community Workers union said the backflow fund managers would face further investigation and a fine .

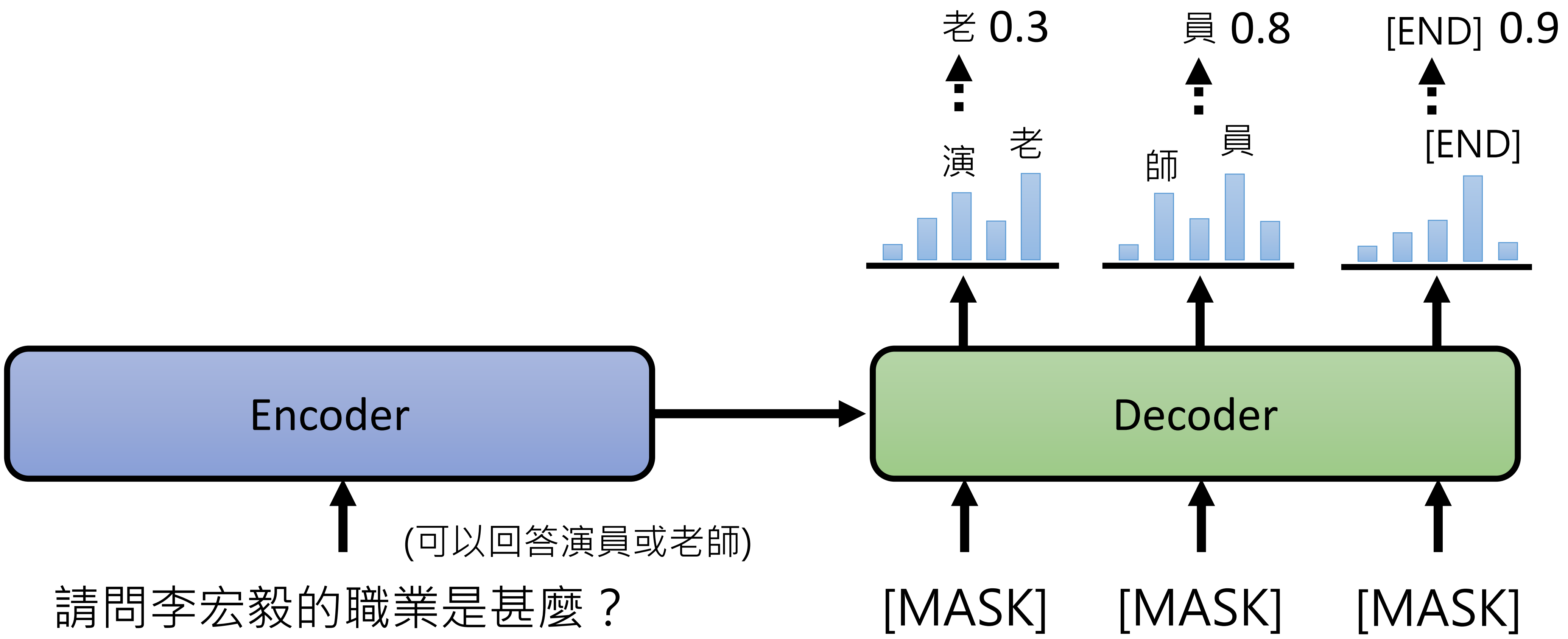
https://arxiv.org/abs/2107.03006


各個擊破 + 一次到位
一隻在
雪地的貓
一次
到位
一次
到位
......
「一次到位」改成
「 N次到位」
......
一次
到位
疑？這聽起來很像 Diffusion Model

之前上課投影片

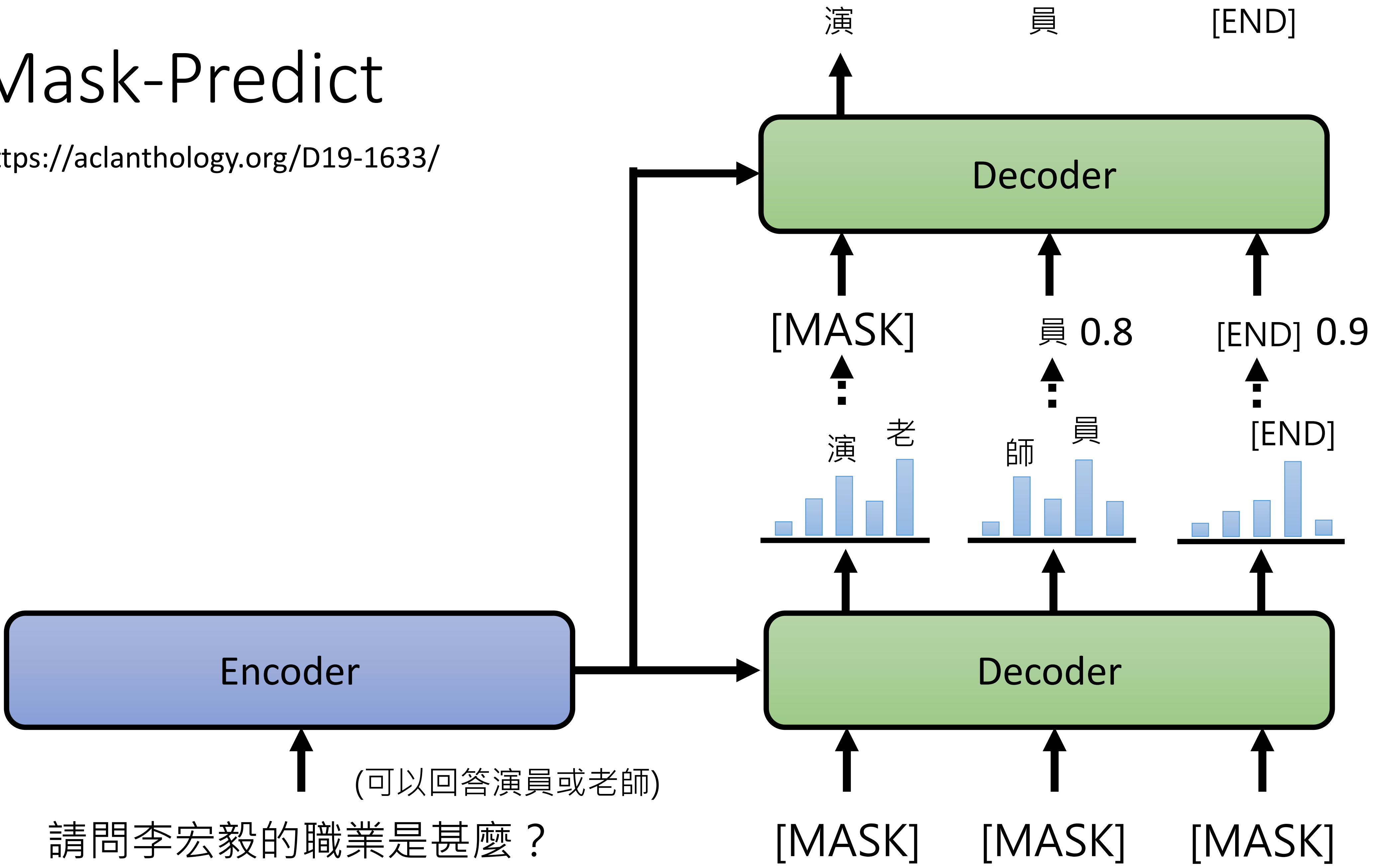
Mask-Predict

https://aclanthology.org/D19-1633/



Mask-Predict

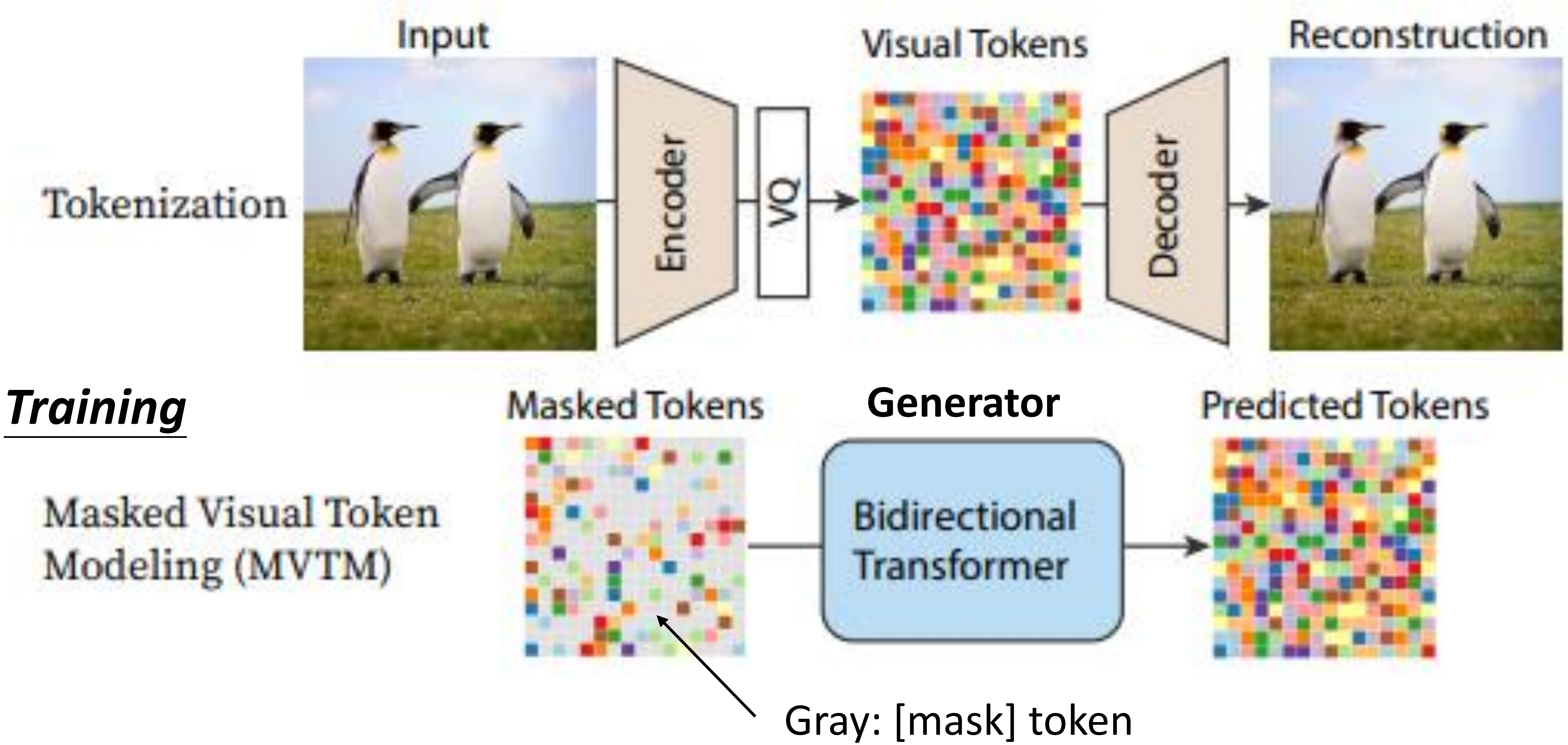
https://aclanthology.org/D19-1633/

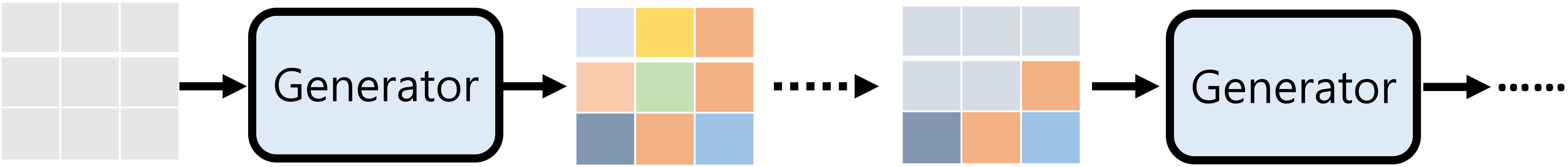


Mask-Predict

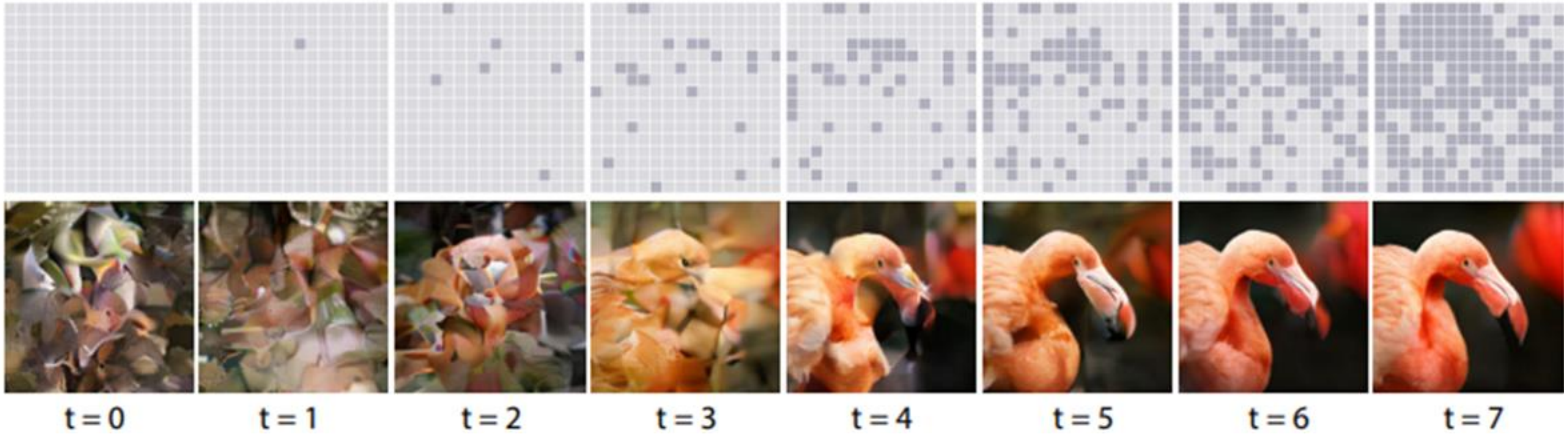
https://arxiv.org/abs/2202.04200

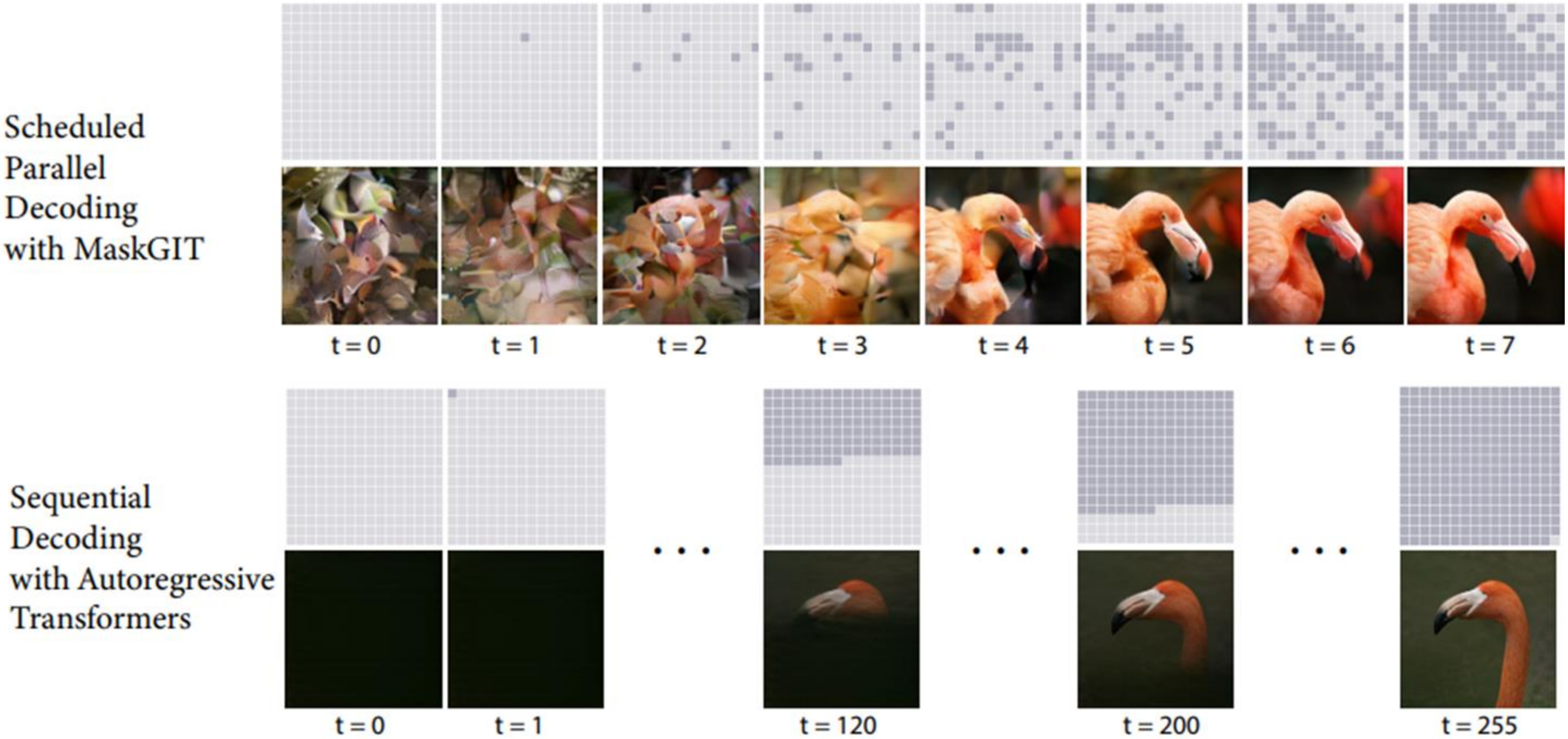
https://arxiv.org/abs/2301.00704





Scheduled Parallel Decoding with MaskGIT




Scheduled Parallel Decoding with MaskGIT
t = 0
t = 1
t = 2
t = 3
t = 4
t = 5
t = 6
t = 7
Sequential Decoding with Autoregressive Transformers
t = 0
t = 1
t = 120
t = 200
t = 255