# Diffusion Model 扩散模型

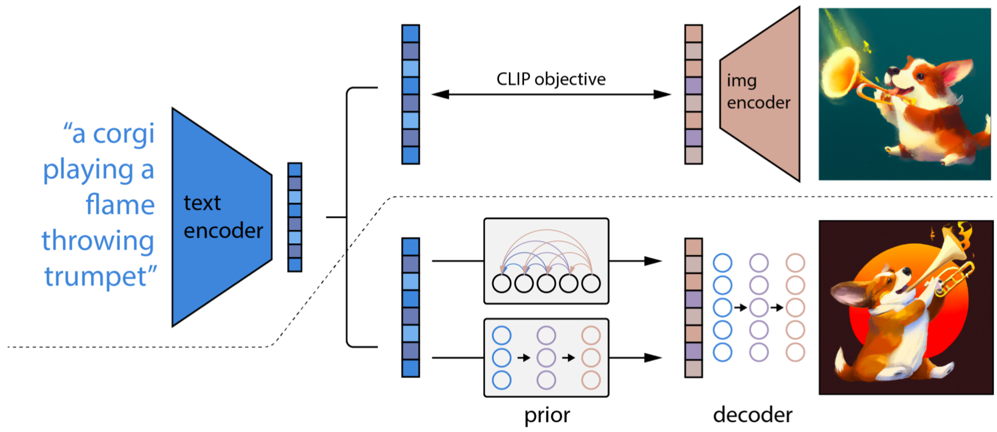
😎 Edited at 2022-10-28 by **Song1xinn**

## 1. Introduce

### 1.1 DALL·E 2

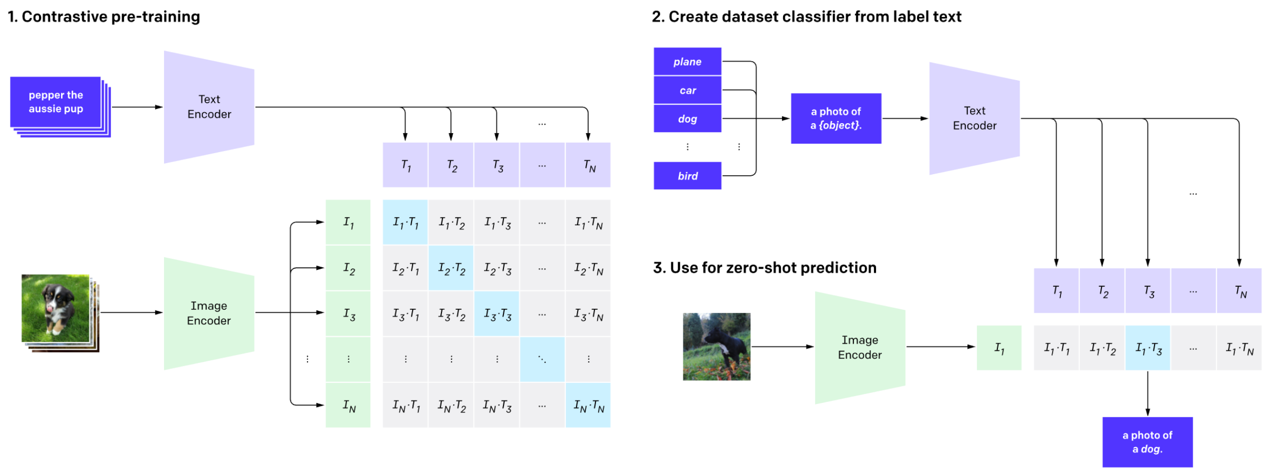
> DALL·E2：https://openai.com/dall-e-2/  DALL·E mini：https://huggingface.co/spaces/dalle-mini/dalle-mini
> Imagen / Parti - Google

DALL·E 2  CLIP + diffusion model

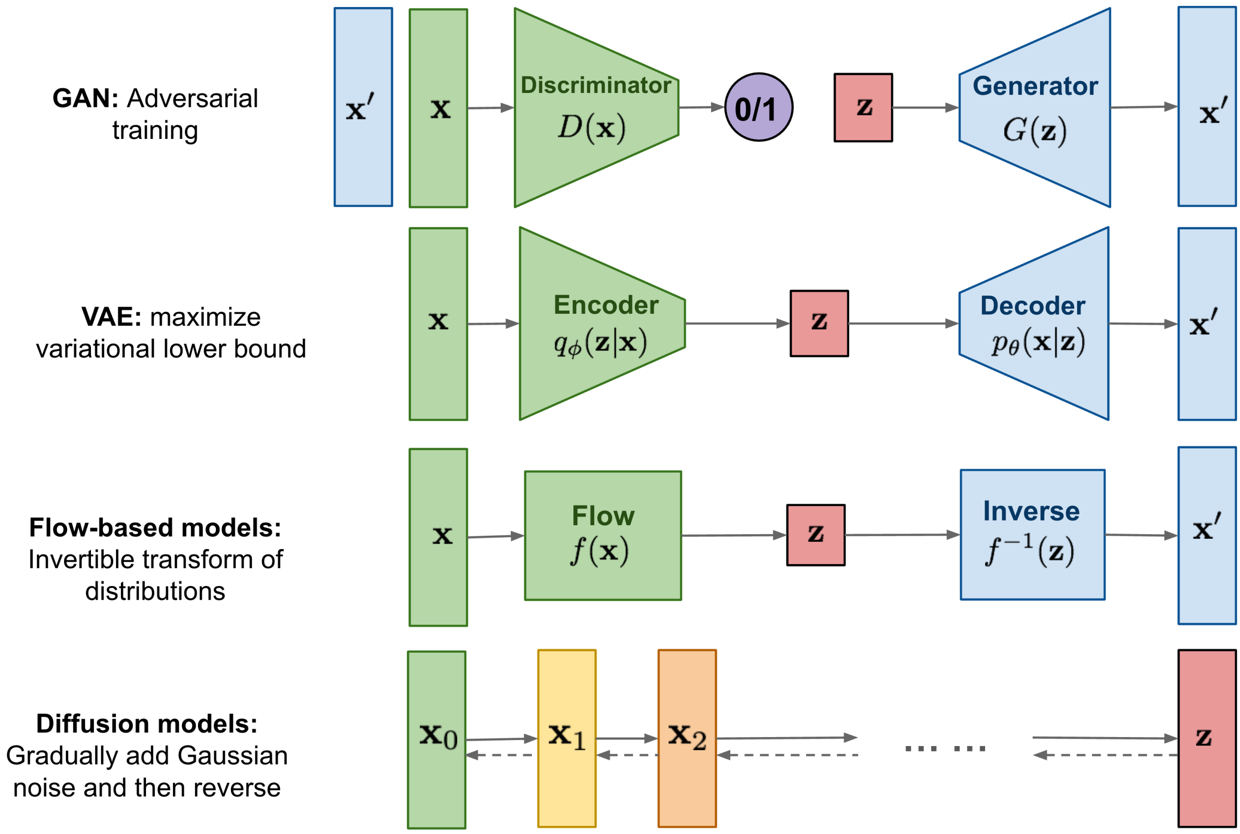



CLIP

> 1 CLIP pre-trains an image encoder and a text encoder to predict which images were paired with which texts in our dataset. 2 Then use this behavior to turn CLIP into a **zero-shot classifier**. 3 Convert all of a dataset's classes into captions such as "a photo of a *dog*" and **predict the class of the caption** with a given image.



## 1.2 Generation Models

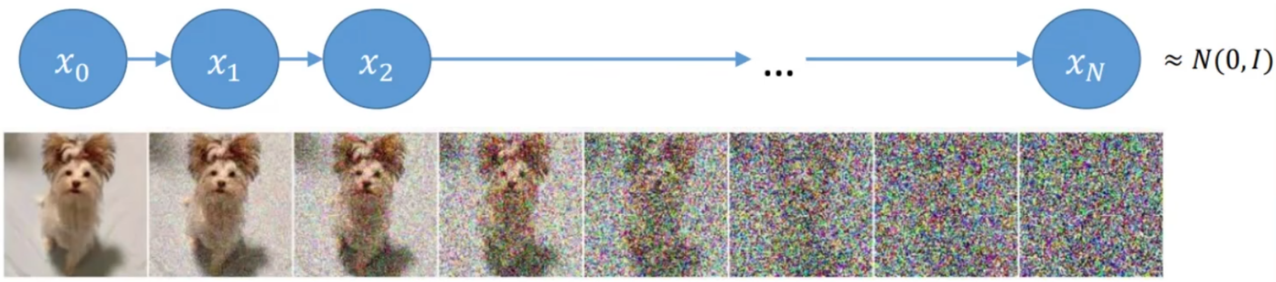



## 2. What's Diffusion Model

前提：所有的图像都满足自然中的分布（distribution），比如所有带有小猫的图都遵循一种分布、所有带有小狗的图都遵循一种分布。

### 2.1 Forward diffusion process（Training Process ONLY）

> Given a data point sampled from a real data distribution $x_0 \sim q(x)$, let us define a ***forward diffusion process*** in which we add small amount of **Gaussian noise** to the sample in $T$ steps, producing a sequence of noisy samples $x_1, \ldots, x_T$. The data sample $x_0$ gradually loses its distinguishable features as the step $t$ becomes larger. Eventually when $T \to \infty$, $x_T$ is equivalent to an isotropic Gaussian distribution.




**目标**：$q(x_T|x_0)$

给定如下公式，其中 $\beta_t \in (0,1)_{t=1}^{T}$，可以理解为添加的噪声的占比，是自定的函数，所以可以看作已知量。

$$\alpha_t = 1 - \beta_t \tag{1}$$

那么，如果已知 $x_{t-1}$，我们设定 $x_t$ 为下述公式，其中 $\epsilon_t$ 表示时刻 $t$ 加的噪声：

$$x_t = \sqrt{\alpha_t} x_{t-1} + \sqrt{1-\alpha_t}\epsilon_t \tag{2}$$

同理，$x_{t-1}$ 可以由 $x_{t-2}$ 表示，再由于每一次添加噪声都是从高斯分布中采样的噪声，即 $\epsilon_t \sim N(0, \boldsymbol{I})$，基于此，我们还能推理得到 $x_t$ 与 $x_{t-2}$ 的关系，其中 $\epsilon$ 合并了两个高斯分布：

$$\begin{aligned} x_t &= \sqrt{\alpha_t}(\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{1-\alpha_{t-1}}\epsilon_{t-1}) + \sqrt{1-\alpha_t}\epsilon_t \\ &= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{\alpha_t}\sqrt{1-\alpha_{t-1}}\epsilon_{t-1} + \sqrt{1-\alpha_t}\epsilon_t \\ &= \sqrt{\alpha_t\alpha_{t-1}}x_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\epsilon \end{aligned} \tag{3}$$

**数学解释**

- 关于 $\epsilon_t$ 的高斯分布可以写作：$\epsilon_t \sim N(0, \sigma_1^2)$，乘上 $w$ 后方差变为 $\sigma_1^2 * w^2$，加上 $b$ 后均值变为 $0 + b$。
- 如果两个相互独立的高斯分布$\epsilon_1 \sim N(\mu_1, \sigma_1^2), \epsilon_2 \sim N(\mu_2, \sigma_2^2)$，那么 $\epsilon = (a\epsilon_1 \pm b\epsilon_2) \sim N(a\mu_1 \pm b\mu_2, a^2\sigma_1^2 + b^2\sigma_2^2)$
- 现在有两个高斯分布：$\sqrt{\alpha_t(1-\alpha_{t-1})}\epsilon_{t-1} \sim N(0, \alpha_t(1-\alpha_{t-1}))$，$\sqrt{1-\alpha_t}\epsilon_t \sim N(0, 1-\alpha_t)$ 两个分布相加可以得到：$\sqrt{\alpha_t(1-\alpha_{t-1})}\epsilon_{t-1} + \sqrt{1-\alpha_t}\epsilon_t \sim N(0, 1-\alpha_t\alpha_{t-1})$

可以推理得到 $x_t$ 与 $x_0$ 的关系，其中 $\bar{\alpha}_t$ 表示累乘：

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon \tag{4}$$

**回到概率分析**

给定初始的数据分布 $x_0 \sim q(x)$，可以不断地向分布中添加高斯噪声，该噪声的方差以固定值 $\beta_t$ 确定，均值以 $\beta_t$ 和当前时刻 $t$ 的数据 $x_t$ 决定。基于前一时刻去预测后一时刻是一个条件概率分布，给定 $x_0$，$x_1$ 到 $x_T$ 的联合概率分布可以写为条件概率分布相乘：

$$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1}) \qquad q(x_t|x_{t-1}) = N(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t\boldsymbol{I}) \tag{5}$$

公式 (5) 中可以看出这个分布的均值是 $\sqrt{1-\beta_t}x_{t-1}$，方差是 $\beta_t$，可以得到由 $x_{t-1}$ 表示的 $x_t$，也就是公式 (2)。和前面的推理原理相同，通过对高斯分布的相加，得到 $x_t$ 关于 $x_0$ 的条件概率分布。

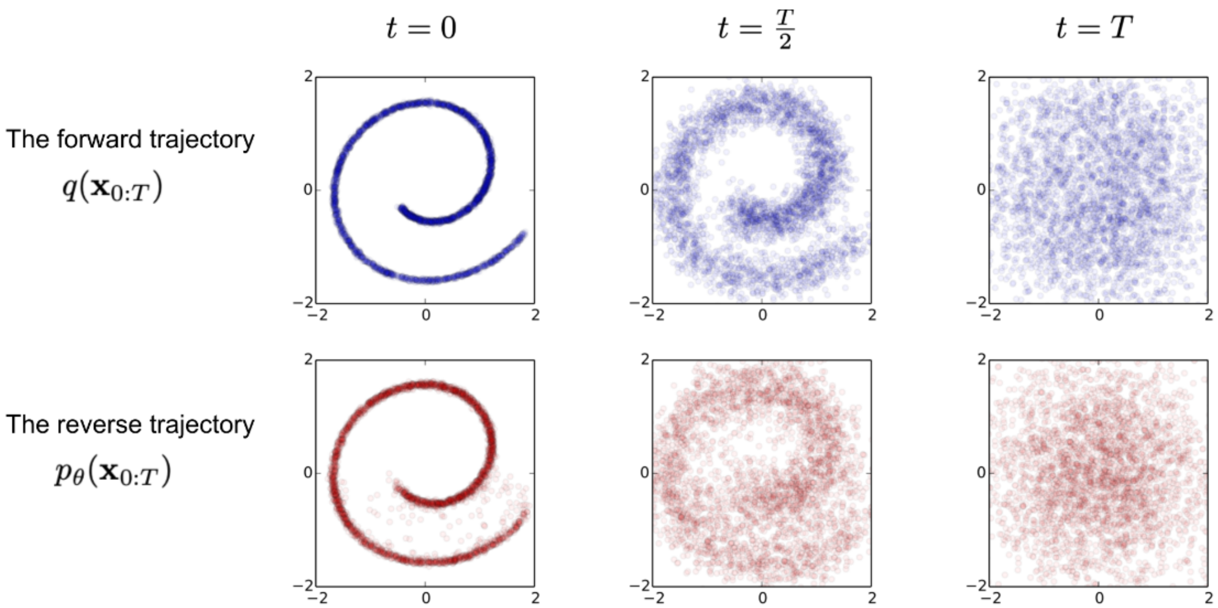
$$q(x_t|x_0) = N(x_t; \sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_t)\boldsymbol{I}) \tag{6}$$

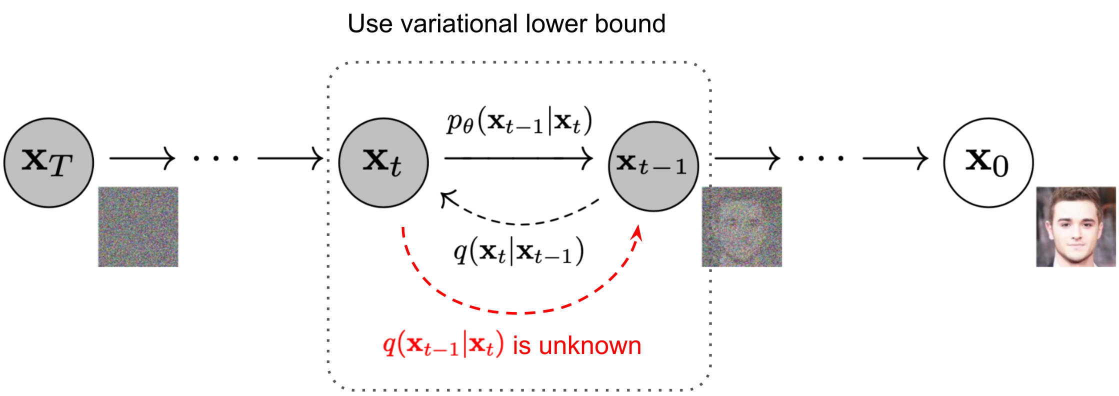
随着 $t$ 的不断增大，当 $T \to \infty$，最终数据分布 $x_T$ 变成了一个各向独立的高斯分布。
注意，前向过程不包括任何需要学习的参数。

🤔 Question **Why forward diffusion process ?**

## 2.2 Reverse diffusion process

> if we can reverse the above process and sample from $q(x_{t-1}|x_t)$, we will be able to recreate the true sample from a Gaussian noise input, $x_T \sim N(0, I)$. Note that if $\beta_t$ is small enough, $q(x_{t-1}|x_t)$ will also be Gaussian. Unfortunately, we cannot easily estimate $q(x_{t-1}|x_t)$ because it needs to use the entire dataset and therefore we need to learn a **model** $p_\theta$ to approximate these conditional probabilities in order to run the *reverse diffusion process*.




**目标：** $p_\theta(x_0|x_T)$

逆过程是从高斯噪声中回复原始数据，所以可以假设其也是一个高斯分布，在这里需要构建一个模型 $p_\theta$ 来通过给定的噪声来预测出训练集的分布，从而可以通过从分布中采样来生成新的样本。

$$p_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t) \qquad p_\theta(x_{t-1}|x_t) = N(x_{t-1};\mu_\theta(x_t,t),\Sigma_\theta(x_t,t)) \tag{7}$$

由于反向过程没办法直接求得 $x_0$ 与 $x_t$ 之间的关系，即无法直接从噪声到图像，那么我们转换方式，我们可以先求 $x_{t-1}$，$x_{t-2}$ ... 直到得到$x_0$，即先求 $q(x_{t-1}|x_t)$，再进一步建模。若给定 $x_t, x_0$ 后验扩散条件概率 $q(x_{t-1}|x_t,x_0)$ 分布用公式表达：

$$q(x_{t-1}|x_t,x_0) = N(x_{t-1};\tilde{\mu}_t(x_t,x_0),\tilde{\beta}_t \boldsymbol{I}) \tag{8}$$

根据贝叶斯公式，有：

$$q(x_{t-1}|x_t,x_0) = q(x_t|x_{t-1},x_0)\frac{q(x_{t-1},x_0)}{q(x_t,x_0)} \tag{9}$$

将上式用分布表示，同时进行展开

$$\begin{aligned}(9)\ &\propto exp(-\frac{1}{2}(\frac{(x_t-\sqrt{\alpha_t}x_{t-1})^2}{\beta_t}+\frac{(x_{t-1}-\sqrt{\alpha_{t-1}}x_0)^2}{1-\bar{\alpha}_{t-1}}-\frac{x_t-\sqrt{\bar{\alpha}_t}x_0)^2}{1-\bar{\alpha}_t}))\\ &= exp(-\frac{1}{2}(\frac{x_t^2-2\sqrt{\alpha_t}x_t x_{t-1}+\alpha_t x_{t-1}^2}{\beta t}+\frac{x_{t-1}^2-2\sqrt{\bar{\alpha}_{t-1}}x_0x_{t-1}+\bar{\alpha}_{t-1}x_0^2}{1-\bar{\alpha}_{t-1}}-\frac{(x_t-\sqrt{\bar{\alpha}_t}x_0)^2}{1-\bar{\alpha}_t}))\\ &= exp(-\frac{1}{2}((\frac{\alpha_t}{\beta_t}+\frac{1}{1-\bar{\alpha}_{t-1}})x_{t-1}^2-(\frac{2\sqrt{\alpha_t}}{\beta_t}x_t+\frac{2\bar{\alpha}_{t-1}}{1-\bar{\alpha}_{t-1}}x_0)x_{t-1}+C(x_t,x_0)))\end{aligned} \tag{10}$$

**数学解释**

- 根据前向过程，可以得到：
  $q(x_t|x_{t-1},x_0) = \sqrt{\alpha_t}x_{t-1}+\sqrt{1-\alpha_t}\epsilon \sim N(\sqrt{\alpha_t}x_{t-1},1-\alpha_t)$
  $q(x_{t-1},x_0) = \sqrt{\bar{\alpha}_{t-1}}x_0+\sqrt{1-\bar{\alpha}_{t-1}}\epsilon \sim N(\sqrt{\bar{\alpha}_{t-1}}x_0,1-\bar{\alpha}_{t-1})$
  $q(x_t,x_0) = \sqrt{\alpha_t}x_0+\sqrt{1-\bar{\alpha}_t}\epsilon \sim N(\sqrt{\alpha_t}x_0,1-\bar{\alpha}_t)$
- 高斯分布的概率密度函数：$f(x) = \frac{1}{\sqrt{2\pi\sigma}}exp(-\frac{1}{2}(\frac{x-\mu}{\sigma})^2)$，于是有 $N(\mu,\sigma^2) \propto exp(-\frac{1}{2}(\frac{x-\mu}{\sigma})^2)$，展开后在 $exp$ 中，乘法就是相加，除法就是相减。

又因为 $exp(-\frac{1}{2}(\frac{x-\mu}{\sigma})^2) = exp(-\frac{1}{2}(\frac{1}{\sigma^2}x^2-\frac{2\mu}{\sigma^2}x+\frac{\mu^2}{\sigma^2}))$，所以根据 (10) 可以得到关于 $x_{t-1}$ 的分布方差和均值：

$$
\begin{aligned}
\tilde{\beta}_t &= \frac{1}{(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}})} = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \cdot \beta_t \\
\tilde{\mu}_t(x_t, x_0) &= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t} x_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t} x_0
\end{aligned} \tag{11}
$$

由于当前的已知是 $x_t$，在前向过程中推理了 $x_t$ 与 $x_0$ 的关系，那么利用公式 (4) 将 $x_0$ 用 $x_t$ 来近似，有:

$$
x_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1-\bar{\alpha}_t}\epsilon_t) \tag{12}
$$

$$
\tilde{\mu}_t = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_t) \tag{13}
$$

😳 Question **How to get $\epsilon_t$ ?** 🙌 *Train a model to predict it.*

## 2.3 Algrithms

### 2.3.1 Training (Predict the noise)

| **Algrithm 1 Training** | **Note** |
| --- | --- |
| 1: **repeat** | |
| 2: $x_0 \sim q(x_0)$ | $x_0$ 为分布 $q$ 中随机采样的图像（数据集中取数据） |
| 3: $t \sim Uniform(\{1, \dots, T\})$ | $t$ 即扩散次数，从 0 到 $T$，对不同的图像是不固定的 |
| 4: $\epsilon \sim N(0, I)$ | $\epsilon$ 高斯分布 $N(0, I)$ 中随机采样的噪声（从前向过程获得） |
| 5: Take gradient descent step on $\gradient_\theta \|\|ϵ−ϵ_θ(\sqrt{\bar α_t}x_0+\sqrt{1−\bar α_t}ϵ,t)\|\|^2 $ | $\epsilon_\theta$ 即训练的模型，括号内是输入：时间以及 $x_t$ |
| 6: **until** converged | |

### 2.3.2 Sampling (To get $x_0$)

| **Algrithm 2 Sampling** | **Note** |
|---|---|
| 1: $x_T \sim N(0, I)$ | $x_T$ 高斯分布 $N(0, I)$ 中随机采样的噪声 |
| 2: **for** $t = T, \ldots, 1$ **do** | |
| 3: $z \sim N(0, I)$ **if** $t > 1$ **, else** $z = 0$ | $t = 1$ 即 $x_0$ 时刻没有噪声，其他时刻都有从分布中采样的噪声（重参数） |
| 4: $x_{t-1} = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t)) + \sigma_t z$ | |
| 5: **end for** | |
| 6: **return** $x_0$ | |

## 3. Code

- diffusion model demo
- diffusion in DALL·E 2 （image generation）

## References:

[1] Radford A, Kim J W, Hallacy C, et al. Learning transferable visual models from natural language supervision[C]//International Conference on Machine Learning. PMLR, 2021: 8748-8763.
[2] **Ho J, Jain A, Abbeel P. Denoising diffusion probabilistic models[J]. Advances in Neural Information Processing Systems, 2020, 33: 6840-6851.**
[3] https://openai.com/dall-e-2/
[4] https://huggingface.co/spaces/dalle-mini/dalle-mini
[5] https://lilianweng.github.io/posts/2021-07-11-diffusion-models/
[6] https://www.bilibili.com/video/BV1b541197HX/?spm_id_from=333.788&vd_source=7020551ede7e34125c5de7acc9417f8d
[7] https://www.bilibili.com/video/BV1tY4y1N7jg/?spm_id_from=333.788.recommend_more_video.1&vd_source=7020551ede7e34125c5de7acc9417f8d
[8] https://github.com/heejkoo/Awesome-Diffusion-Models
[9] https://www.bilibili.com/video/BV1ad4y1c7vY/?spm_id_from=333.337.search-card.all.click&vd_source=7020551ede7e34125c5de7acc9417f8d