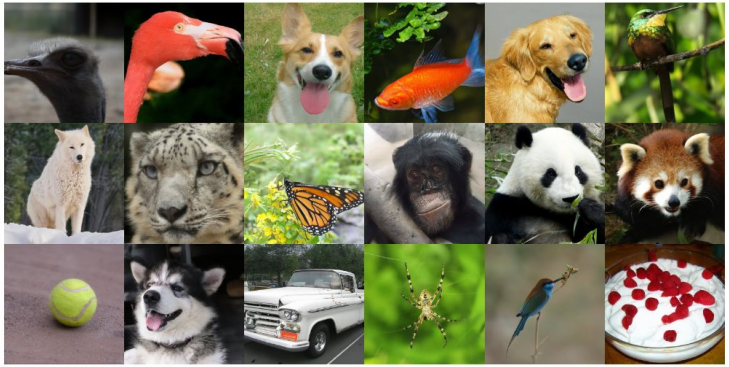
Deep Learning Architectures

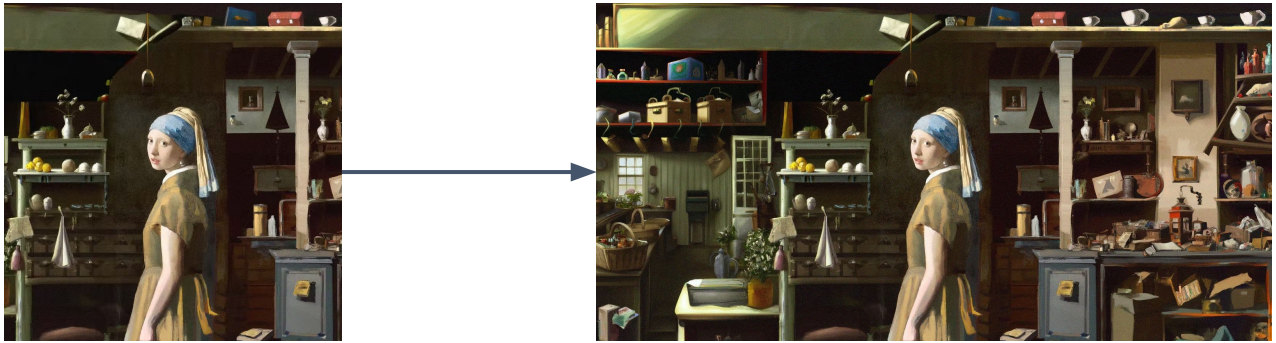
Diffusion model

INSTITUT DU DÉVELOPPEMENT ET DES RESSOURCES EN INFORMATIQUE SCIENTIFIQUE



Dhariwal & Nichol, 2021

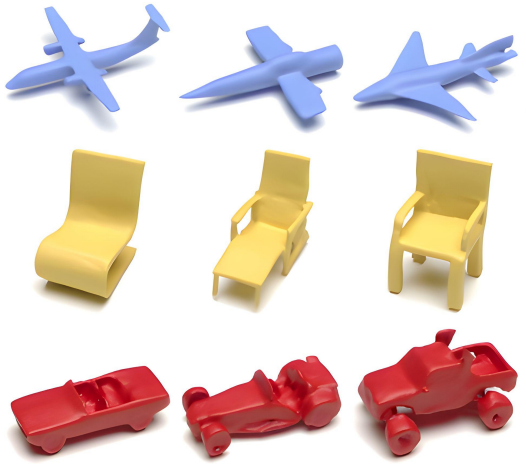
Source : https://github.com/bentoml/stable-diffusion-bentoml



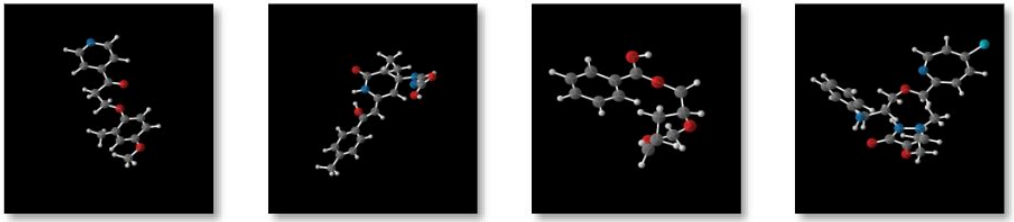
Source : Dall-E 3

DPM Landscape

Source : https://ai.meta.com/blog/emu-text-to-video-generation-image-editing-research/

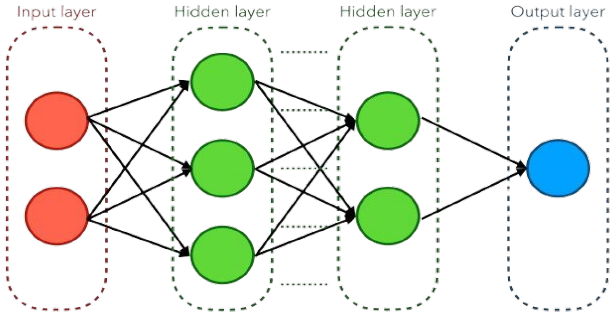


Source : https://arxiv.org/pdf/2210.06978.pdf



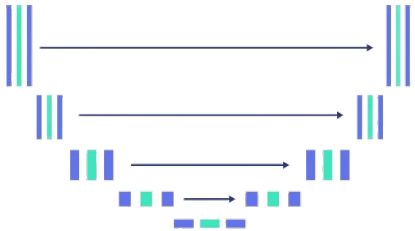
Source : https://arxiv.org/pdf/2305.01140.pdf

Generation of videos, of molecules, of …

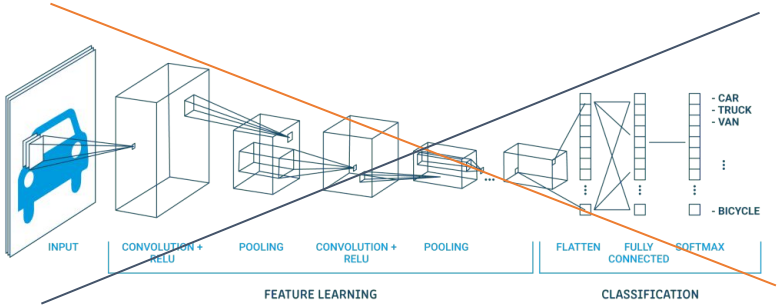


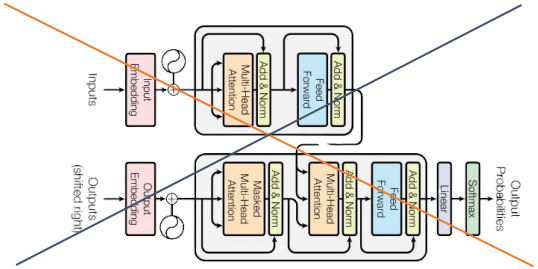
$q(Y|x)$

$q(x)$



Generation vs Classification





$q(x)$

$\mathcal{N}(0,1)$

$\mathcal{N}(0,1)$

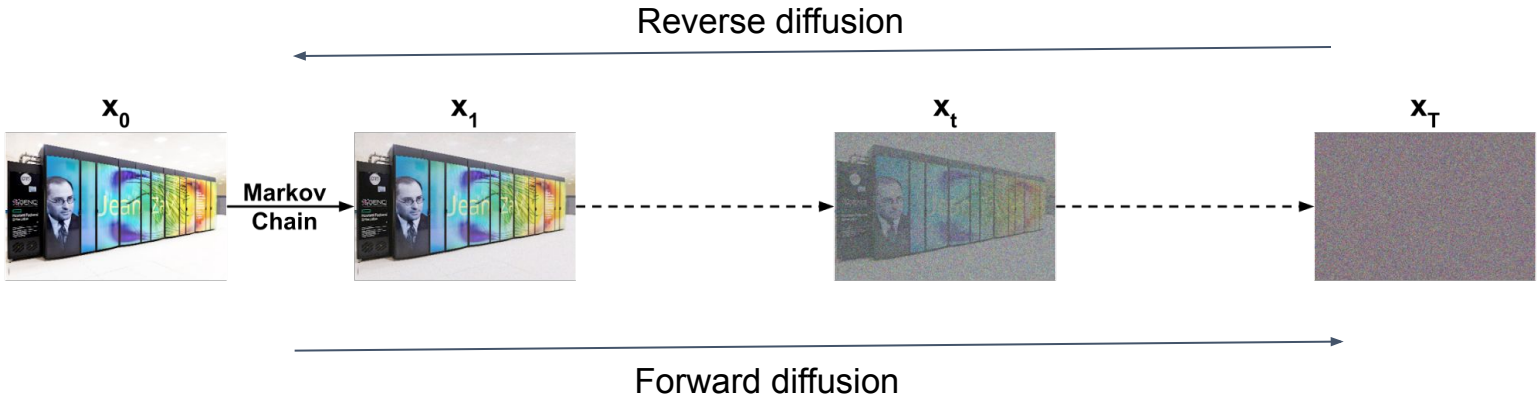
$q(x)$

CNN/Transformer/GNN vs Diffusion Model

Denoising diffusion probabilistic models (DDPM) consist of two processes:

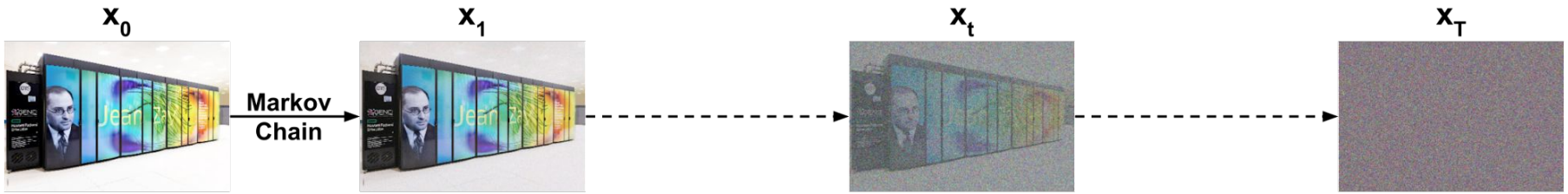
• Forward diffusion process that gradually adds noise to input

• Reverse denoising process that learns to generate data by denoising



DDPM Principle

Forward Diffusion Process



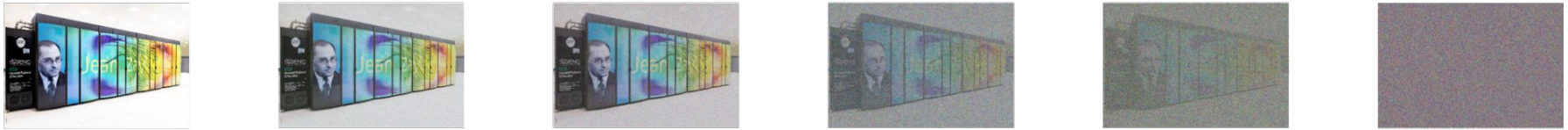
This process will add a small noise to any image gradually

$0 \leq t \leq T$; T is a hyperparameter

DDPM Principle 2

Forward Diffusion Process

t=0 t=5 t=10 t=50 t=100 t=T=1000



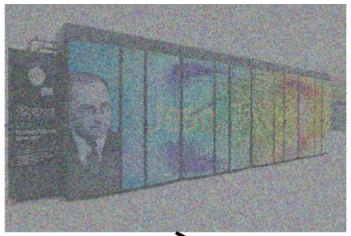
Denoising Diffusion Probabilistic Models (DDPM)

Here we choose T=1000, but it can be different values (it's an hyperparameter)

DDPM Principle 3

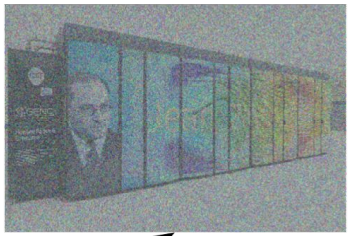
Reverse Diffusion Process

x_t

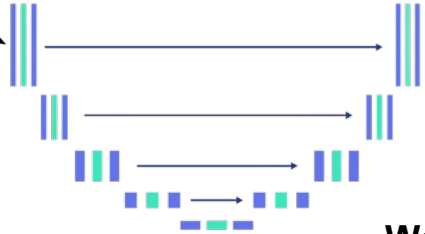


a bit more noisy than x_{t-1}

x_{t-1}



a bit less noisy than x_t

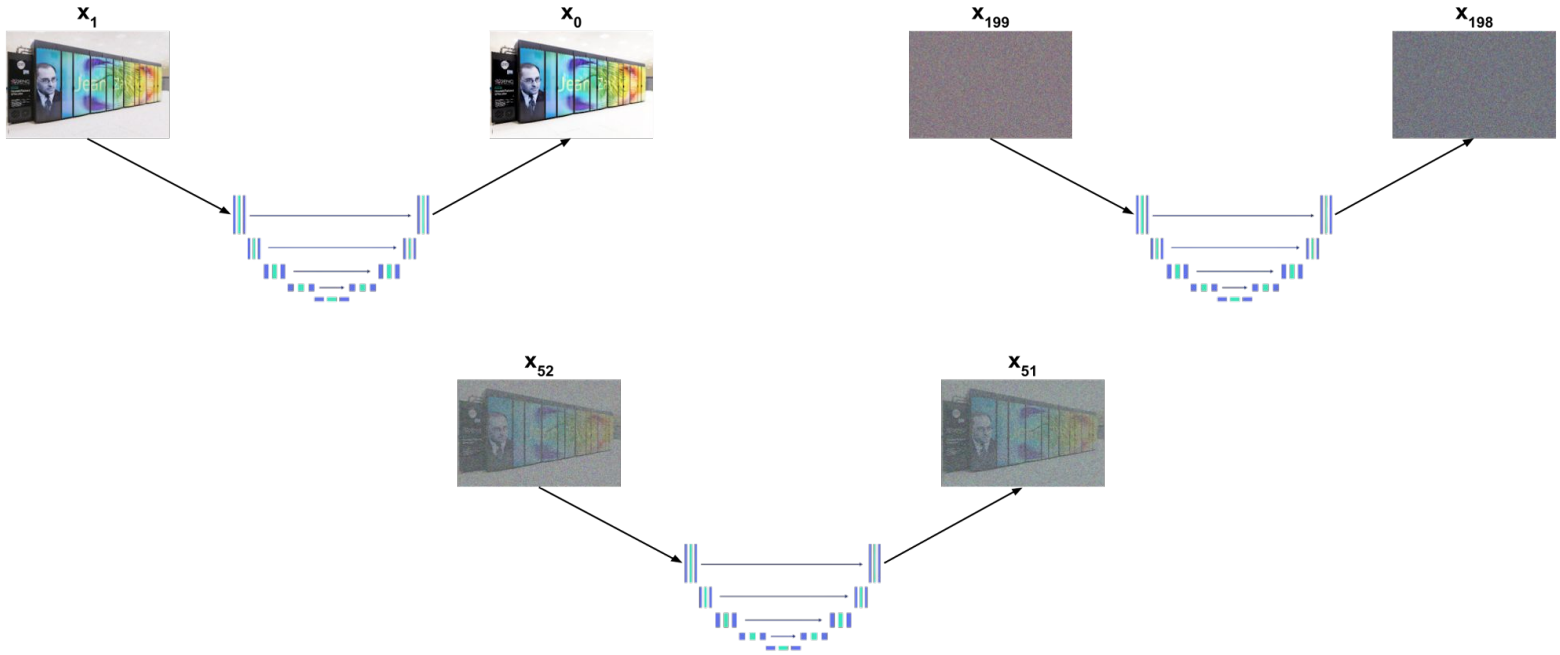


We train a model to predict x_{t-1} from x_t

x_0 is any image from the dataset

DDPM Principle 4

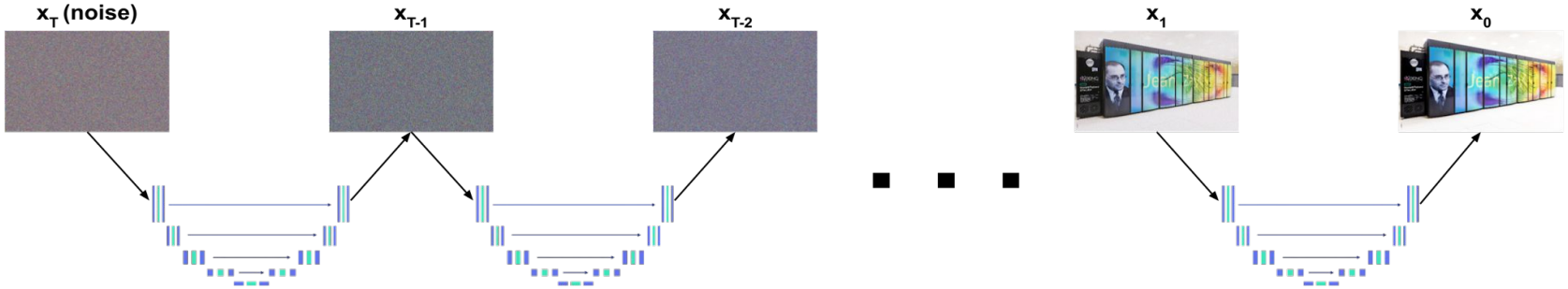
Reverse Diffusion Process



The same model must predict every x_{t-1} from x_t $Model(x_t, t)$

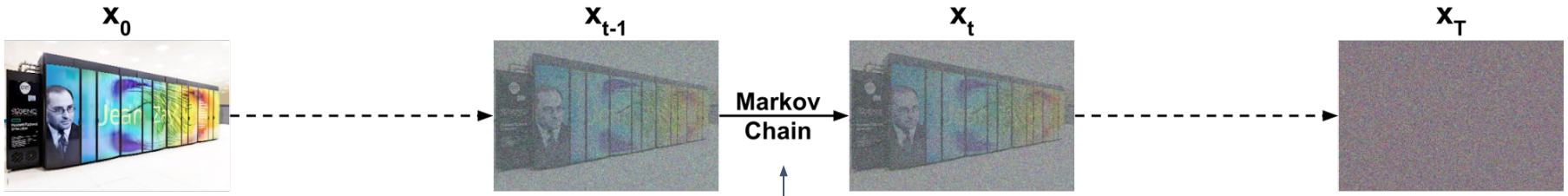
DDPM Principle 5

After the training, the model will generate images from Gaussian noise by following a sampling process :




```
torch.randn(4)
```

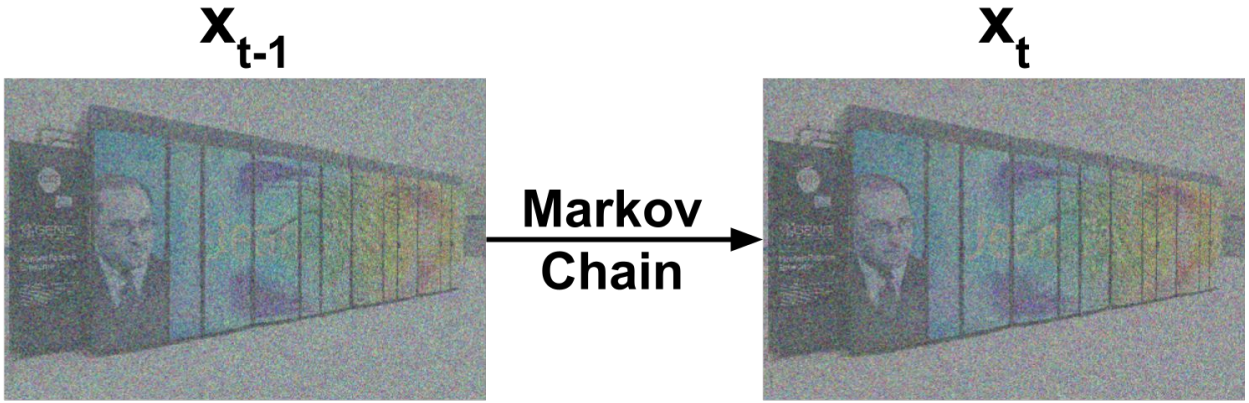
DDPM Principle 6



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

(β_t) **is a hyperparameter**

Forward diffusion 1



$$\mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$$

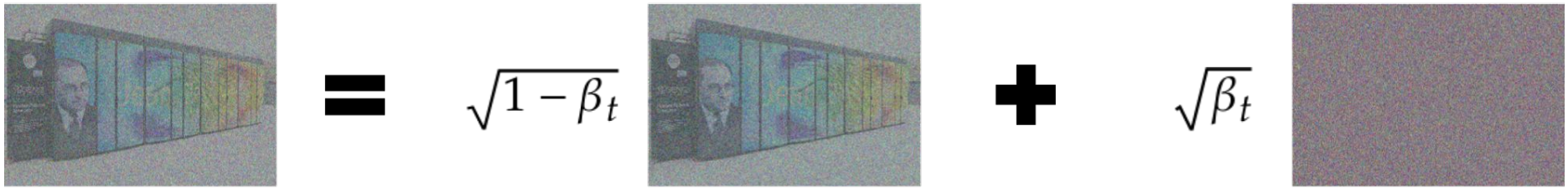
$$x_t = \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}z_{t-1}$$

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

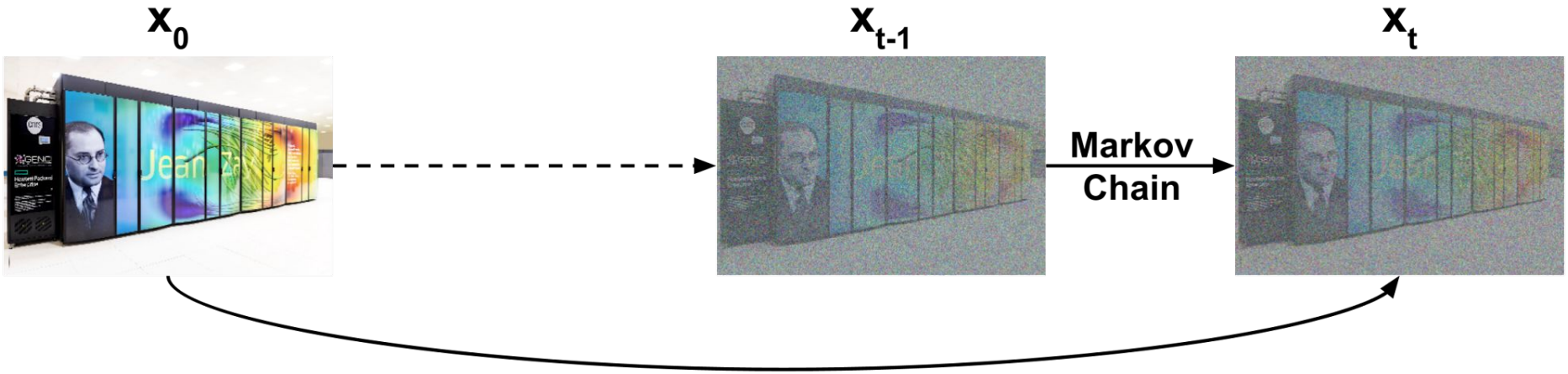
```
torch.randn(4)
```

Forward diffusion 2

x_t = $\sqrt{1-\beta_t}$ x_{t-1} + $\sqrt{\beta_t}$ Gaussian noise



Forward diffusion 3



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

$$where\ \bar{\alpha}_t = \prod_{i=1}^{T}(1-\beta_i)$$

Forward diffusion 4

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

So we can sample a noised image at any time step directly from original image

Forward diffusion 5

β_t (the noise schedule) such that $q(\mathbf{x}_T|\mathbf{x}_0) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$

$\beta_t \epsilon (0,1),\ \beta_t\ following\ a\ schedule\ \beta_1 < \beta_2 < ... < \beta_T$

Linear scheduling

$$(\beta_1, \ldots, \beta_T) = (\beta_1 + (t-1) * \frac{\beta_T - \beta_1}{T-1})_{t \in \{1 \ldots T\}}$$

0.02 — β_1

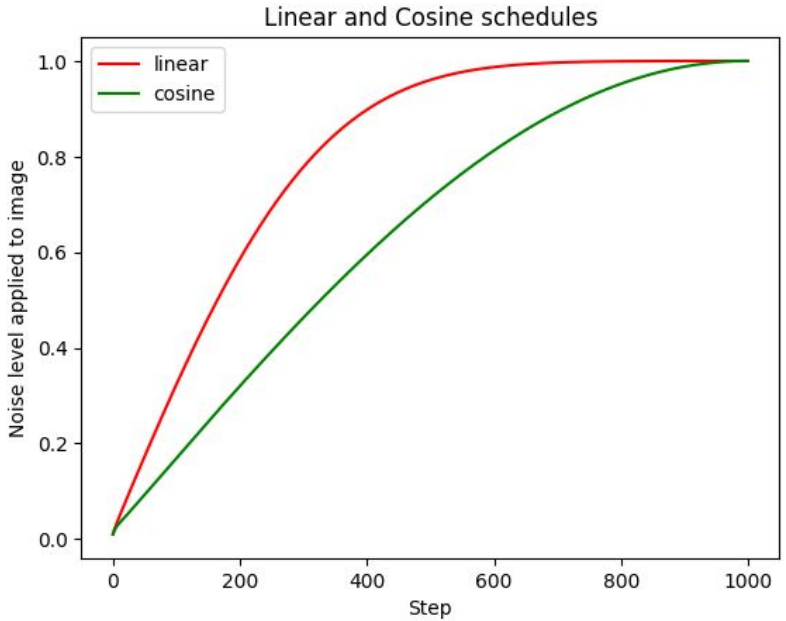
0.0001 — β_T

1000 — T

Cosinus scheduling

$$\bar{\alpha}_t = \frac{f(t)}{f(0)}, \quad f(t) = \cos\left(\frac{t/T + s}{1+s} \cdot \frac{\pi}{2}\right)^2$$

$$where\ \bar{\alpha}_t = \prod_{i=1}^{T} (1 - \beta_i)$$



Beta scheduling

$q(x_0)$

Données

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

Données bruitées par un petit bruit gaussien

$q(x_t|x_0)$

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

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

Computation 1

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

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

$$q(x_t|x_0)$$

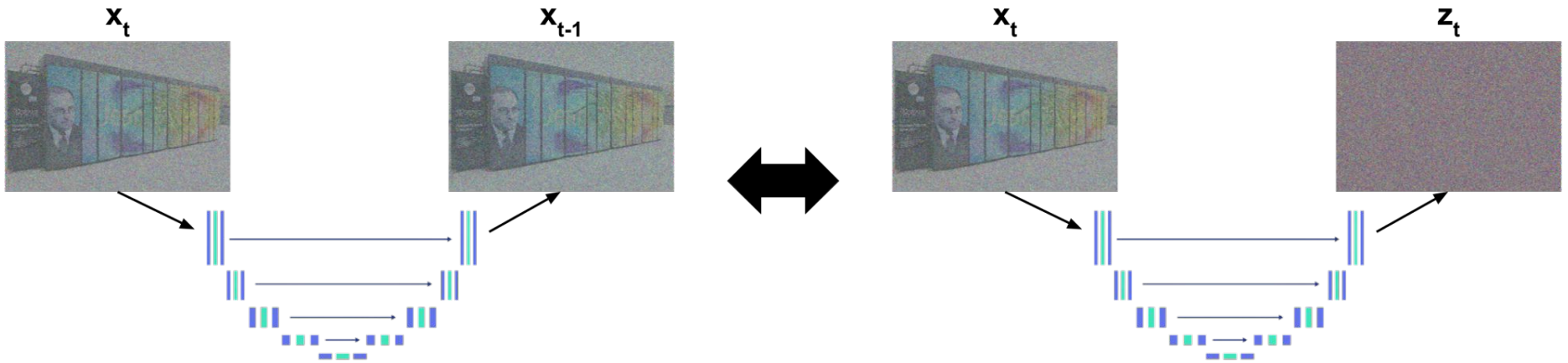
$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}z_t$$

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

$$\tilde{\mu}_t(\mathbf{x_t}, \mathbf{x_0}) = \frac{1}{\sqrt{\alpha_t}}(\mathbf{x_t} - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\mathbf{z_t})$$

$\mathbf{z_t}$ *???*

Computation 2



We can predict x_{t-1} by predicting z_t

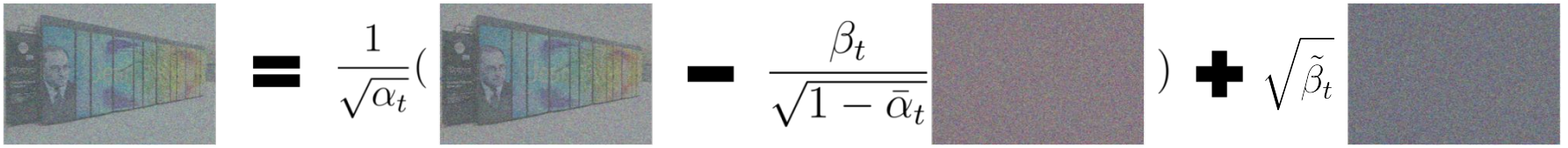
Reverse diffusion 1

$$\tilde{\mu}_t(\mathbf{x_t}, \mathbf{x_0}) = \frac{1}{\sqrt{\alpha_t}}(\mathbf{x_t} - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\mathbf{z_t}) \approx \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\mathbf{z}_\theta(\mathbf{x_t}, \mathbf{t}))$$

Our network

---

x_{t-1} = $\frac{1}{\sqrt{\alpha_t}}($ x_t $-$ $\frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}$ z_t $)$ $+$ $\sqrt{\tilde{\beta}_t}$ z (noise)



Reverse diffusion 2

$$\frac{1}{\sqrt{\alpha_t}}(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\mathbf{z}_\theta(\mathbf{x_t}, \mathbf{t}))$$

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

$$L_{\text{VLB}} = \mathbb{E}_{q(\mathbf{x}_{0:T})}\left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})}\right] \geq -\mathbb{E}_{q(\mathbf{x}_0)} \log p_\theta(\mathbf{x}_0)$$

$$L_{\text{VLB}} = L_T + L_{T-1} + \cdots + L_0$$

$$L_t = \mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{(1-\alpha_t)^2}{2\alpha_t(1-\bar{\alpha}_t)\|\boldsymbol{\Sigma}_\theta\|_2^2}\|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_t, t)\|^2\right]$$

$$L_t^{\text{simple}} = \mathbb{E}_{t\sim[1,T],\mathbf{x}_0,\boldsymbol{\epsilon}_t}\left[\|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2\right]$$

Reverse diffusion 3

Algorithm 1 Training

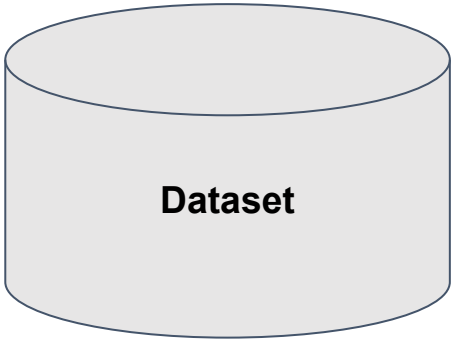
1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(\{1, \dots, T\})$
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: Take gradient descent step on

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

6: **until** converged

https://arxiv.org/abs/2006.11239

Training 1

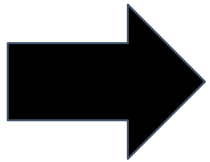


x_0

Training 2

Uniform distribution

Between 1 and T



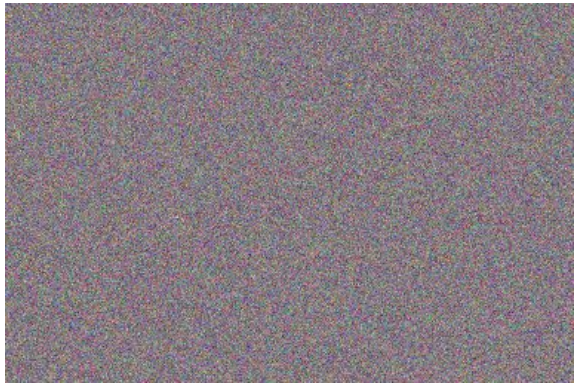
t = 50

x_0

z_t (= ϵ)

Gaussian distribution

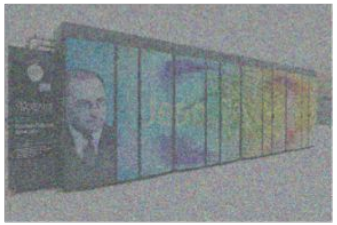
Same shape than x_0

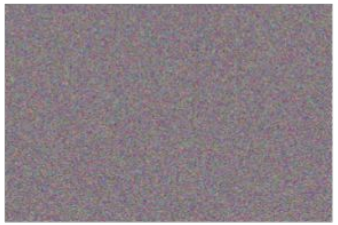


x_0

t = 50

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

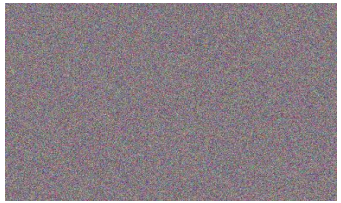




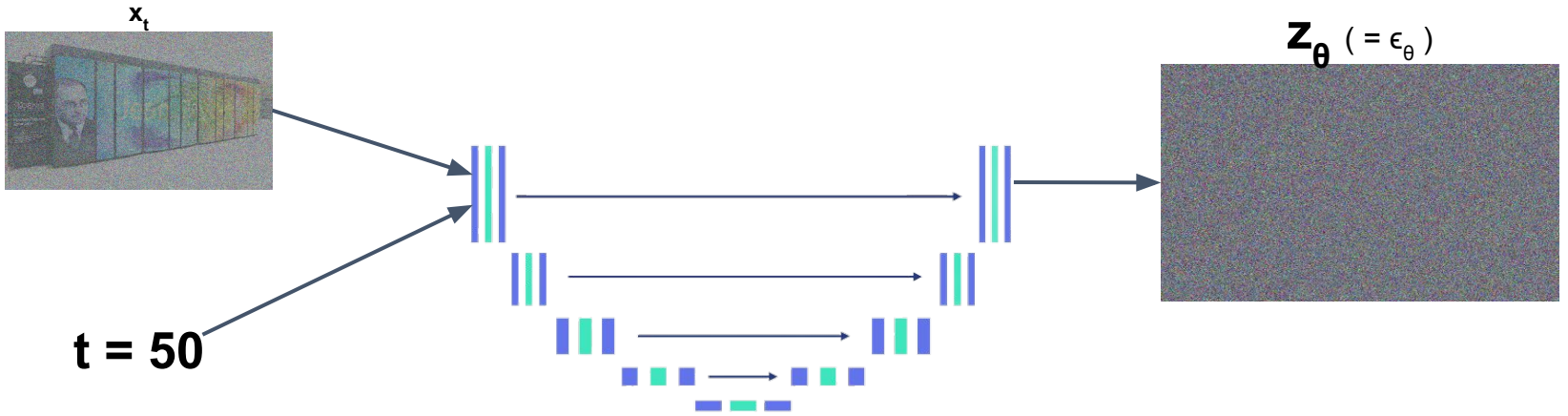
x_0

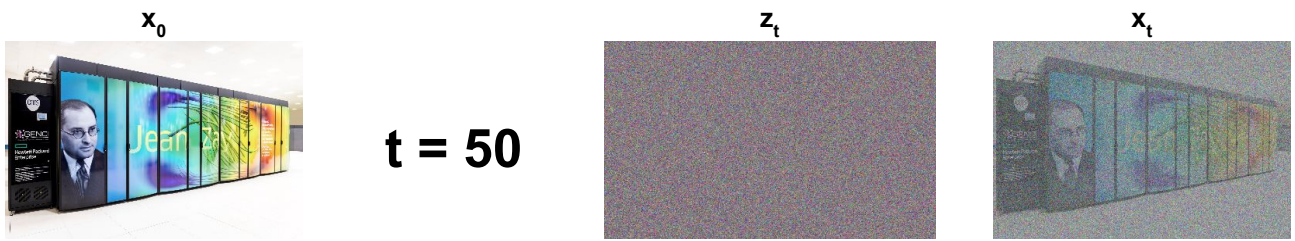
t = 50

z_t



Training 5





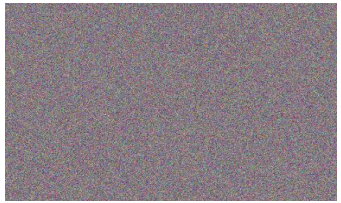
Training 6

$$\text{Loss} = \left\| z_t - z_\theta \right\|^2$$

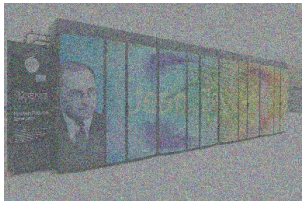
x_0

t = 50

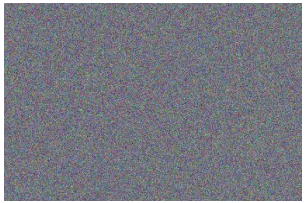
z_t



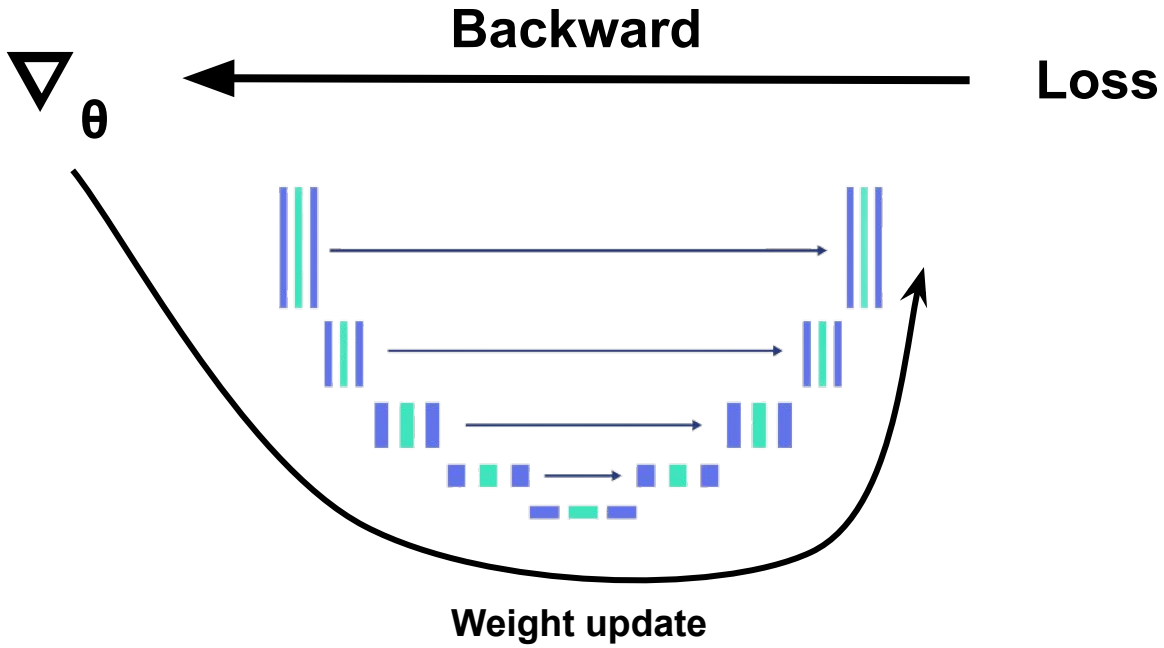
x_t



z_θ



Training 7



Training 8

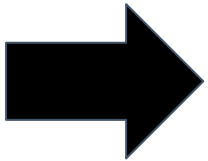
Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
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 $\mathbf{x}_0$

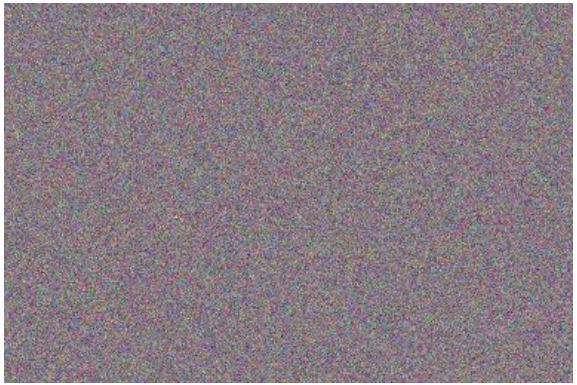
https://arxiv.org/abs/2006.11239

Gaussian distribution

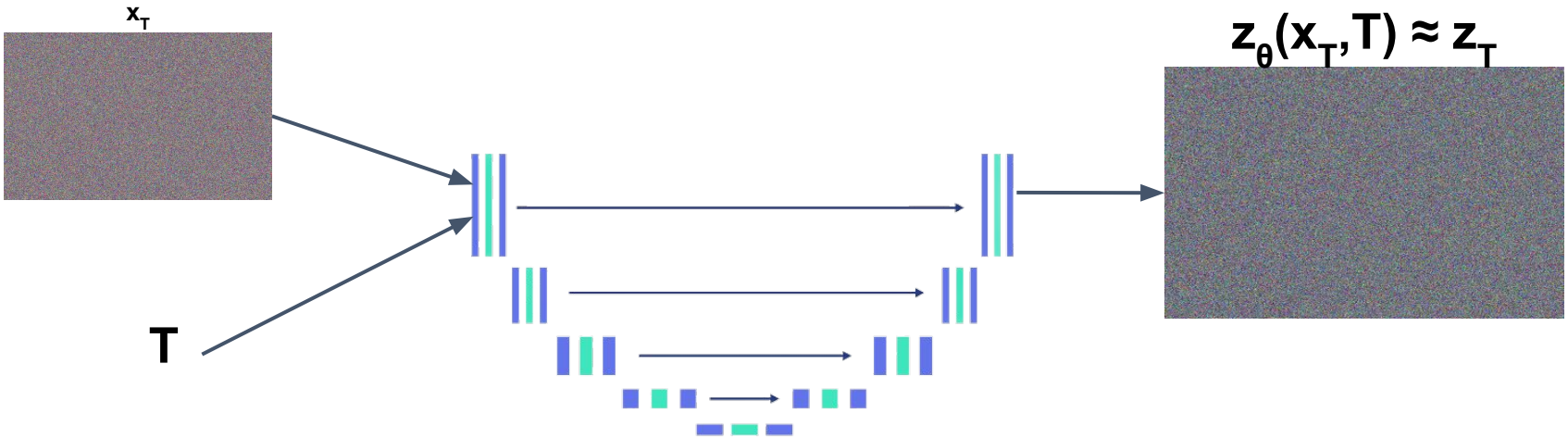
Same shape than training dataset images

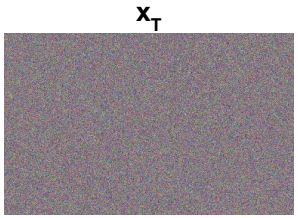


x_T



Sampling 2



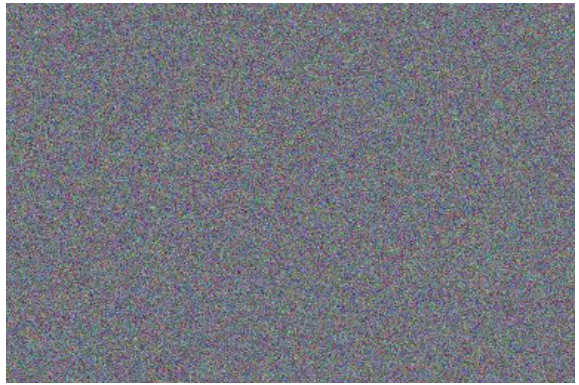


Sampling 3

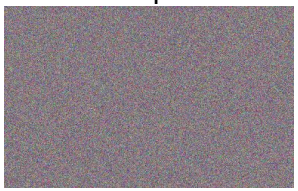
Gaussian distribution

Same shape than training dataset images

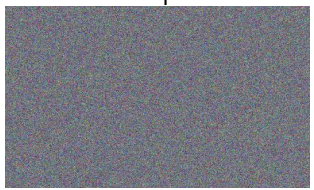
z (noise)



x_T



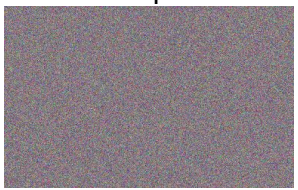
z_T

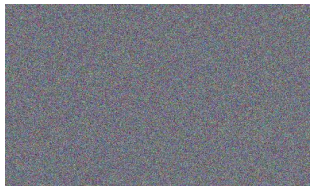


Sampling 3

x_{T-1}  $\approx \frac{1}{\sqrt{\alpha_T}}($ x_T  $- \frac{\beta_T}{\sqrt{1-\bar{\alpha}_T}}$ $z_\theta(x_T, T)$  $) + \tilde{\beta}_T$ z (noise) 

---

x_T 

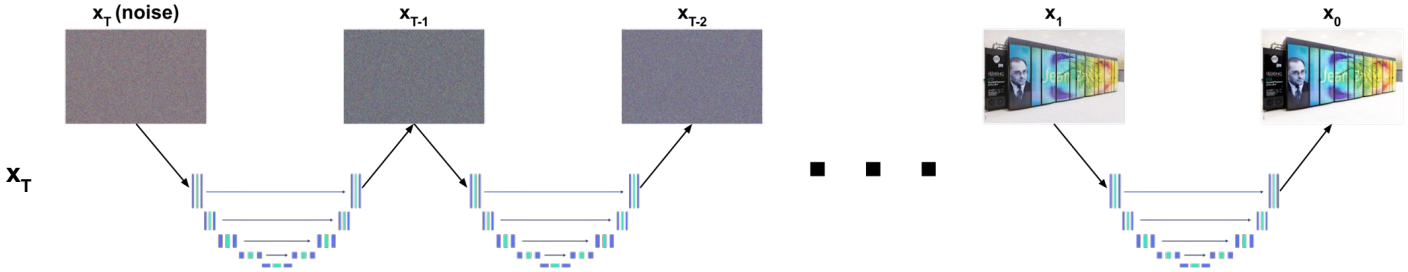
z_T 

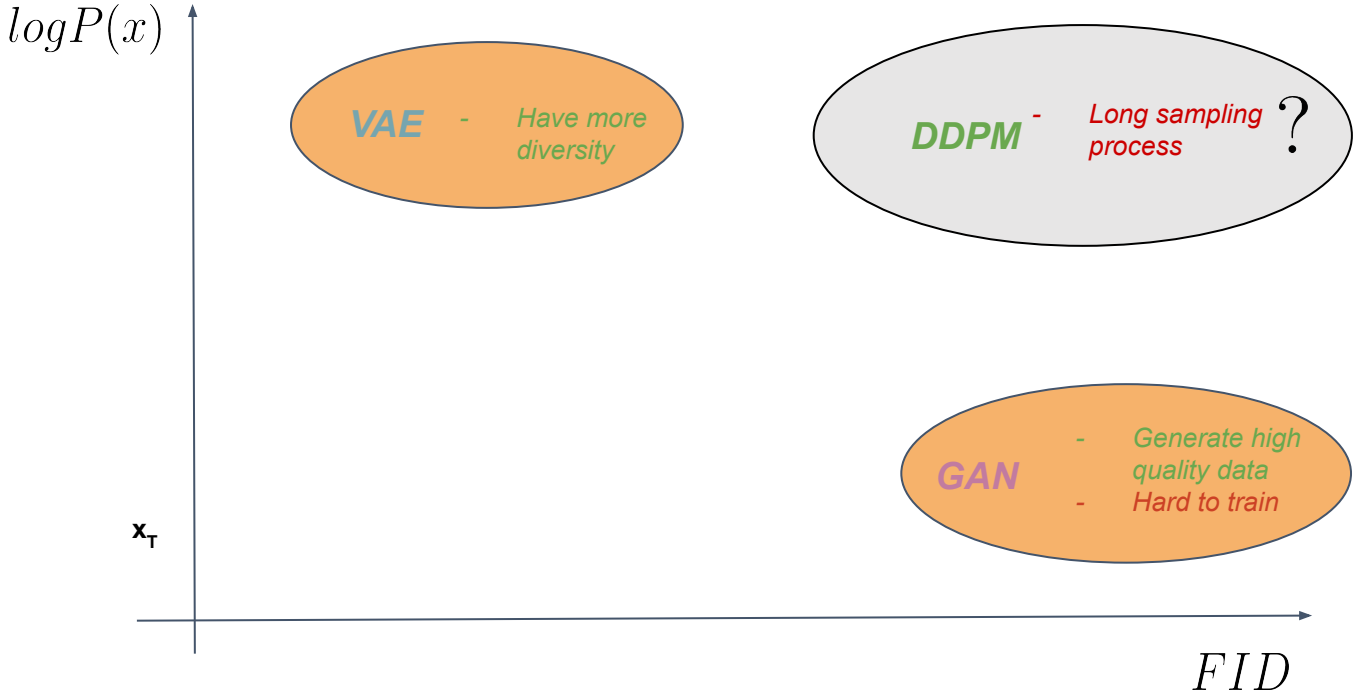
z (noise) 

Sampling 4

and repeat !

Don’t generate x_T, replace it by x_{T-1} and T by T-1… and do it again T time.

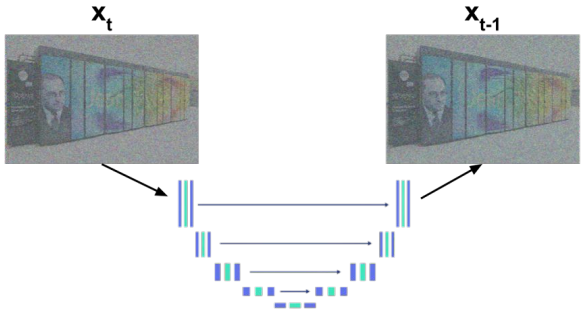


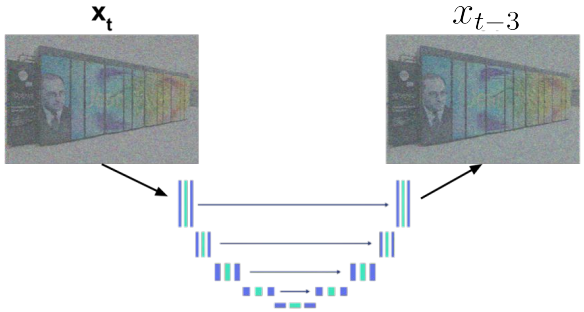


Limitations :

"For example, it takes around 20 hours to sample 50k images of size 32 x 32 from a DDPM, but less than a minute to do so from a GAN on a Nvidia 2080 Ti GPU." (DDIM, 2021)

DDPM vs GAN vs VAE





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

$$x_{t-3} = \sqrt{\bar{\alpha}_{t-3}} x_0 + \sqrt{1 - \bar{\alpha}_{t-3}} z$$

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

$$x_{t-3} = \sqrt{\bar{\alpha}_{t-3}} * \frac{x_t - \sqrt{1 - \bar{\alpha}_t} z_t}{\sqrt{\bar{\alpha}_t}} + \sqrt{1 - \bar{\alpha}_{t-3}} z$$

Reduce the sampling step

Generalisation to a bigger class of inverse process (non-Markovian)

$$q_\sigma(x_{t-1}|x_t, x_0) = \mathcal{N}(\sqrt{\bar{\alpha}_{t-1}}x_0 + \sqrt{1-\bar{\alpha}_{t-1}-\sigma_t^2}.\frac{x_t - \sqrt{\bar{\alpha}_t}x_0}{\sqrt{1-\bar{\alpha}_t}}, \sigma_t^2 I)$$

$$\sigma_t^2 = \tilde{\beta}_t \quad \Rightarrow \quad DDPM$$

Important :

Same network and training as a DDPM

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

DDIM 1

$$\sigma_t^2 = \tilde{\beta}_t \quad \Rightarrow \quad DDPM$$

$$\sigma_t^2 = \eta.\tilde{\beta}_t \qquad \eta \in [0, 1]$$

$$\eta = 0 \qquad \text{=> DDIM}$$

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

FID

DDIM 2

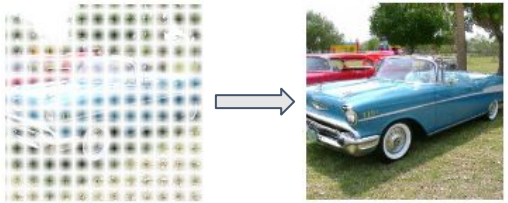
Source *Lugmayr, Andreas, et al. "Repaint: Inpainting using denoising diffusion probabilistic models." Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition. 2022.*

Diffusion models can solve a variety of tasks. We already know about image generation, as well as conditional image generation (for instance with a short paragraph describing the picture)

Other tasks:

➔ Inpainting

➔ Super-resolution



➔ Outpainting

Other task 1

We can solve many of these tasks through the usage of a mask

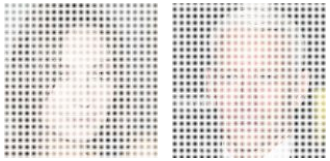
➔ Wide mask

➔ Thin mask

➔ Outer mask for expanding the image

➔ Right side mask for halving the image

➔ Every second pixel in both directions for super-resolution

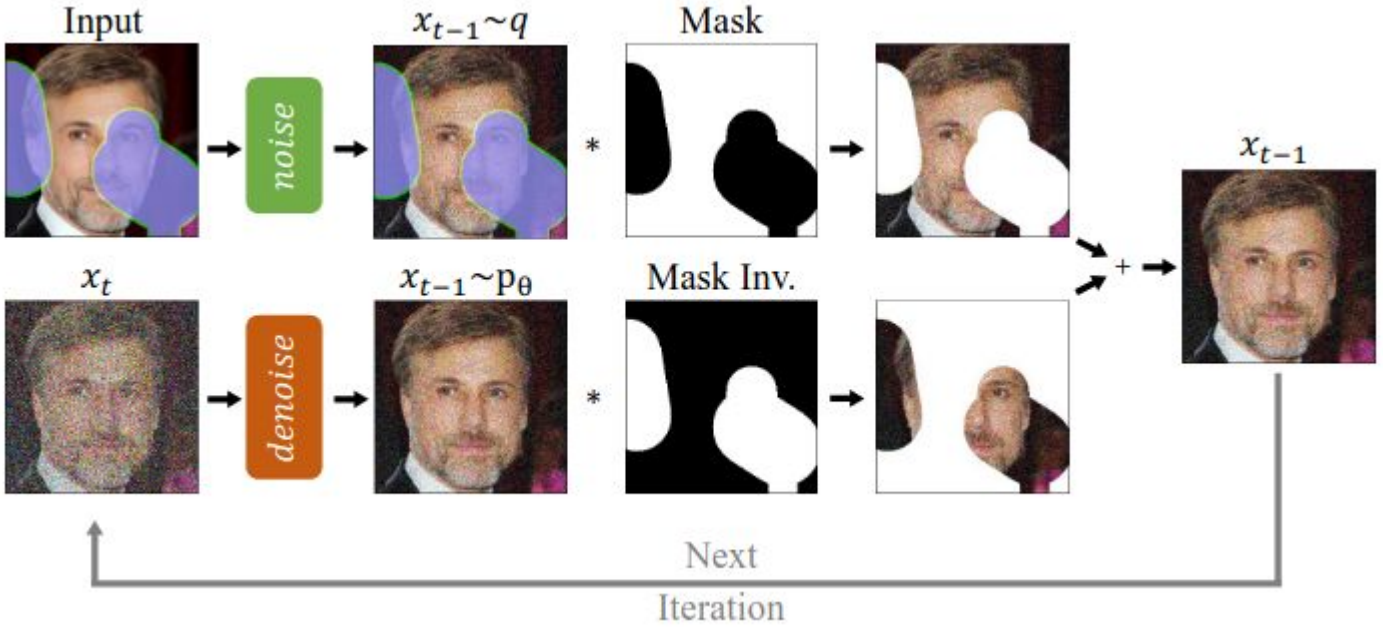


➔ Every second row of pixels for alternating lines

Source *Lugmayr, Andreas, et al. "Repaint: Inpainting using denoising diffusion probabilistic models." Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition. 2022.*

Other task 2

Step t :

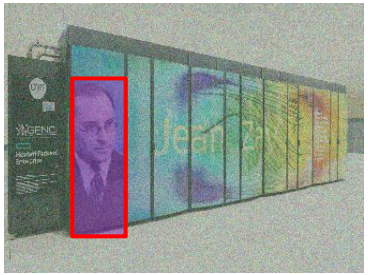


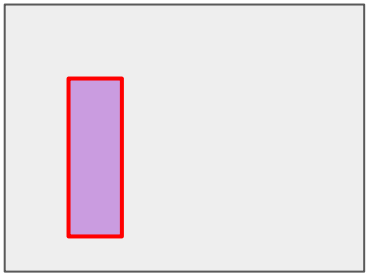
Source *Lugmayr, Andreas, et al. "Repaint: Inpainting using denoising diffusion probabilistic models." Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition. 2022.*

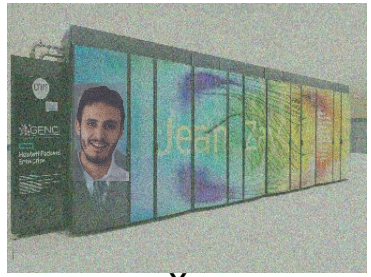
Other task 3

x_0

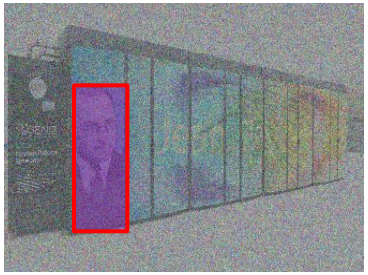
+noise





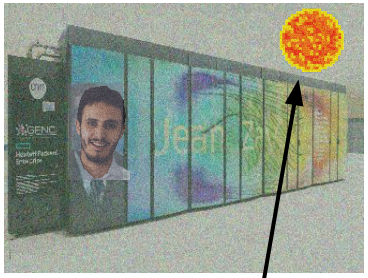


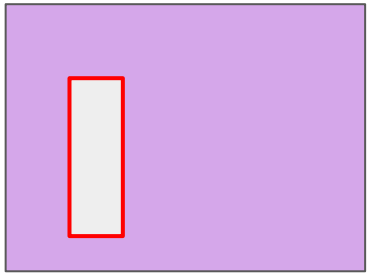
x_{t-1}



x_t

+diffusion





New artifacts added (in this coarse example, our diffusion model drew a sun), so we force the known background again!

Other task 4

Papers:

- Deep Unsupervised Learning using Nonequilibrium Thermodynamics (DPM) (https://arxiv.org/abs/1503.03585)
- Denoising Diffusion Probabilistic Models (DDPM) (https://arxiv.org/abs/2006.11239)
- Improved Denoising Diffusion Probabilistic Models (IDDPM) (https://arxiv.org/abs/2102.09672)
- Denoising Diffusion Implicit Models (DDIM) (https://arxiv.org/abs/2010.02502)
- Diffusion Models Beat GANs on Image Synthesis (https://arxiv.org/abs/2105.05233)
- High-Resolution Image Synthesis with Latent Diffusion Models (LDM) (https://arxiv.org/abs/2112.10752)
- Repaint: Inpainting using denoising diffusion probabilistic models (https://arxiv.org/pdf/2201.09865)
- Diffusion Models in Vision: A Survey (https://arxiv.org/abs/2209.04747)
- Diffusion Models: A Comprehensive Survey of Methods and Applications(https://arxiv.org/abs/2209.00796)

Other resources:

- Lilian Weng's article (https://lilianweng.github.io/posts/2021-07-11-diffusion-models)
- Yang Song's article (https://yang-song.net/blog/2021/score)
- Outlier video (https://www.youtube.com/watch?v=HoKDTa5jHvg)

Online Resources