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Diffusion models

Olivier Bernard

UNIVERSITÉ DE LYON | INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES LYON | CREATIS

olivier.bernard@insa-lyon.fr

What is the purpose of diffusion models?

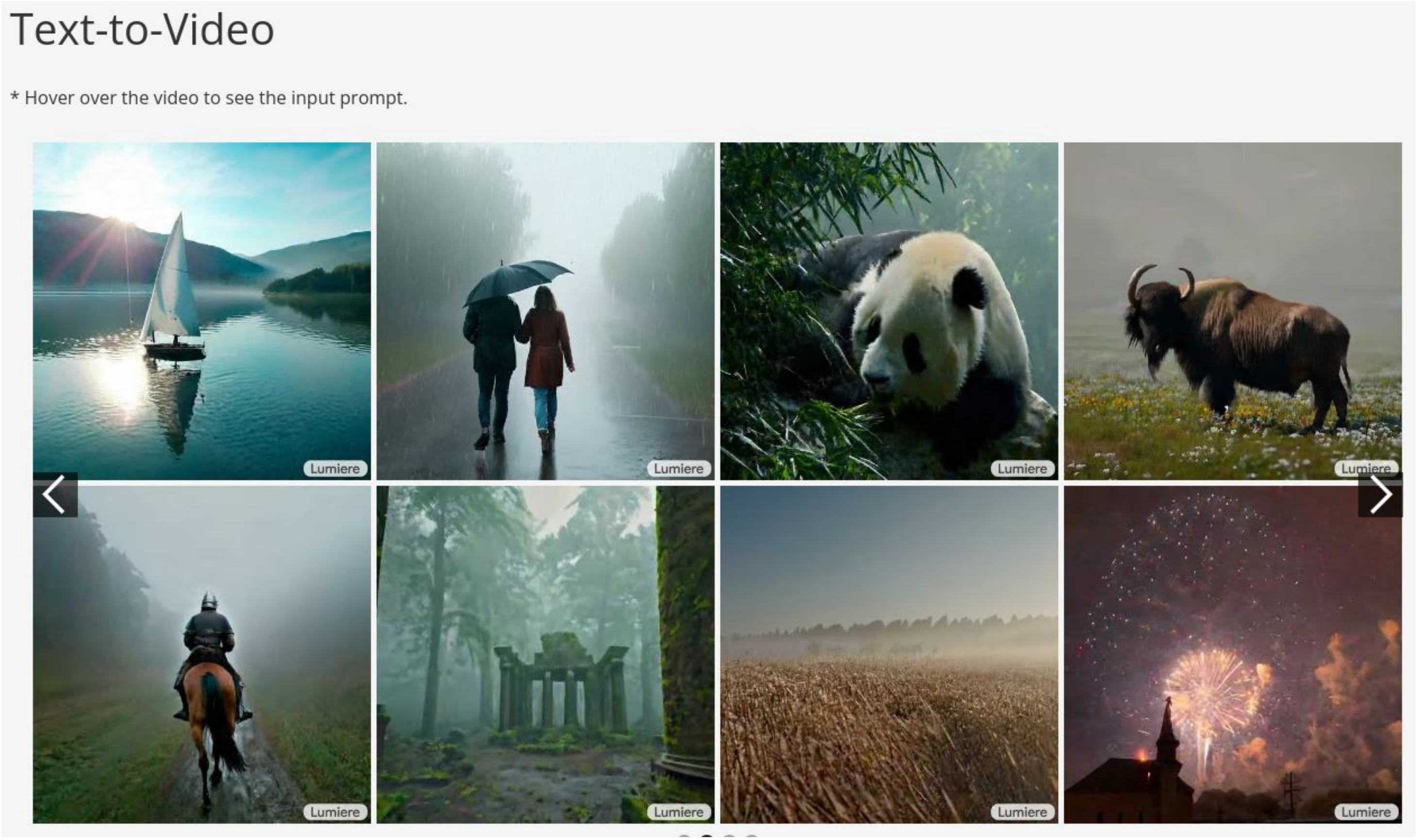
- Best current methods for synthetic image generation
- Allows generating images in a *conditioned* form
- Many software solutions, such as Midjourney, DALL-E

An Asian girl in ancient coarse linen clothes rides a giant panda and carries a wooden cage. A chubby little girl with two buns walks on the snow. High-precision clothing texture, real tactile skin, foggy white tone, low saturation, retro film texture, tranquil atmosphere, minimalism, long-range view, telephoto lens

What is the purpose of diffusion models?

- Recent extensions for video synthesis

  https://lumiere-video.github.io/#section_image_to_video



What is the purpose of diffusion models?

- Recent extensions for video synthesis

  https://lumiere-video.github.io/#section_image_to_video

Image-to-Video

* Hover over the video to see the input image and prompt.

What is the purpose of diffusion models?

- Family of diffusion networks

Denoising Diffusion Probabilistic models

Score-based methods

Normalizing flow methods

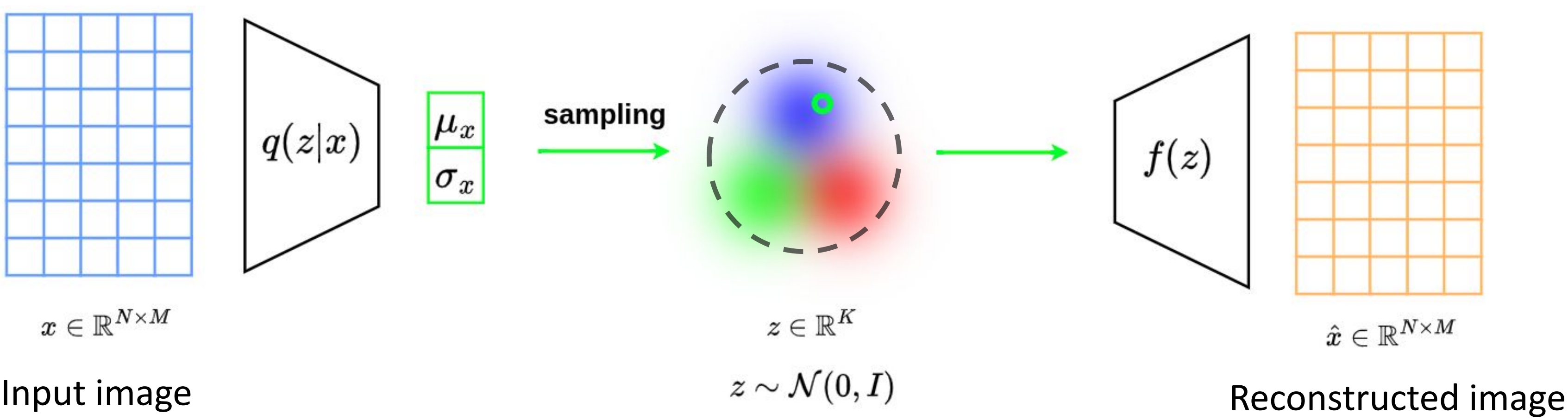
Intuition behind diffusion models

- Interpretation of the loss function

$$\text{loss} = D_{KL}\left(\mathcal{N}\left(g(x), diag\left(h(x)\right)\right), \mathcal{N}\left(0, I\right)\right) + \alpha\|x - f(z)\|^2$$

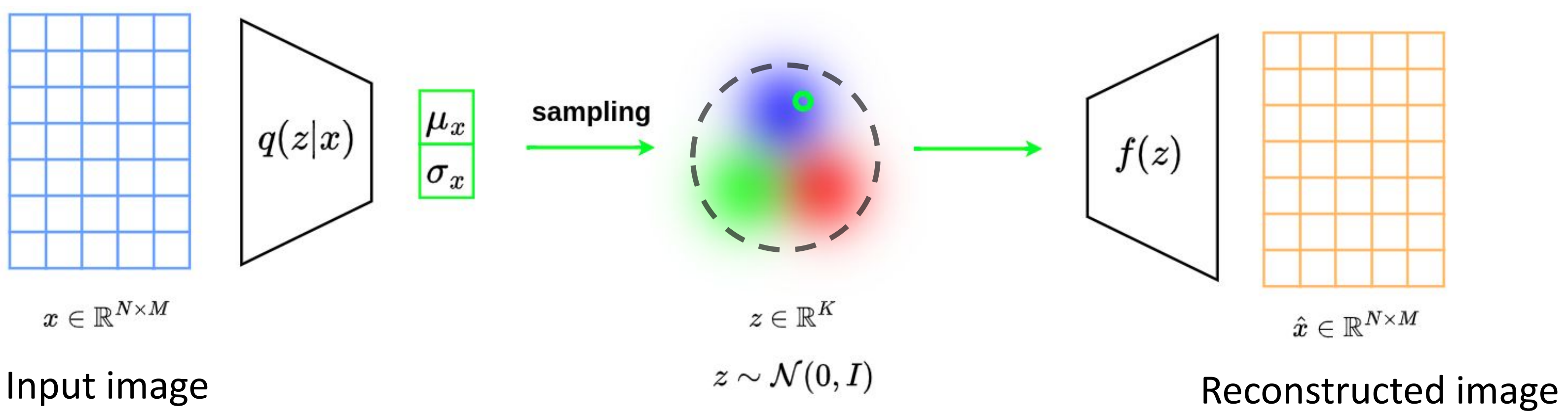
imposes a local *continuity* constraint

imposes a global *completeness* constraint



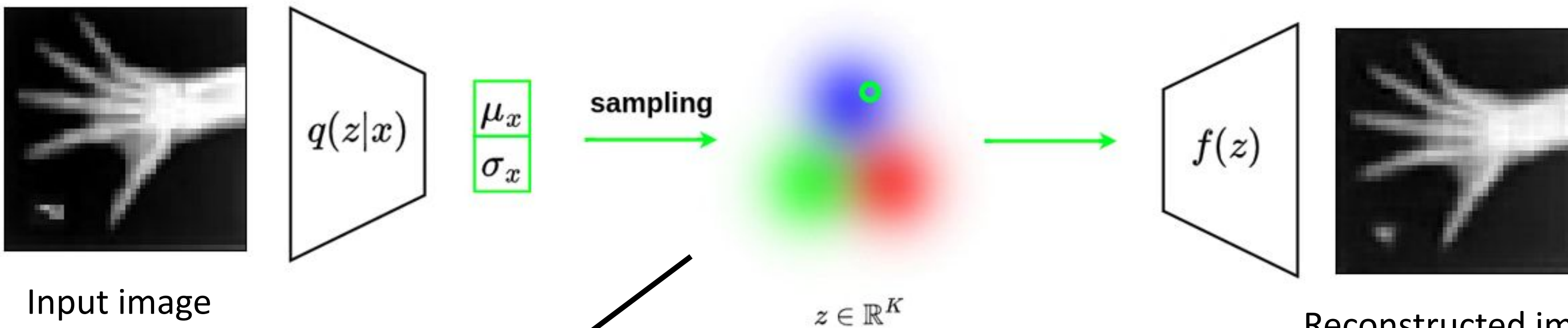
- Completeness is expressed as a ***soft constraint*** !

$\mathcal{N}\left(g(x), diag(h(x))\right)$ and $\mathcal{N}(0, I)$ should remain close in terms of distributional distance



Sampling from the latent space $\mathcal{N}(0, I)$ does not guarantee to obtain a reconstructed image from the target distribution

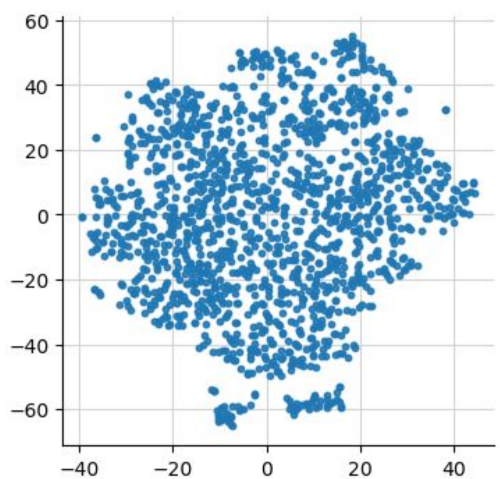
- Illustration from Mednist dataset
  - (train,valid,test) = (1491,373,223)
  - Input image size: 48x48 / latent space K=432 (compression factor around 5)



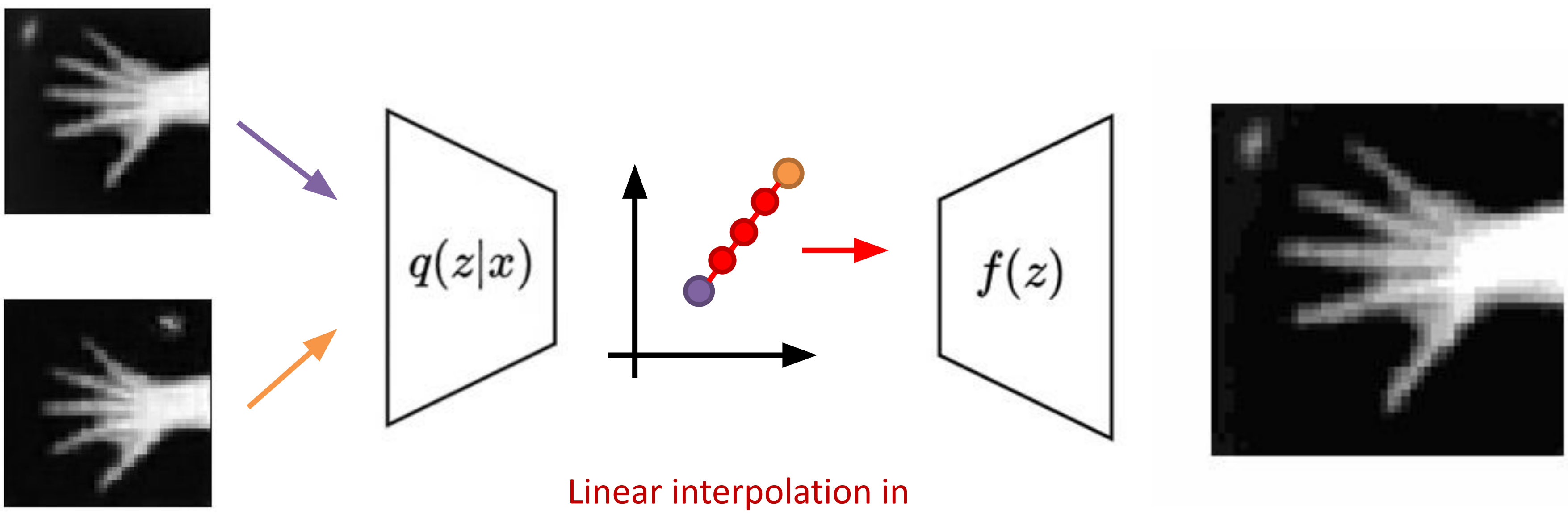
Input image

Reconstructed image

t-SNE visualization of the latent space using the training data as sample points



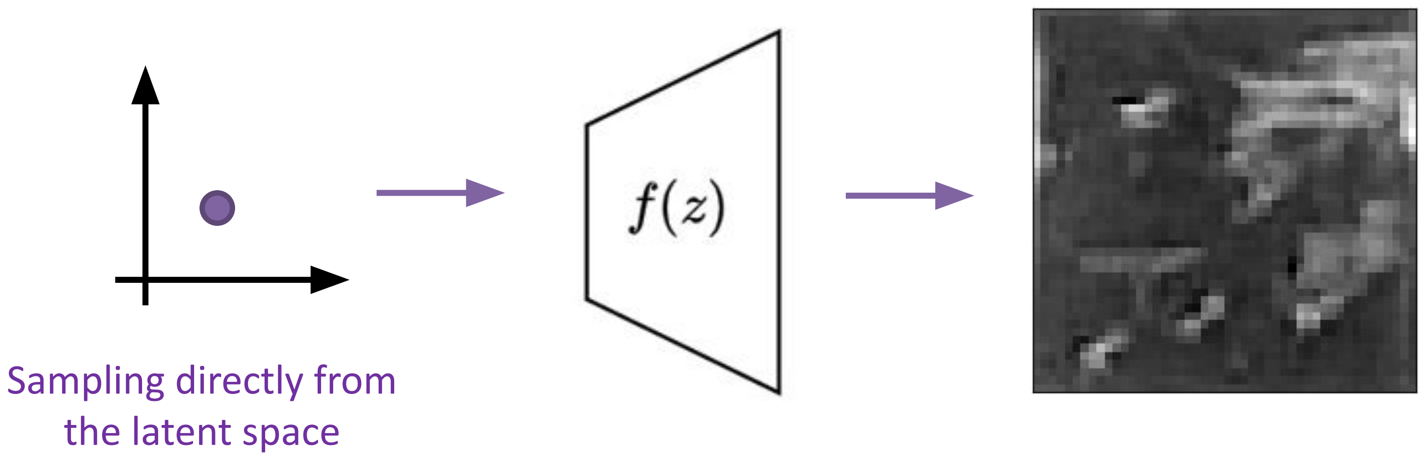
- Linear interpolation between two real images



Linear interpolation in the latent space

- Sampling directly from the latent space

$$z \in \mathbb{R}^{(K)} \quad \text{with} \quad z_i \sim \mathcal{N}(0, I)$$



A soft constraint on the latent space to remain close to $\mathcal{N}(0, I)$ is not sufficient to build generative models that effectively learn a target distribution

The denoising diffusion probabilistic models

DDPM

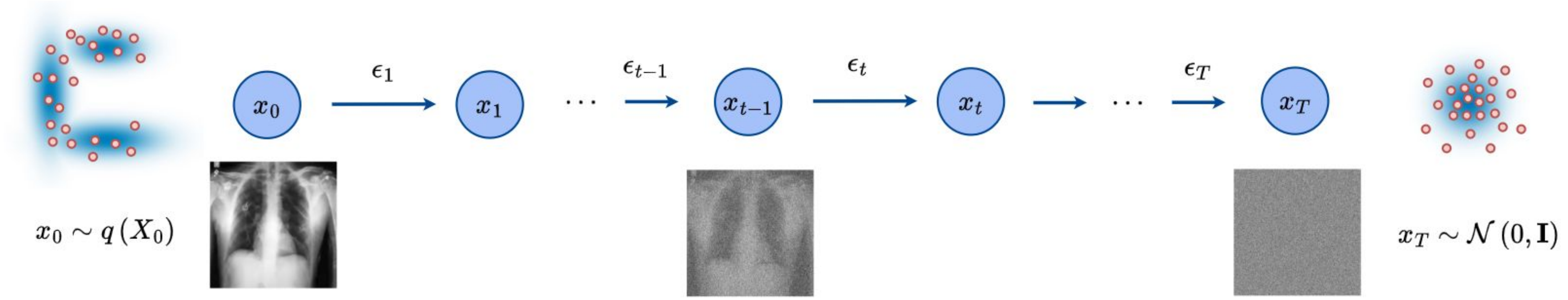
All the mathematics are described in the following blog

https://creatis-myriad.github.io/tutorials/2023-11-30-tutorial-ddpm.html

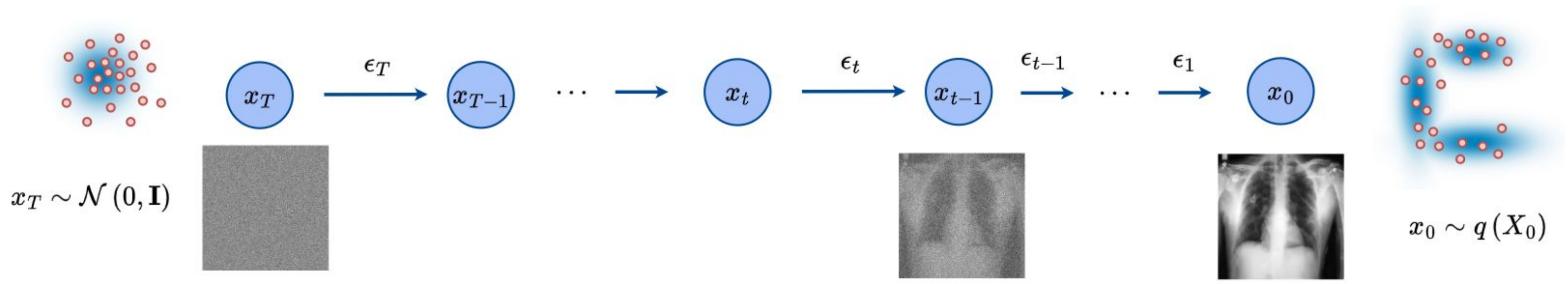
Basic idea of denoising diffusion model

How can a hard constraint be enforced to ensure a direct transformation from the latent space (modeled as a Gaussian) to the target distribution?

- Noising process



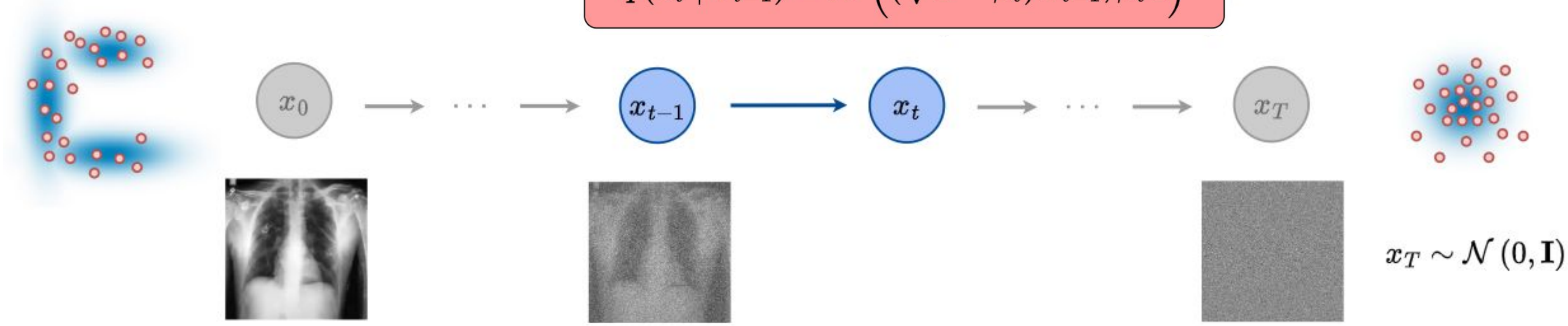
- Denoising process



Noising process (forward diffusion process)

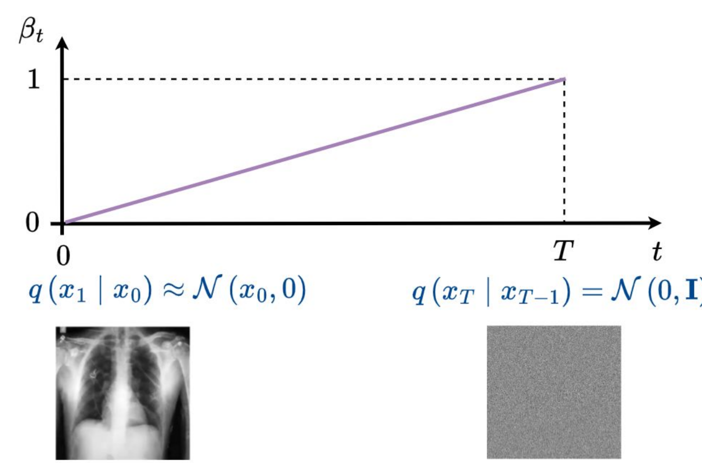
- Modeled as sequence of normal distributions (Markov chain process)

$$q\left(x_t \mid x_{t-1}\right) = \mathcal{N}\left(\left(\sqrt{1-\beta_t}\right) x_{t-1}, \beta_t \mathbf{I}\right)$$



- β_t : variance varying over the iterative process from 0 to 1

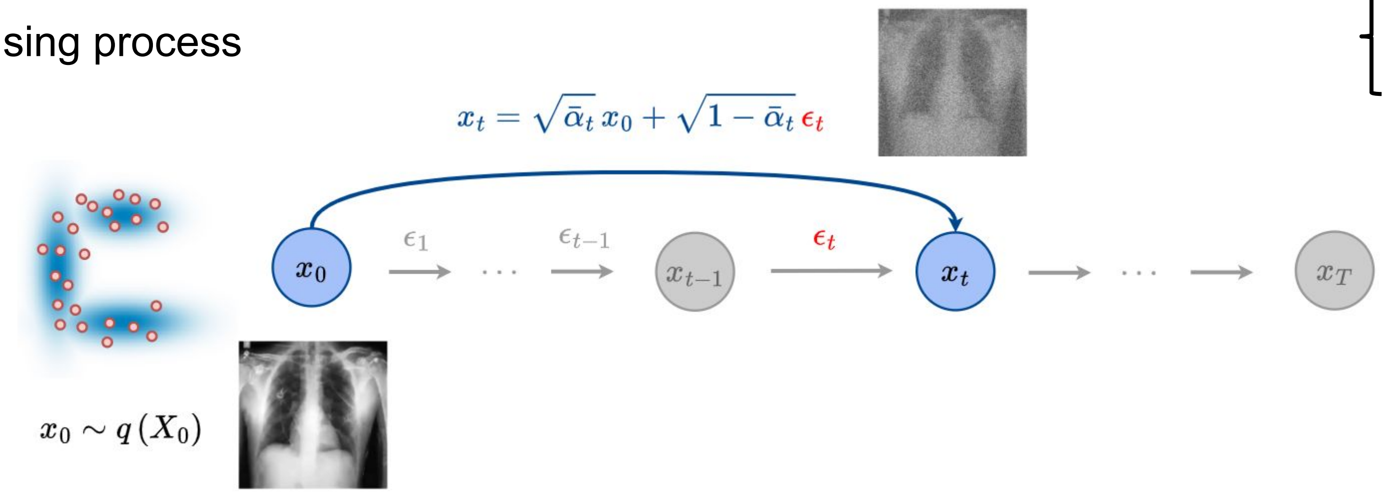
$$\begin{aligned} &\text{if} \quad \beta_t = 0, \quad \text{then} \quad q(x_t \mid x_{t-1}) = x_{t-1} \\ &\text{if} \quad \beta_t = 1, \quad \text{then} \quad q(x_t \mid x_{t-1}) = \mathcal{N}(0, \mathbf{I}) \end{aligned}$$



Noising / denoising processes

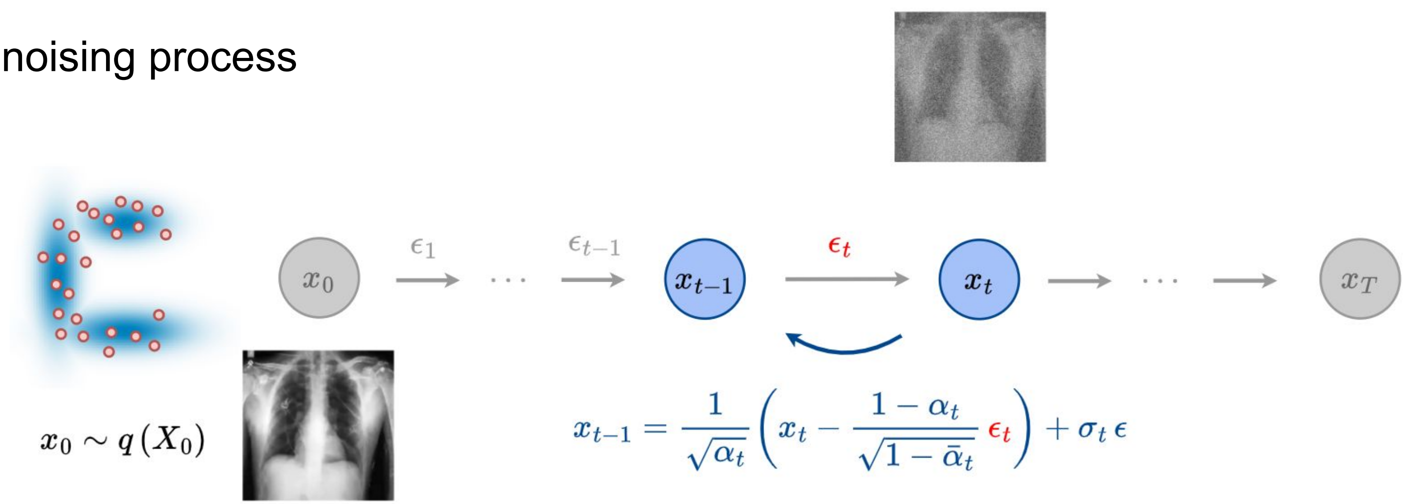
$$\begin{cases} \alpha_t = 1 - \beta_t \\ \bar{\alpha}_t = \prod_{k=1}^{t} \alpha_k \end{cases}$$

- Noising process



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

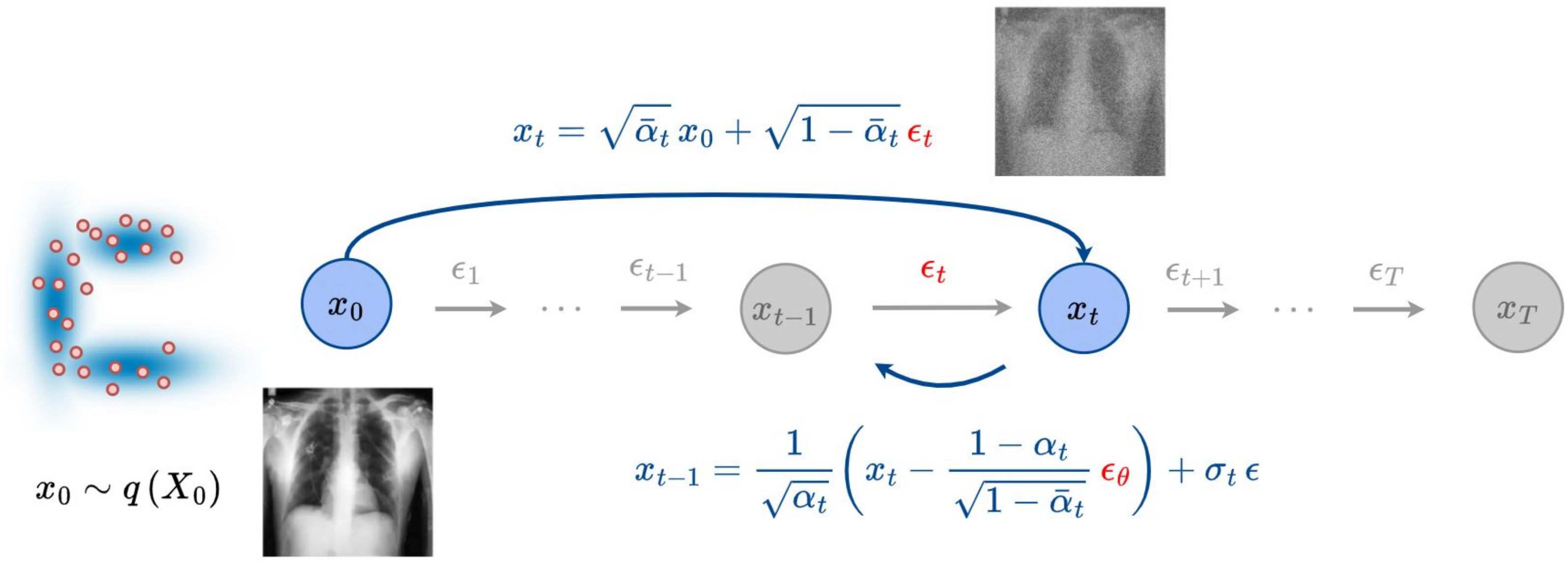
- Denoising process



$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \epsilon_t \right) + \sigma_t \epsilon$$

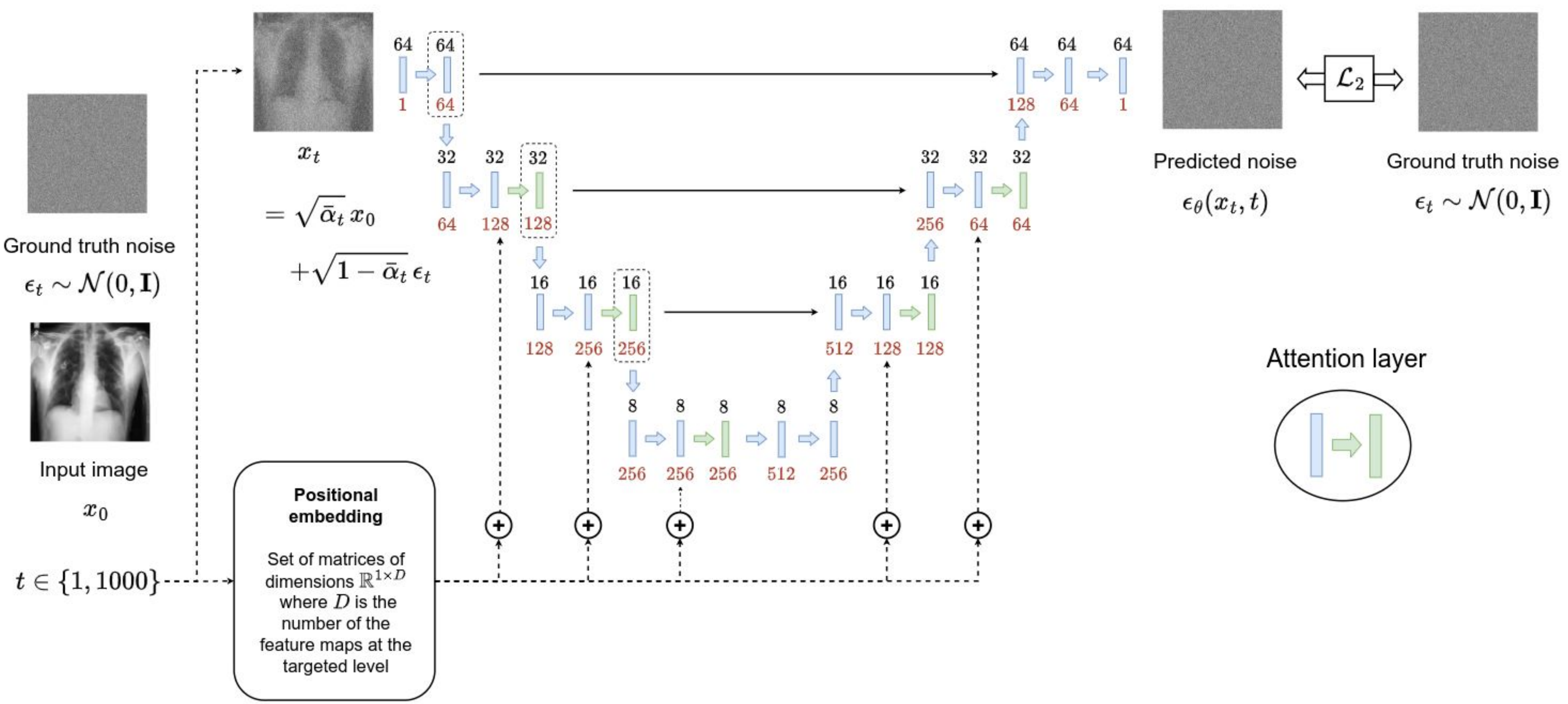
Training procedure

- Choose a random step $t \in \{1,\ldots,T\}$
- Trained a U-Net model to predict ϵ_θ from x_t



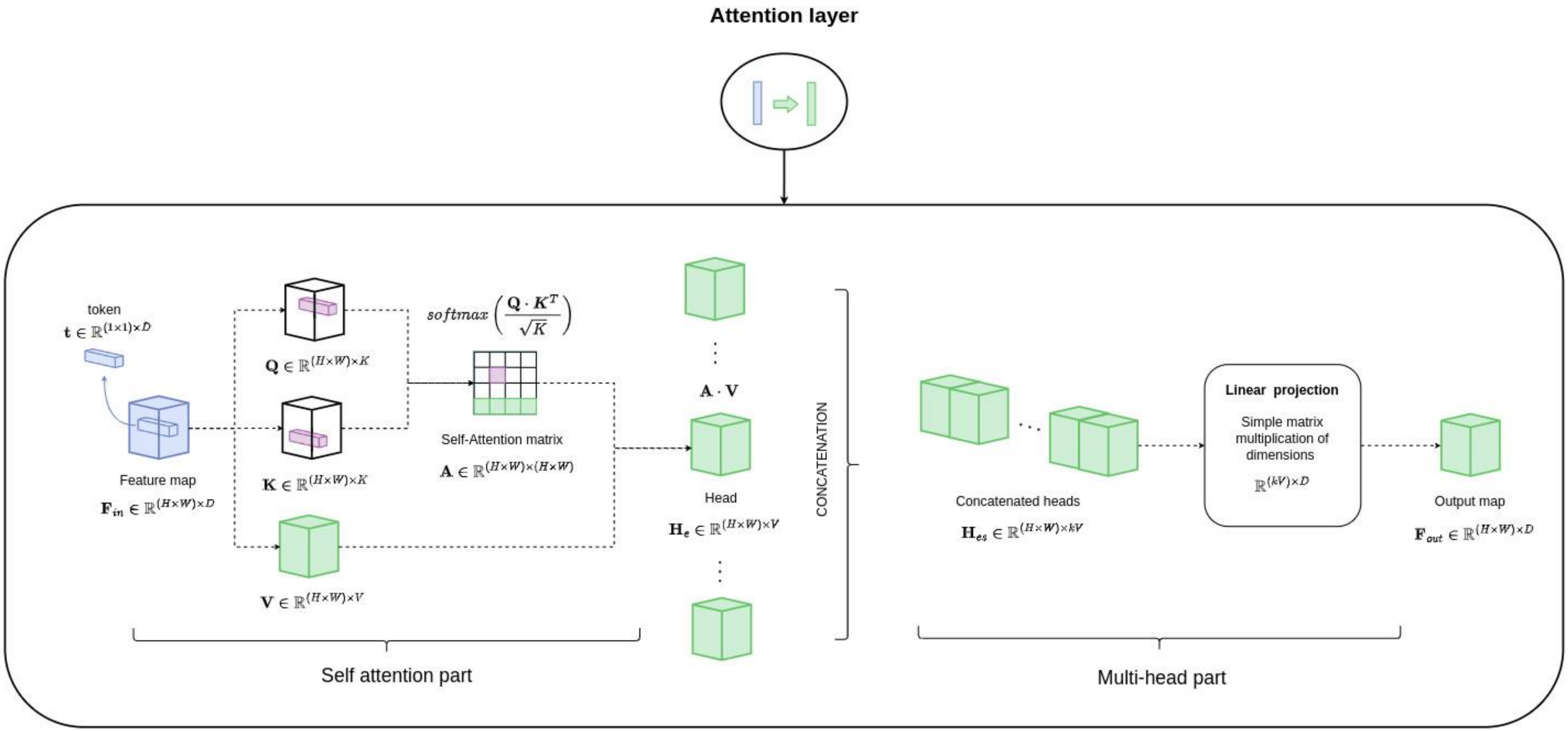
Standard U-Net with attention layers and position encoding to integrate temporal information

➔ Integration of t is necessary because the added noise varies over time

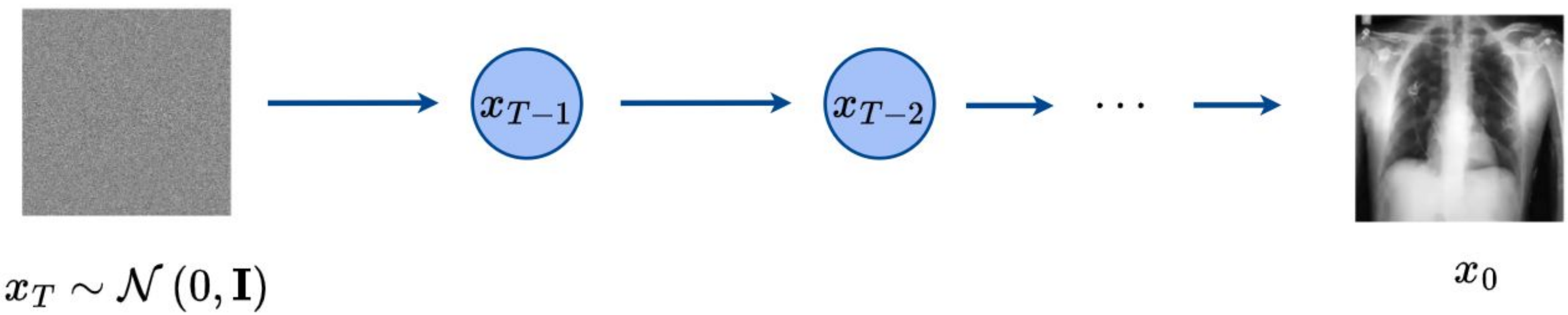


Architecture

- Attention layer



Inference: generation of synthetic data



- Generate a random image $x_T \sim \mathcal{N}(0, I) \in \mathbb{R}^{N \times M}$
- At each step from T to 0, use the U-Net model to compute

$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \epsilon_\theta(x_t, t) \right) + \sigma_t \, \epsilon$$

U-Net

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

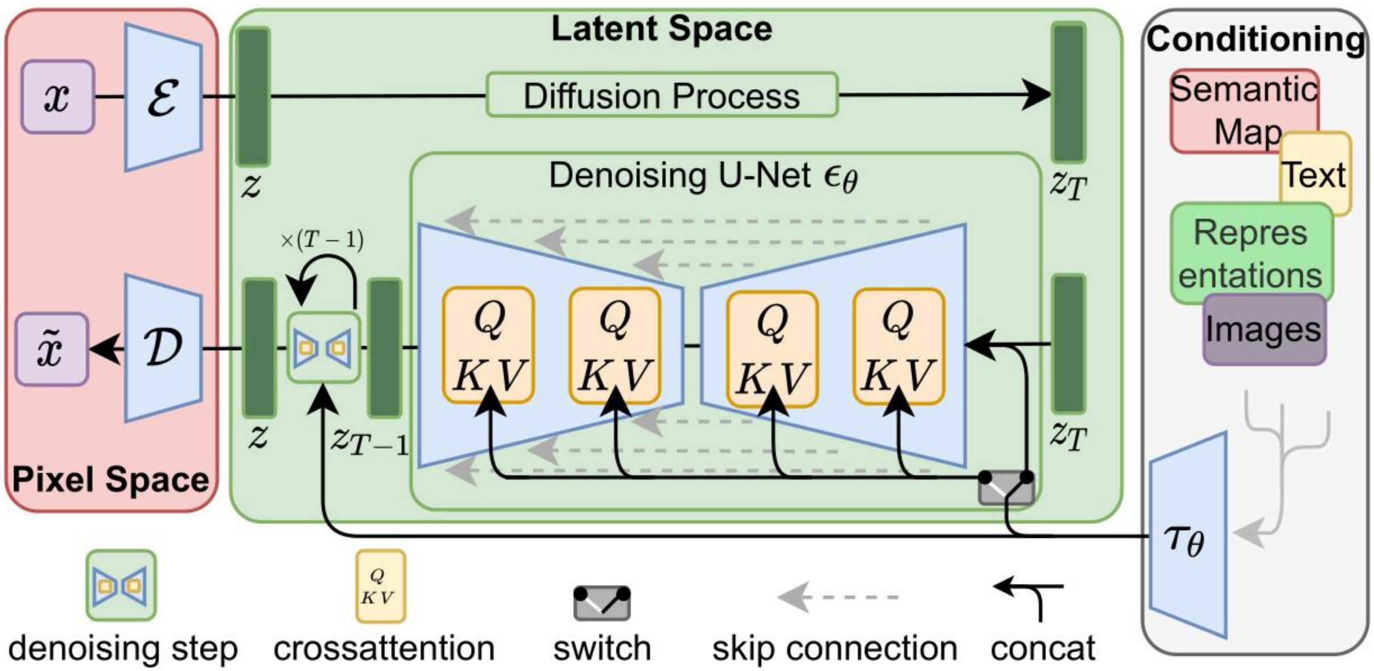
Practical application

Latent diffusion models

Latent diffusion model (LDM)

- VAE is learned independently of DDPM and its architecture is fixed
  - Efficiently reduce the dimensionality of the input space
  - Efficiently initiate the Gaussian diffusion process

- LDM architecture

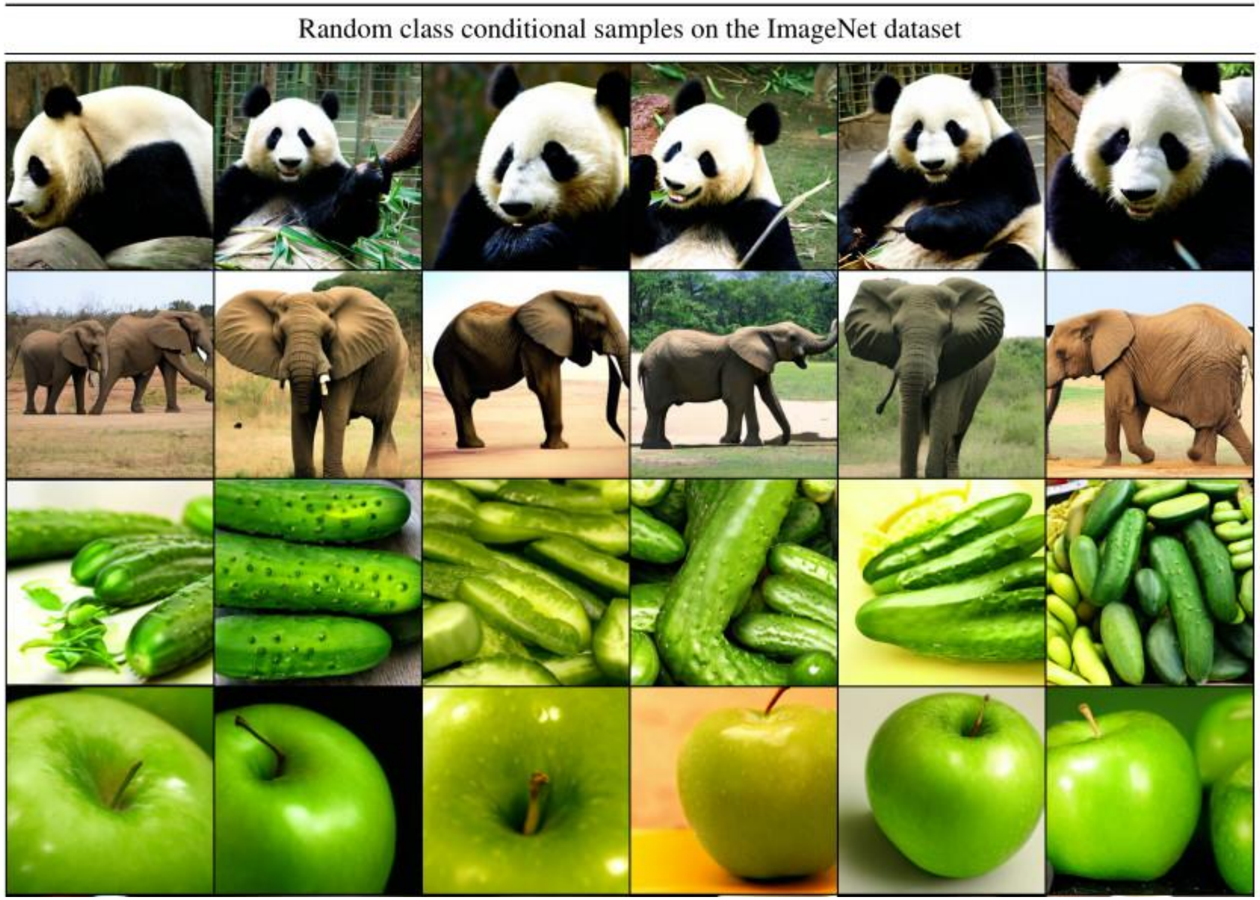


- Random generation of synthetic images *without conditioning* learned from the CelebA-HQ database

Random samples on the CelebA-HQ dataset

Latent diffusion model (LDM)

- Random generation of synthetic images *with conditioning on the class* learned from the ImageNet database



Latent diffusion model (LDM)

- Random generation of synthetic images *with conditioning on masks* learned from the Flickr-landscapes database

Latent diffusion model (LDM)

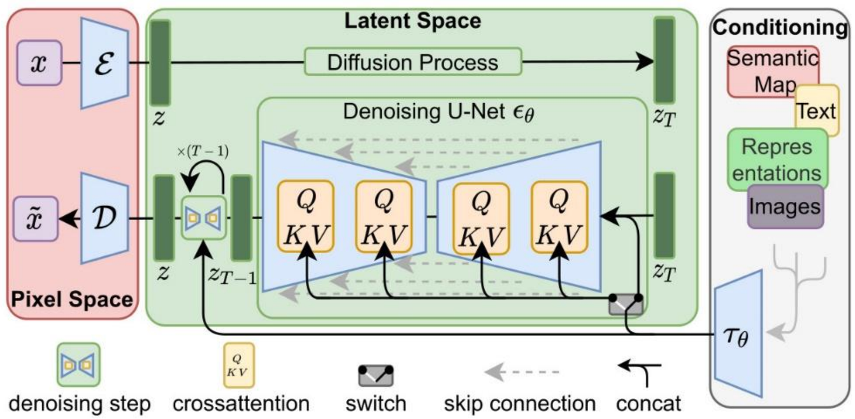
- Random generation of synthetic images *with conditioning on text* learned from LAION-400M database
  - Using the BERT tokenizer
  - This model has over 1.45 billion parameters!

'A painting of the last supper by Picasso.'

Medical applications

Denoising

Data augmentation

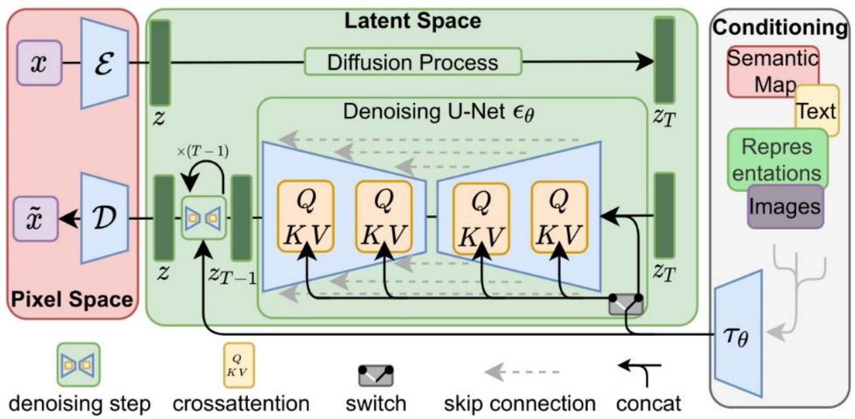


Segmentation

Anomaly detection

Denoising

Data augmentation



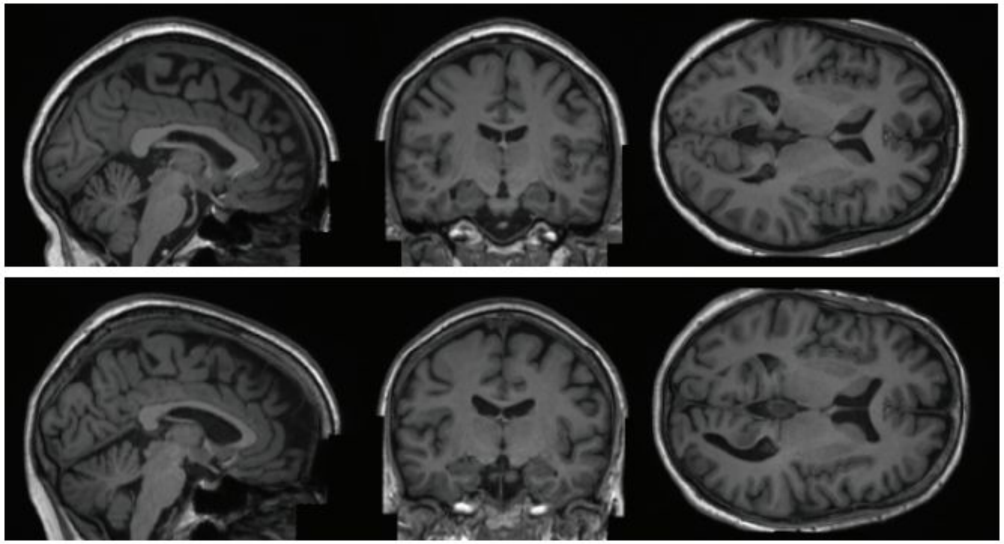
Segmentation

Anomaly detection

Diffusion models for data augmentation

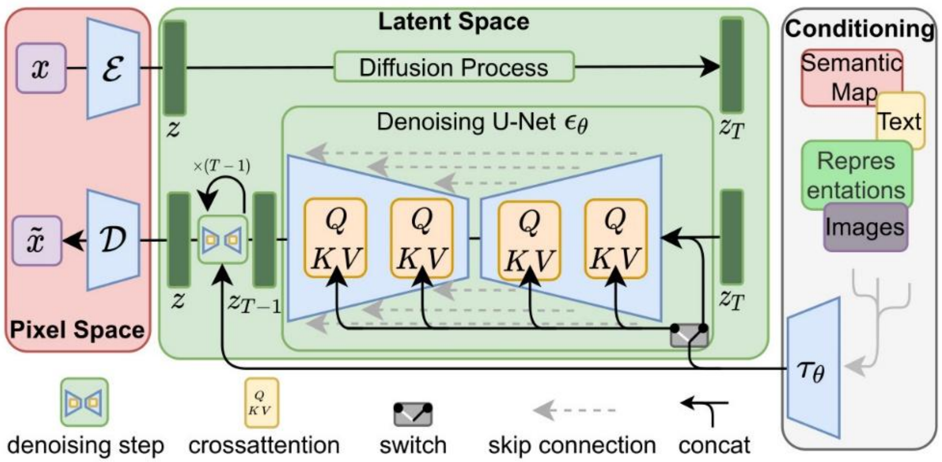
- Synthetic dataset generation for brain MR volumes [Walter et al., MICCAI workshop 2022]

- UK Biobank dataset
  - 3D MR volumes (T1w)
  - Training: 31,740 patients
  - with covariables: age (44 to 82 years), gender (53% women), brain structure volumes
  - Quality of synthetic data measured using FID: Fréchet Inception Distribution



Diffusion models for data augmentation

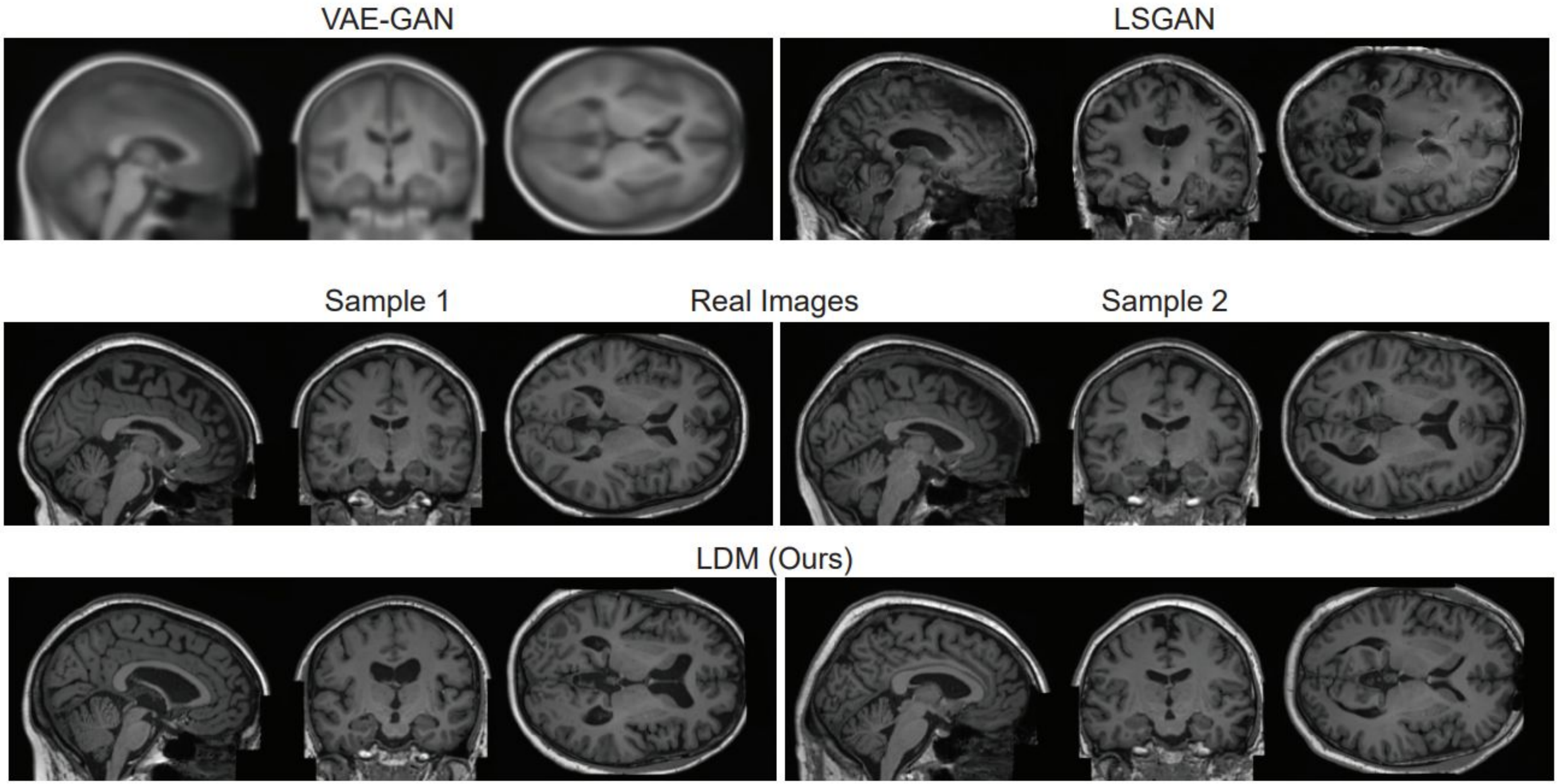
- VAE
  - 3D convolutions
  - Latent space dimension: 20 x 28 x 20
- DDPM
  - 3D convolutions
  - T=1000 time steps
  - Conditioning: vector encoding of each covariable



Diffusion models for data augmentation

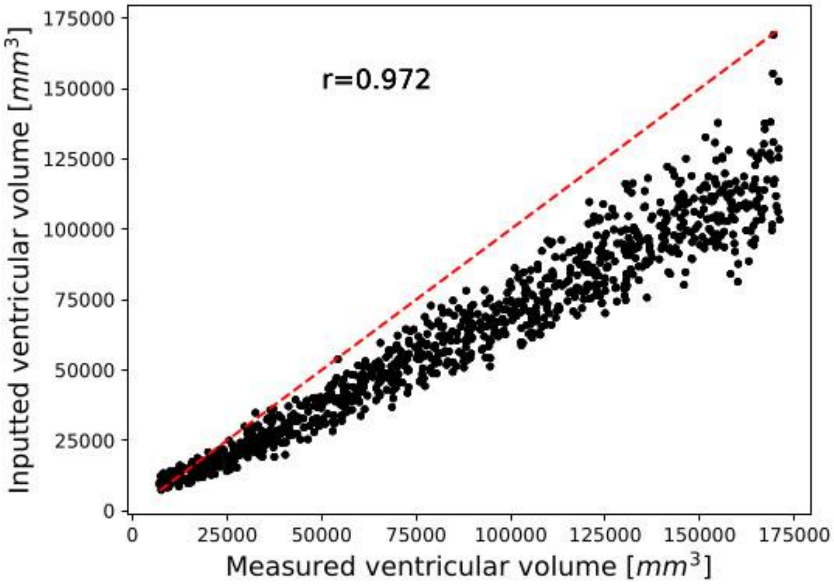
- Results
  - FID: generated from 1,000 samples drawn from each of the two distributions to be compared

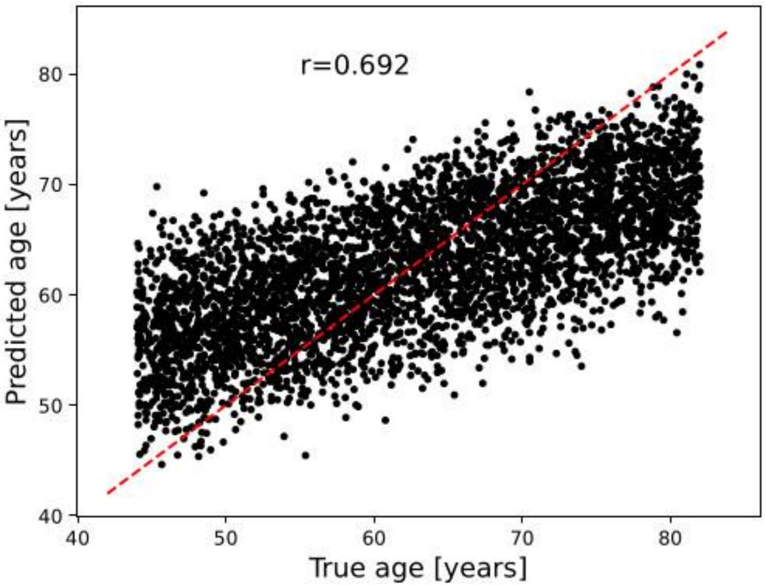
	FID ↓
LSGAN	0.0231
VAE-GAN	0.1576
LDM	**0.0076**
Real images	0.0005



Diffusion models for data augmentation

- Results
  - SynthSeg model was used to automatically measure brain volumes from synthetic data
  - A 3D CNN trained from the UK biobank was used to automatically predict the age from the synthetic data

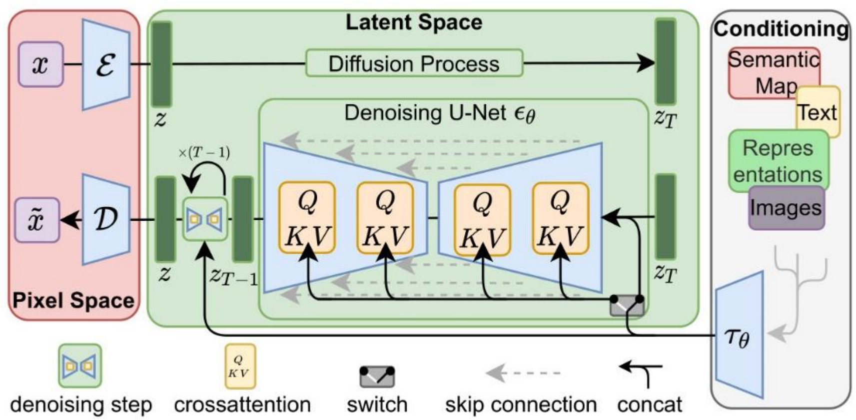




- Synthetic dataset of 100,000 human brain was generated and made publicly available with the conditioning information
- Promote data sharing with privacy guarantees

Denoising

Data augmentation

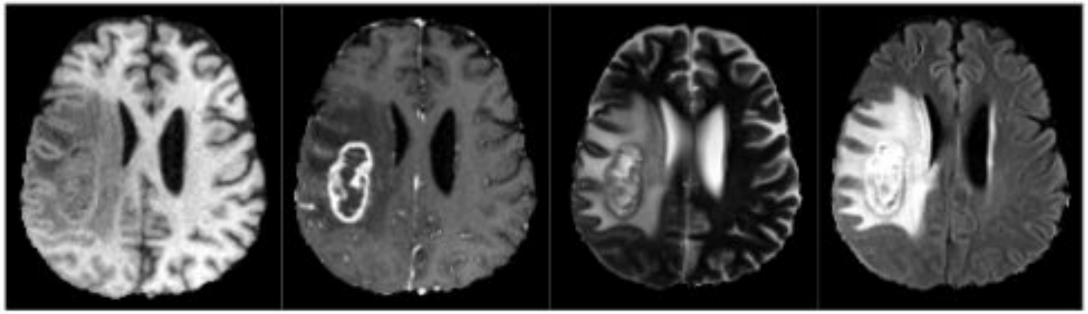


Segmentation

Anomaly detection

Diffusion models for image segmentation

- Segmentation of tumors from MR images [Wolleb et al., MIDL 2022]
- BRATS2020 dataset
  - 4 different MR sequences per patient (T1, T2, T1ce, FLAIR)
  - Training: 332 patients with 3D volumes sequences => 16,998 2D images
  - Testing: 37 patients with 3D volumes sequences => 1,082 2D images

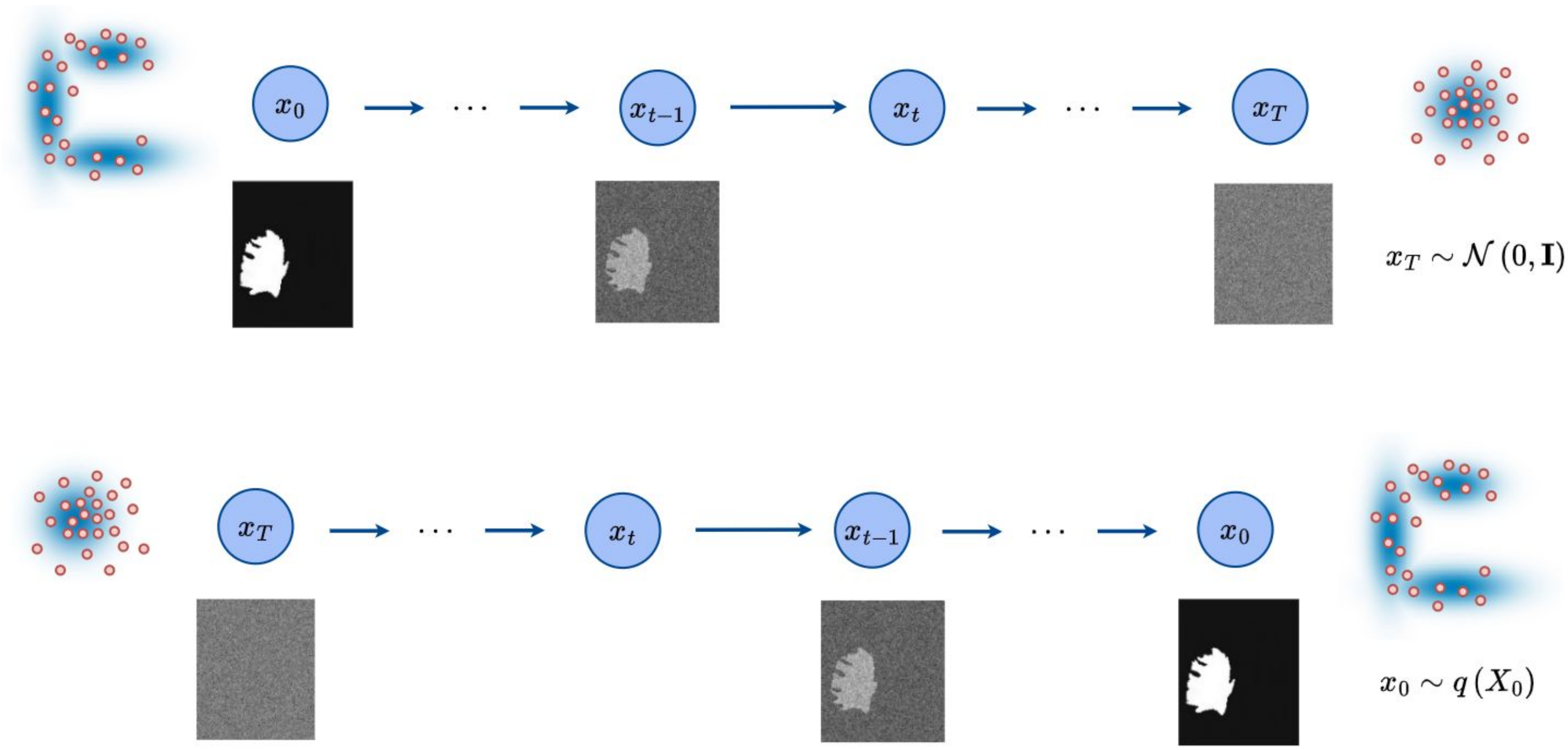


4 MR inputs per patient (T1, T2, T1ec, FLAIR)

Mask output

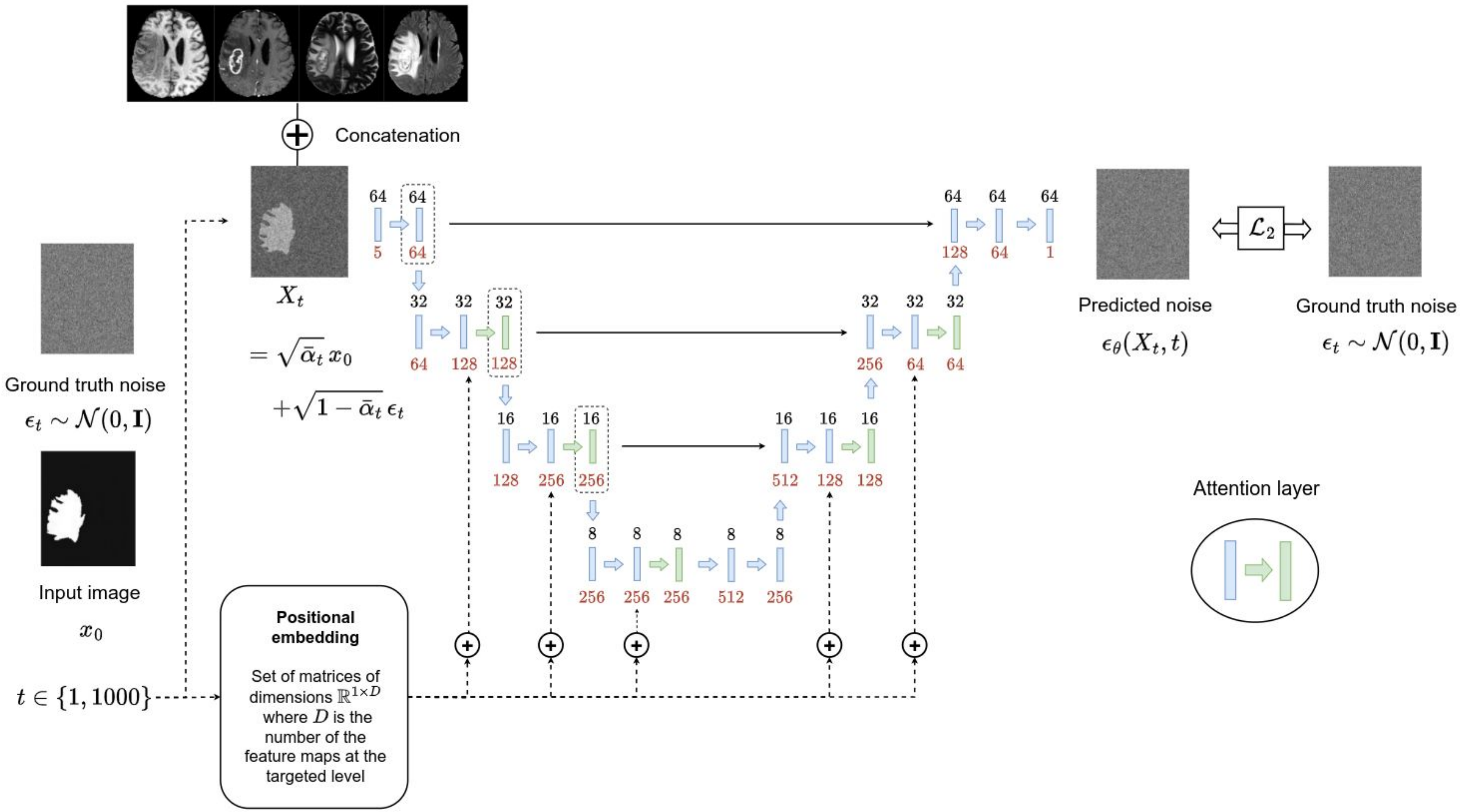
Diffusion models for image segmentation

- Learn the underlying distribution of tumor segmentation masks



Diffusion models for image segmentation

- Conditioning with the 4 MR images using concatenation scheme



Diffusion models for image segmentation

- At inference time: modelling of the segmentation uncertainty

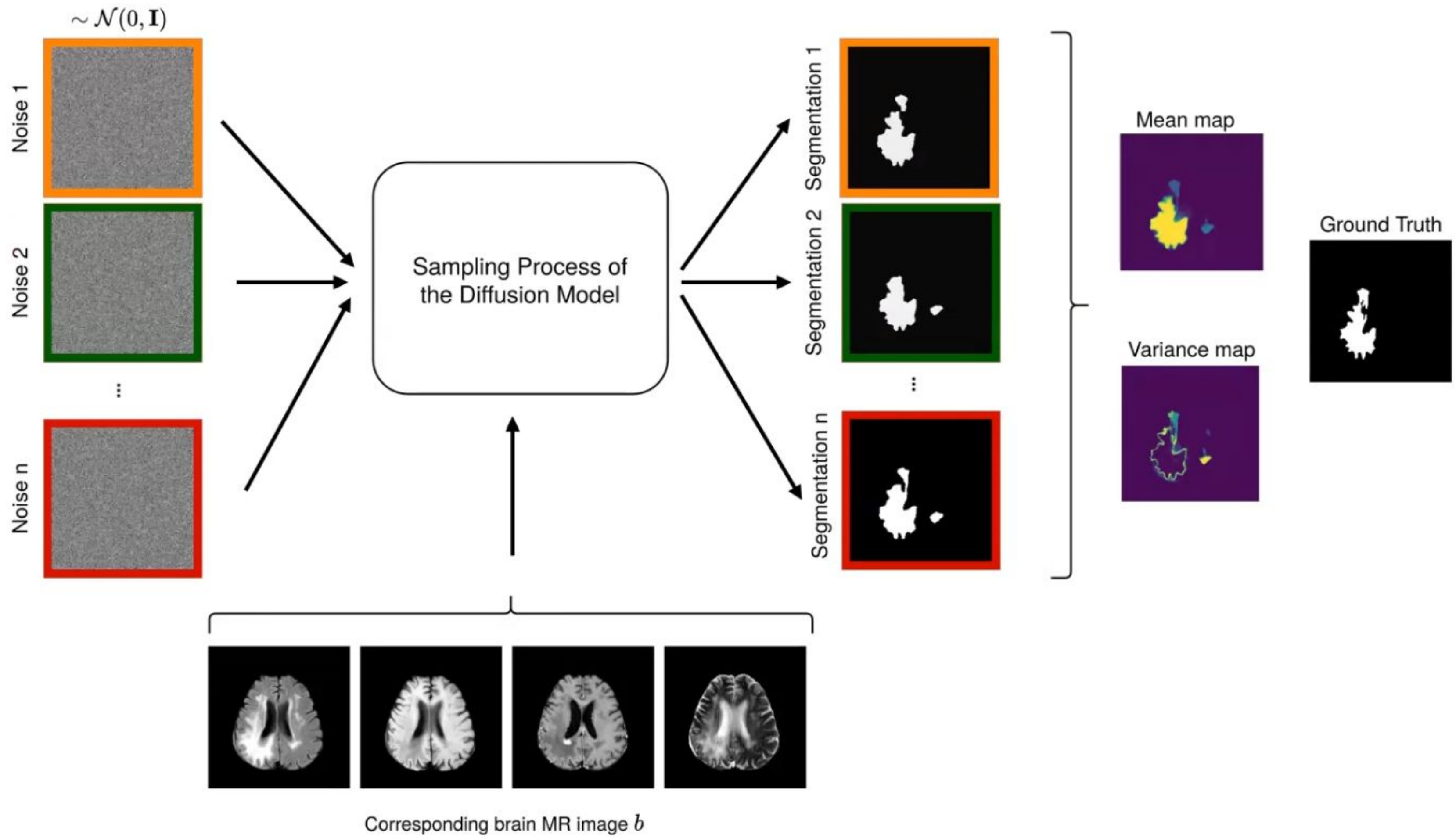


Illustration taken from https://www.youtube.com/watch?v=US9CzPrT2H8

- Results

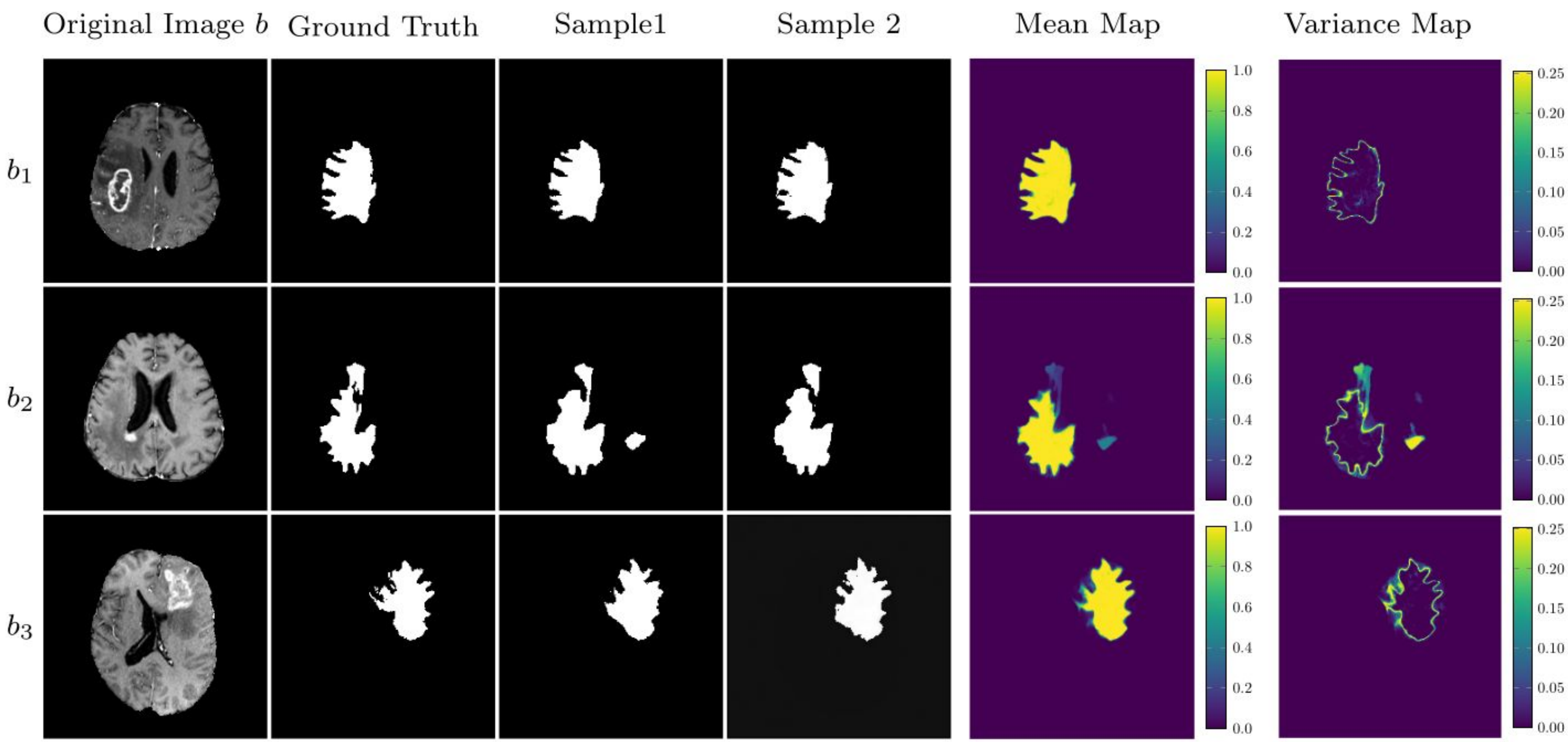
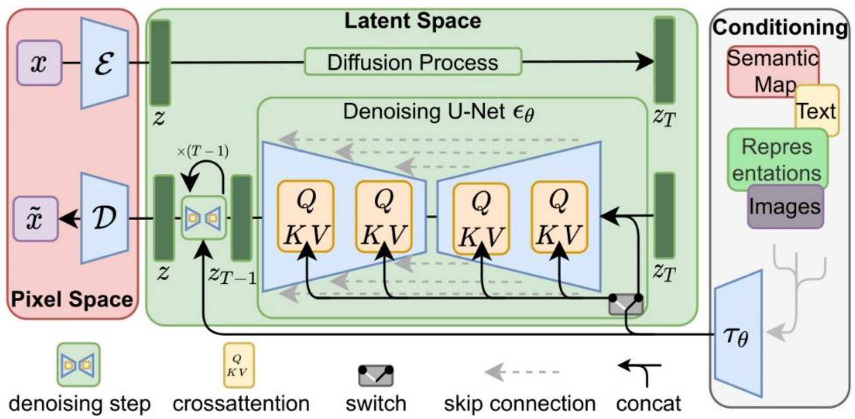


Illustration taken from https://arxiv.org/pdf/2112.03145

Denoising

Data augmentation

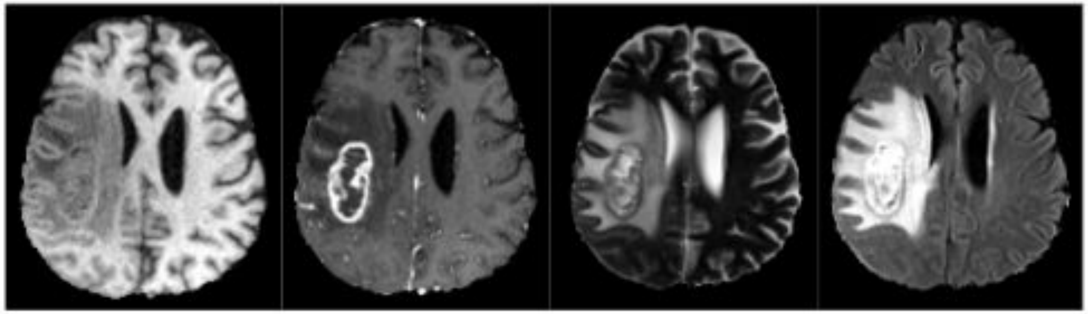


Segmentation

Anomaly detection

- Anomaly detection from MR images [Wolleb et al., MICCAI 2024]

- BRATS2020 dataset
  - 4 different MR sequences per patient (T1, T2, T1ce, FLAIR)
  - Training: 332 patients with 3D volumes sequences => 16,998 2D images
  - 5,598 healthy 2D slices (without tumor) / 10,607 disease 2D slices

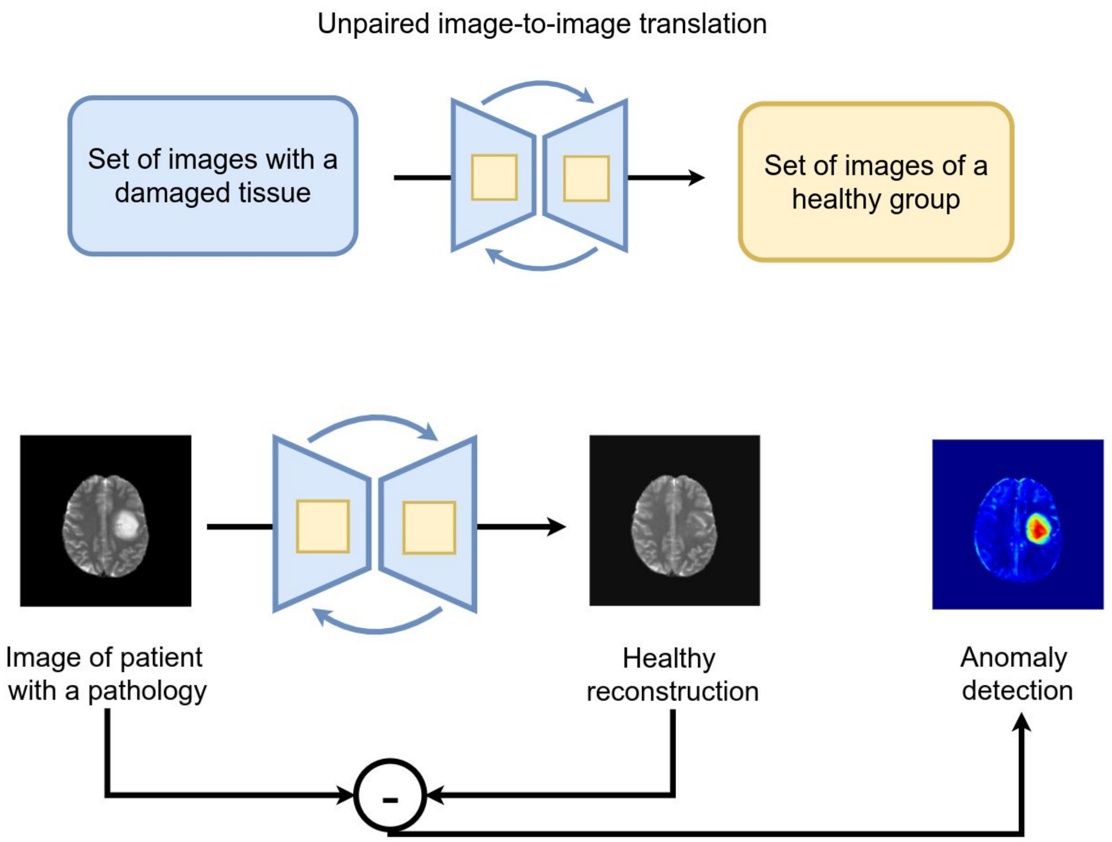


4 MR inputs per patient (T1, T2, T1ec, FLAIR)

Mask output

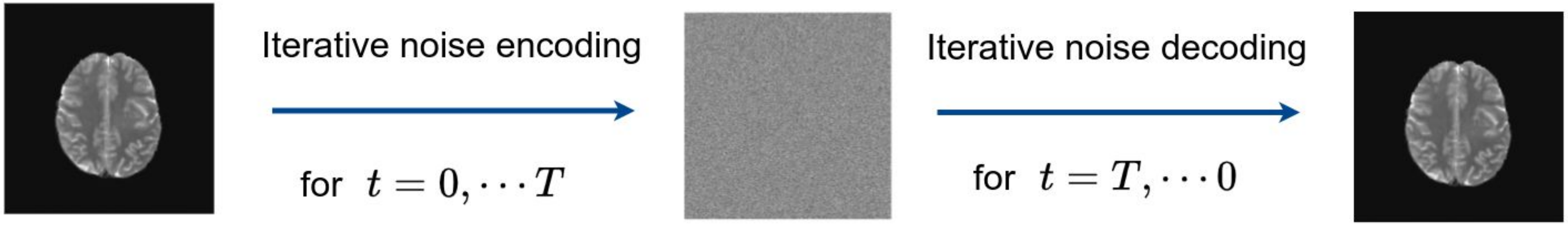
Diffusion models for anomaly detection

- General idea



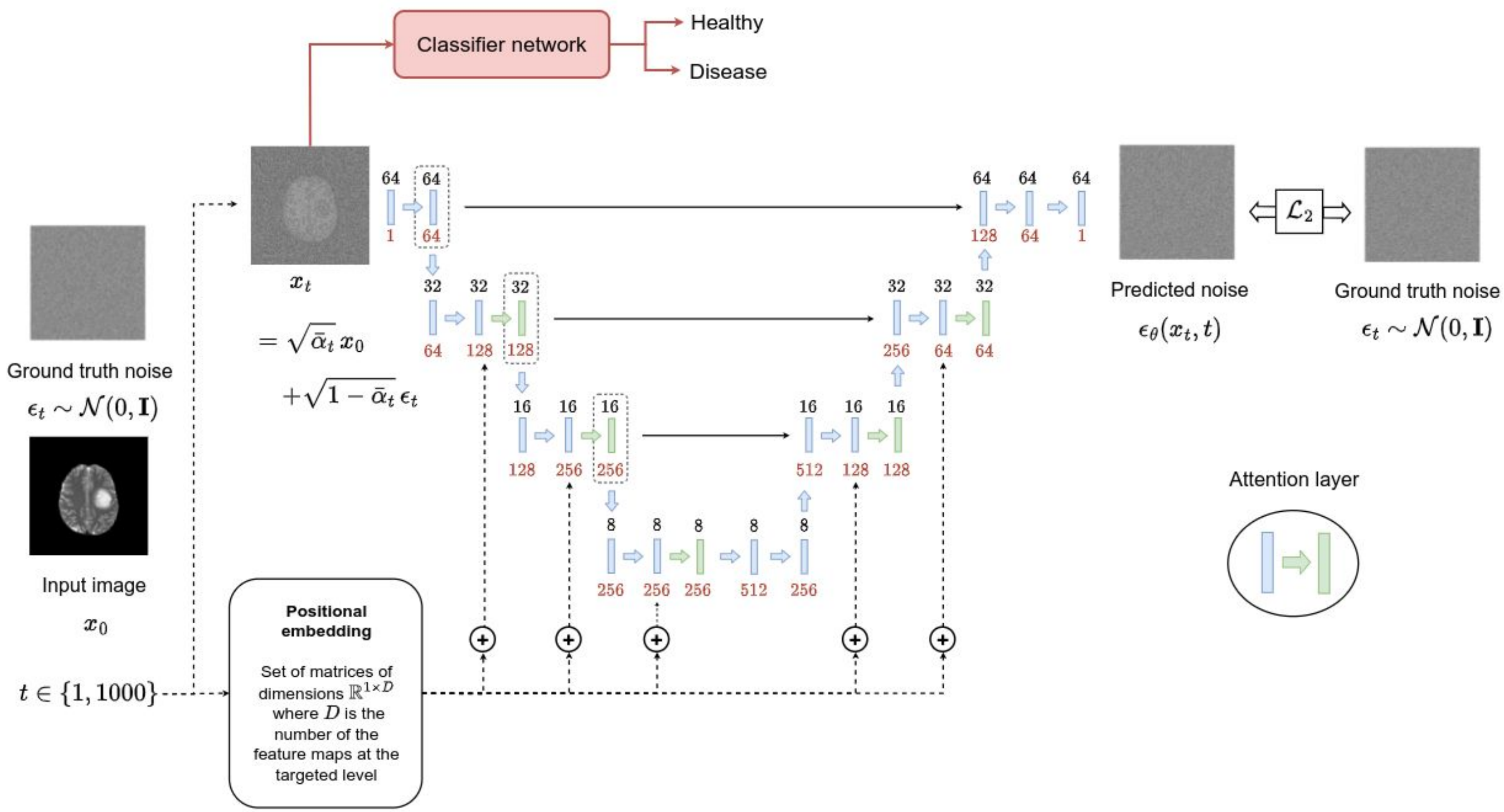
How to preserve spatial anatomical information using a diffusion process?

- Denoising Diffusion Implicit Models (DDIM)
  - Reformulation of the diffusion process
  - Remove the random component $\sigma_t \epsilon$
  - Make the diffusion process deterministic



Diffusion models for anomaly detection

- Main algorithm – part 1
  - Train a classical DDPM on the dataset containing healthy and disease images
  - Train a classifier network C to predict the class label (healthy vs disease) from any noisy images x_t



- Main algorithm – part 2
  - Use DDIM process
  - Compute the gradient of the classifier to guide the removing of anomaly regions

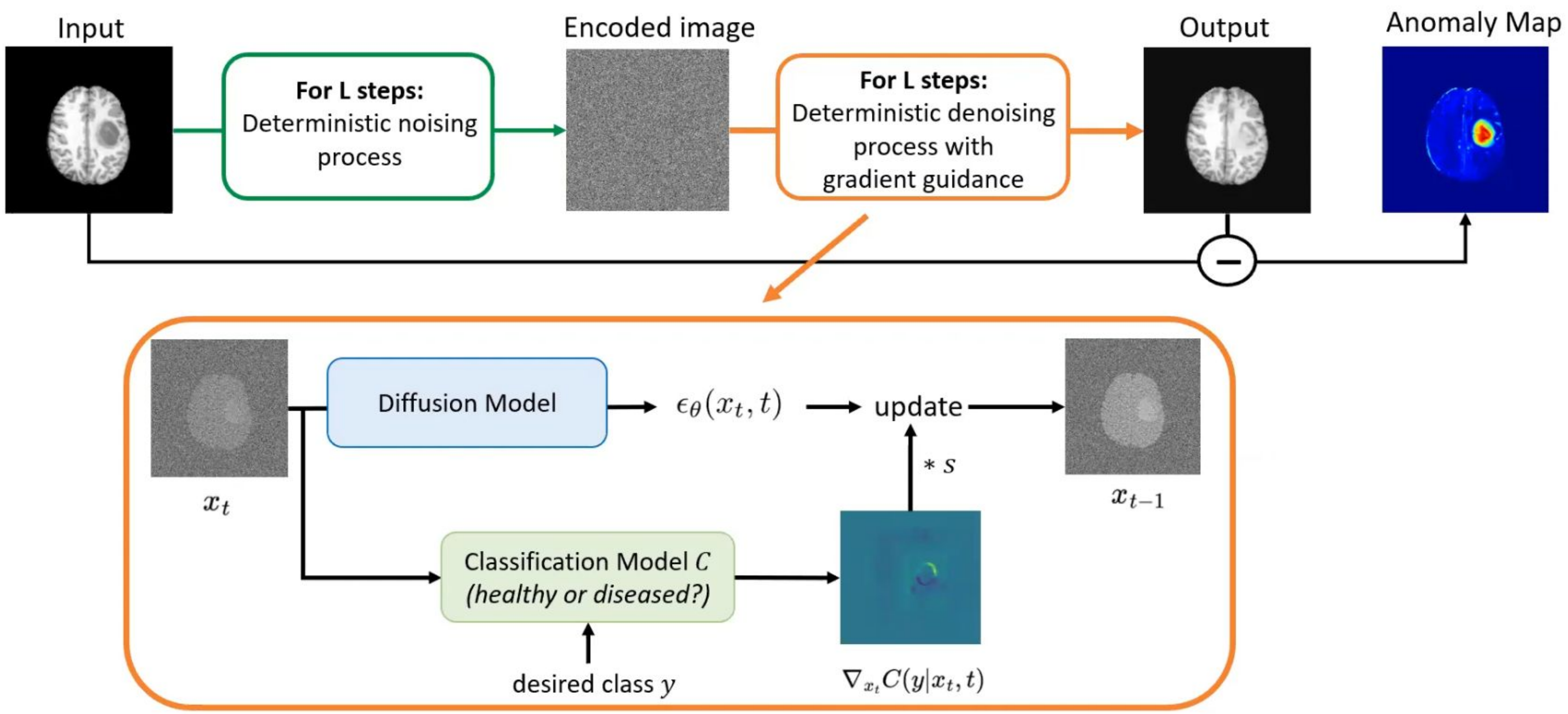
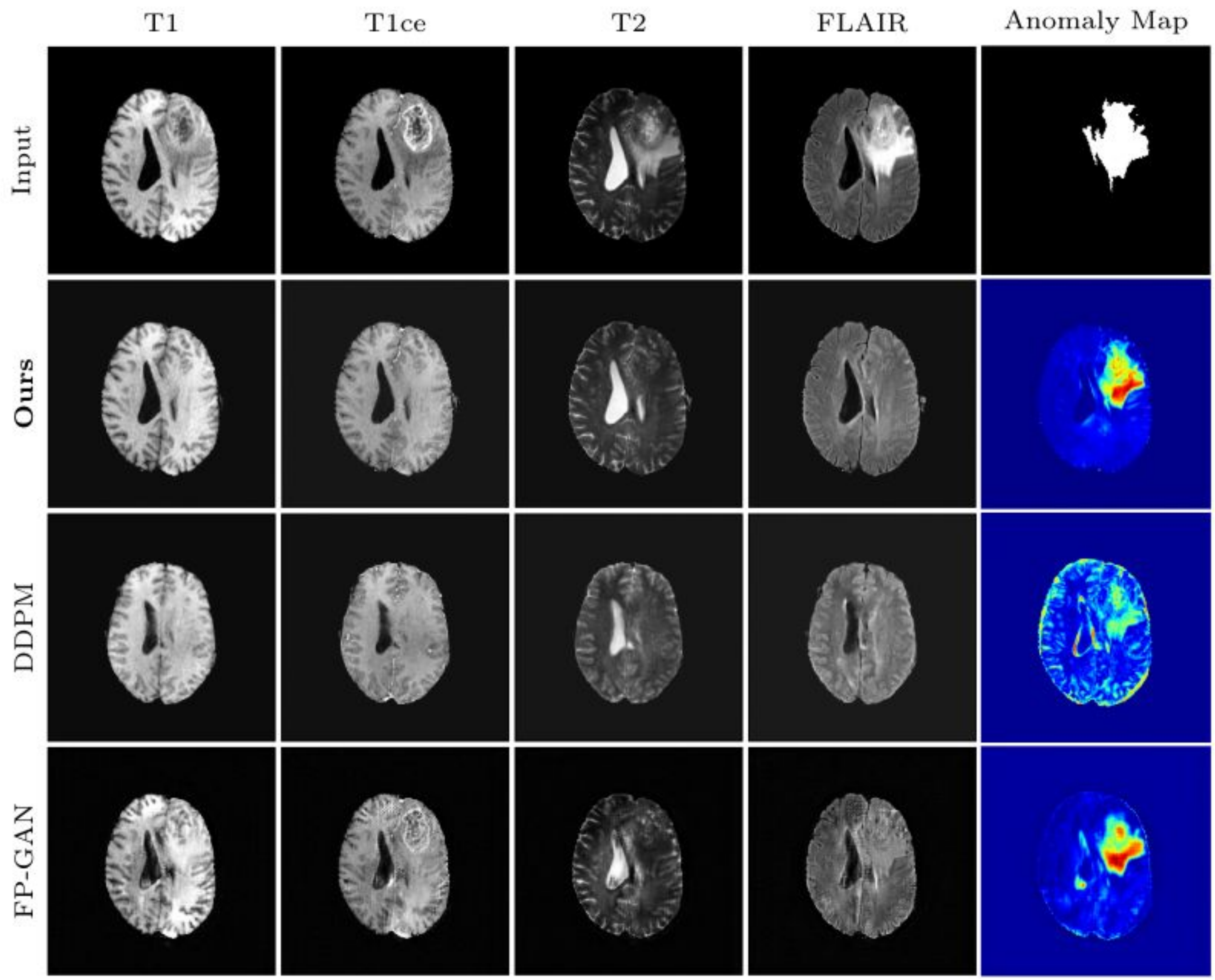


Illustration taken from https://arxiv.org/pdf/2203.04306

Diffusion models for anomaly detection

- Result on an image with a tumor



Diffusion models for anomaly detection

- Result on an image without any tumor

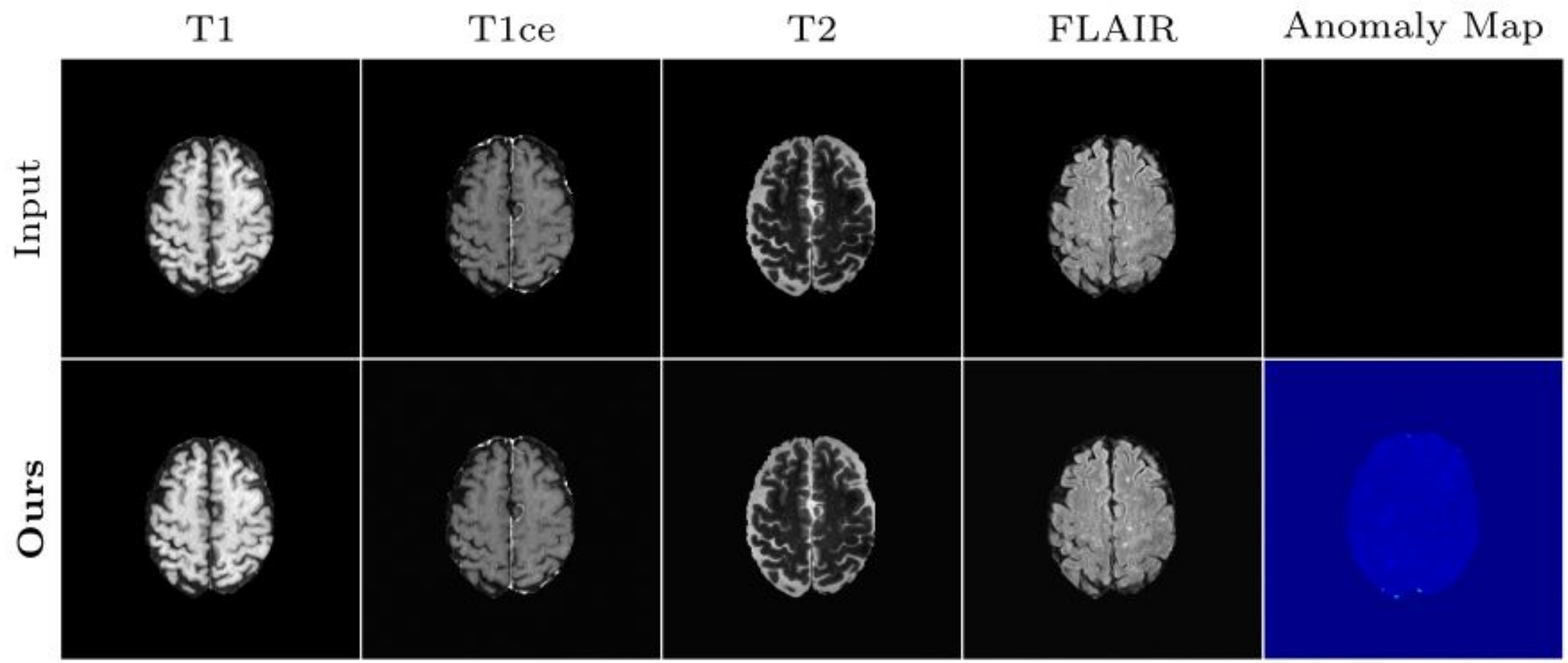


Illustration taken from https://arxiv.org/pdf/2203.04306

That's all folks

- Denoising Diffusion Implicit Models (DDIM)
  - Reformulation of the diffusion process
  - Remove the random component $\sigma_t \epsilon$

$$x_{t-1} = \sqrt{\bar{\alpha}_{t-1}} \left(\frac{x_t - \sqrt{1-\bar{\alpha}_t} \cdot \epsilon_\theta(x_t, t)}{\sqrt{\bar{\alpha}_t}} \right) + \sqrt{1-\bar{\alpha}_{t-1}} \cdot \epsilon_\theta(x_t, t)$$

$$x_{t+1} = x_t + \sqrt{\bar{\alpha}_{t+1}} \left[\left(\sqrt{\frac{1}{\bar{\alpha}_t}} - \sqrt{\frac{1}{\bar{\alpha}_{t+1}}} \right) x_t + \left(\sqrt{\frac{1}{\bar{\alpha}_{t+1}} - 1} - \sqrt{\frac{1}{\bar{\alpha}_t} - 1} \right) \epsilon_\theta(x_t, t) \right]$$

  - Make the diffusion process deterministic