



Videos generated by diffusion models



EN.601.482/682 Deep Learning

# An Introduction to Diffusion Models

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# Agendas

- Recap: Generative Models
  - VAE, GAE, Normalizing Flow, Energy Based Model
- Denoising Diffusion Probabilistic Model
  - Basic Concept & Definitions
  - Method Overview
  - Forward Process
  - Reverse Process
  - Training Objective
  - Denoising Network Architecture
  - Sampling Process
  - Comparisons with other Generative Models
- Conditional Diffusion Model
  - Applications: Text-to-Image, Counterfactual, Inpainting
  - Formulation
  - Network
  - Latent Diffusion Model (*Stable Diffusion*)

Intro Diffusion Models

# Reminder: Generative Models



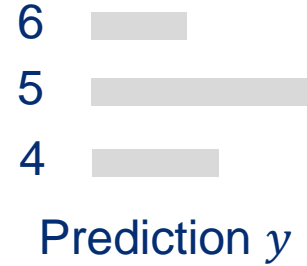
# Discriminative Models



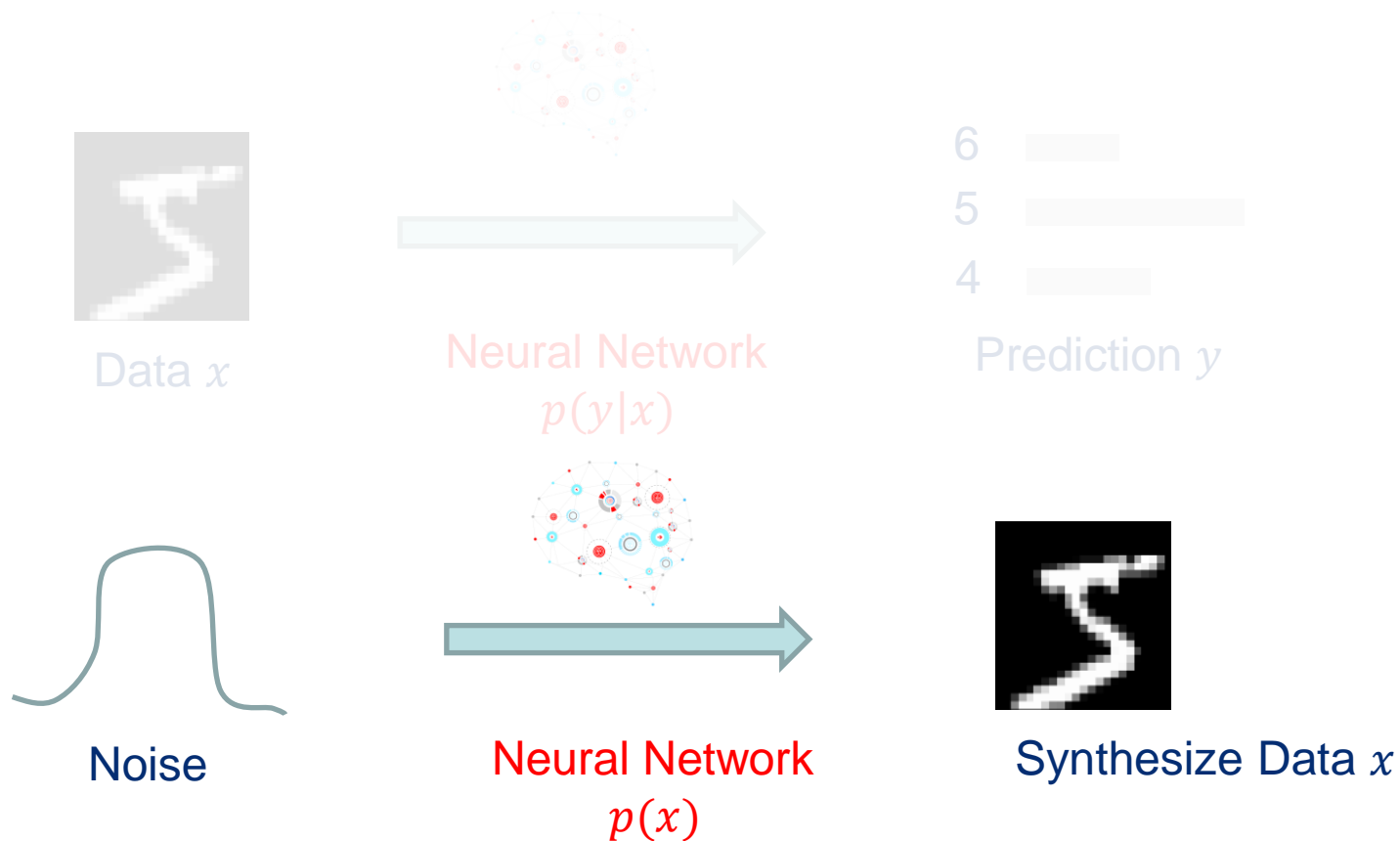
Data  $x$



Neural Network  
 $p(y|x)$



# Generative Models



# Landscape of the Generative Models

Energy-Based Model

Variational  
Autoencoder

Generative  
Adversarial Networks

Normalizing Flow





# Landscape of the Generative Models

Energy-Based Model

Variational  
Autoencoder

Generative  
Adversarial Networks

Normalizing Flow

Diffusion  
Probabilistic Model

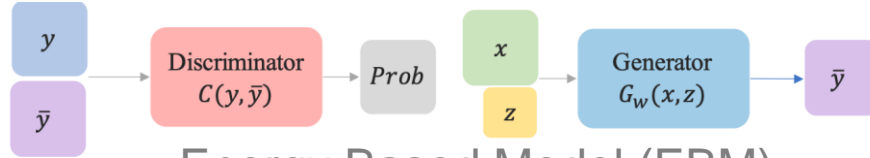




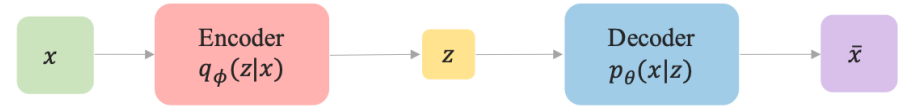
# Why Diffusion Models?



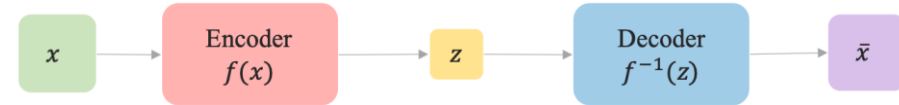
Generative Adversarial Network (GAN):  
training additional discriminators



Energy Based Model (EBM):  
intractable partition functions



Variational Auto Encoder (VAE):  
require aligning posterior distributions



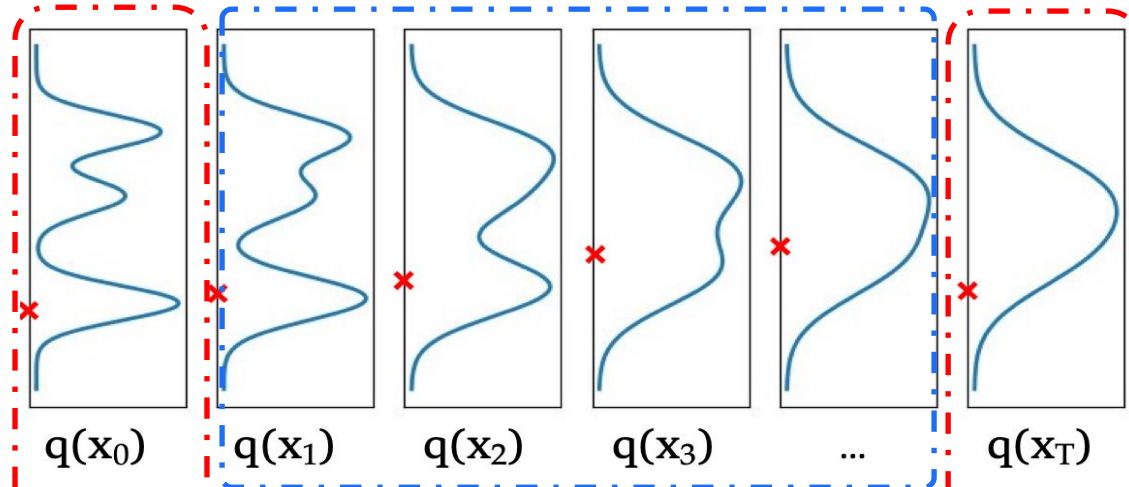
Normalizing Flow (NF):  
imposing network constraints

## Advantages of Diffusion Models:

- Tractable probabilistic parameterization for describing the generation process
- A stable training procedure with sufficient theoretical support
- A unified loss function design with high simplicity

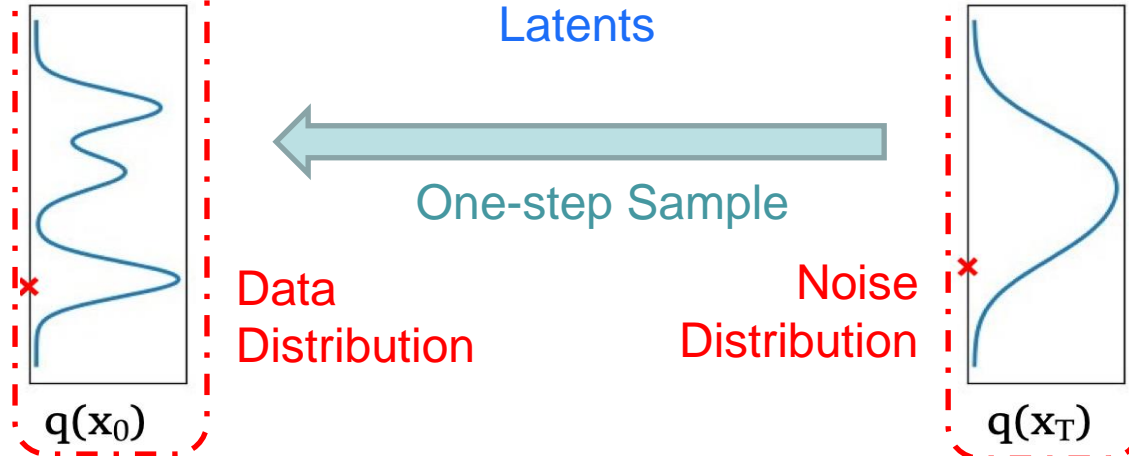
# Why Diffusion Models?

Diffusion Models



Latents

Other Models



# The Power of Diffusion Models: Text-to-Image Generation

## DALL-E 2 (OpenAI)

“A teddy bear on a skateboard in times square”



<https://openai.com/product/dall-e-2>

## Imagen (Google)

“A group of teddy bears in suit in a corporate office celebrating the birthday of their friend. There is a pizza cake on the desk.”



<https://imagen.research.google>

# The Power of Diffusion Models: Text-to-Image Generation

## Stable Diffusion (Stability AI)

'A street sign that reads  
"Latent Diffusion" '



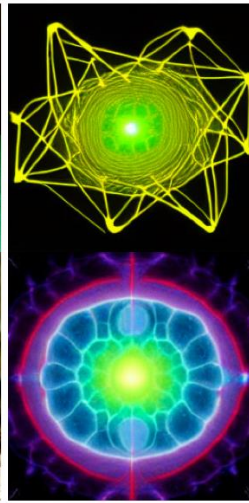
'A zombie in the  
style of Picasso'



'An image of an animal  
half mouse half octopus'



'An illustration of a slightly  
conscious neural network'



'A painting of a  
squirrel eating a burger'



'A watercolor painting of a  
chair that looks like an octopus'



'A shirt with the inscription:  
"I love generative models!" '



<https://stability.ai/blog/stable-diffusion-public-release>

[High-Resolution Image Synthesis with Latent Diffusion Models](#) CVPR 2022

# The Power of Diffusion Models: Text-to-Image Generation

## Midjourney v5





# The Power of Diffusion Models: Text-to-Image Generation

## Midjourney v5



- **Wider Stylistic Range**
- **Higher Resolution**
- **Greater Clarity and Precision**
- **Broader Aspect Ratio Options**

Intro Diffusion Models

# Denoising Diffusion Probabilistic Model (DDPM)

# Basic Concept of Diffusion

- **Diffusion** is the movement of anything (atoms, ions, molecules, energy) generally from a region of higher concentration to a region of lower concentration.

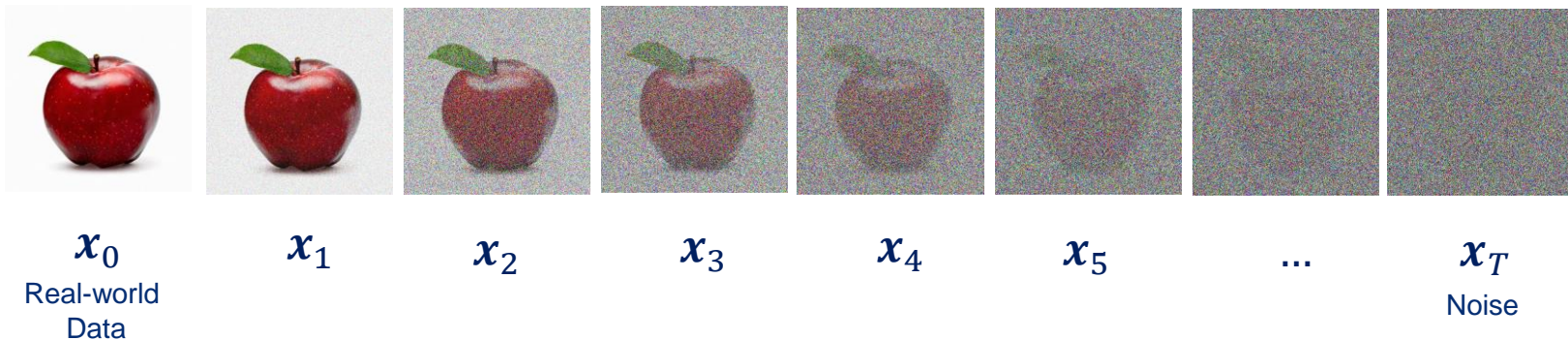


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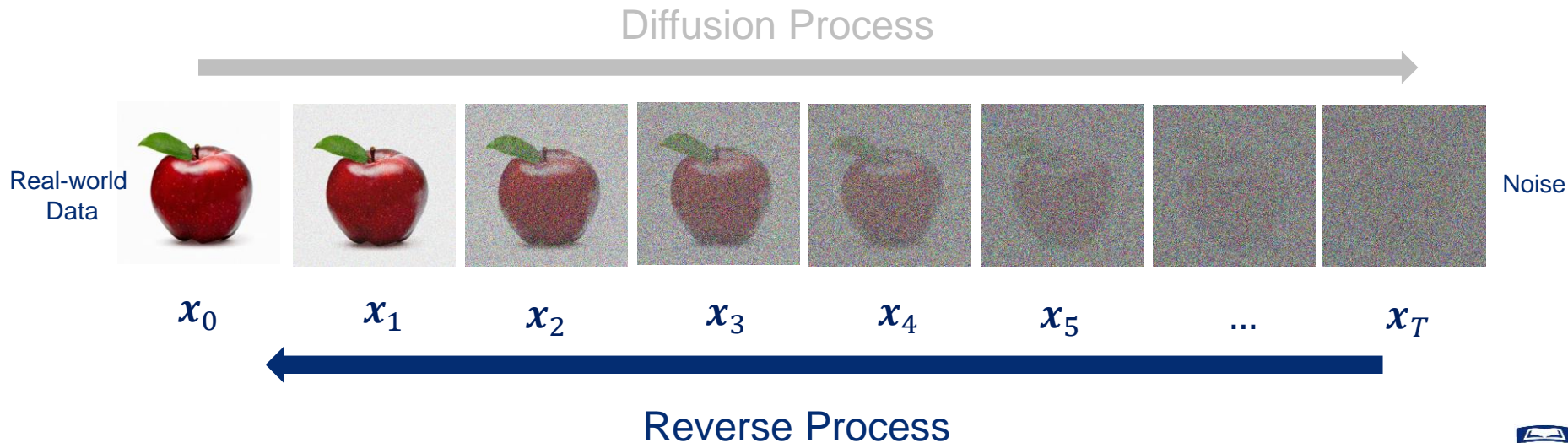


Diffusion Process



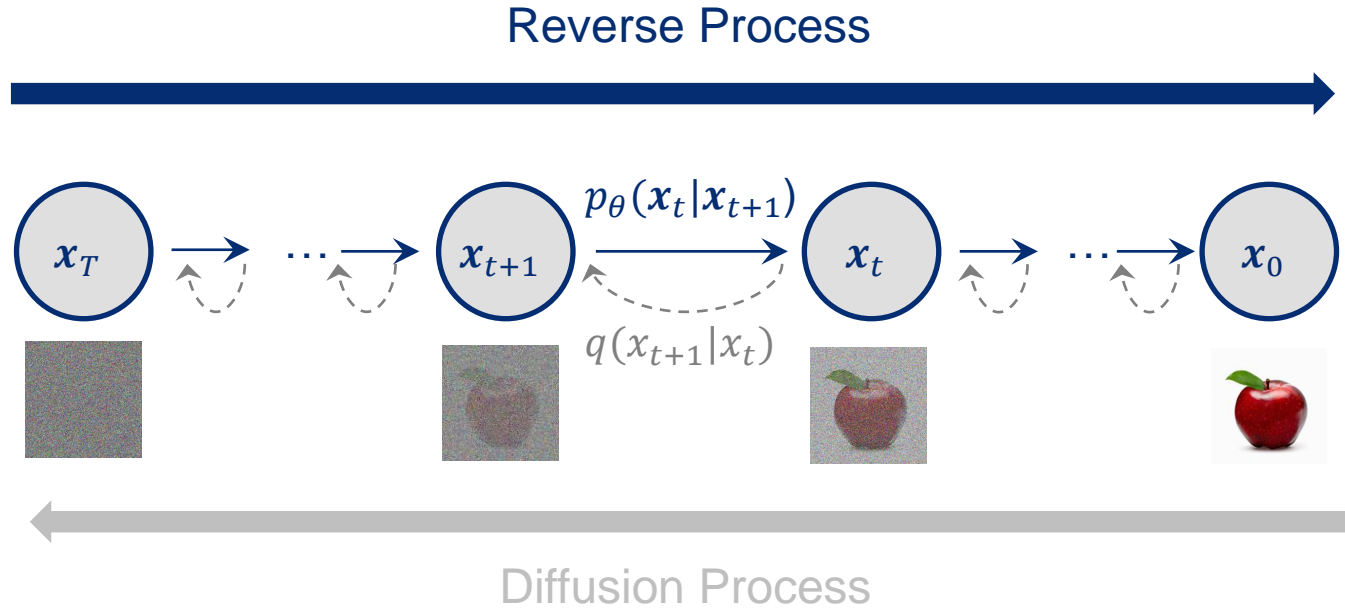
# What is Diffusion Probabilistic Model?

- Consists of two processes.
  - Diffusion/Forward process: gradually add noise to the input
  - Reverse process: learns to denoise -> generate new data

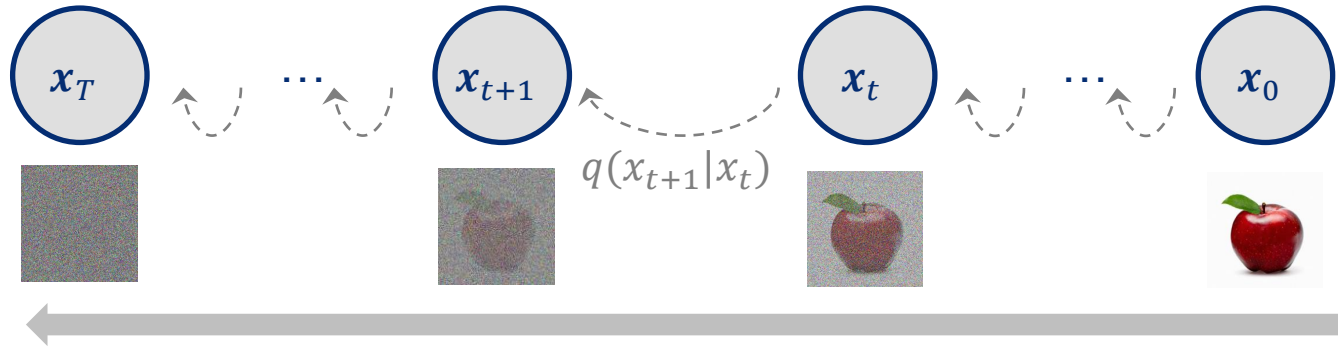




# DDPM In the View of a Directed Graph

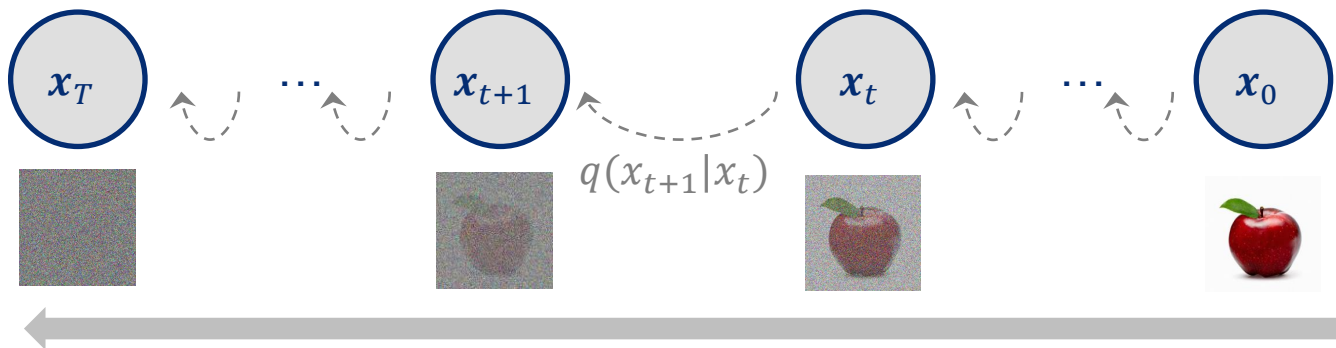


# Diffusion/Forward Process (1/3)



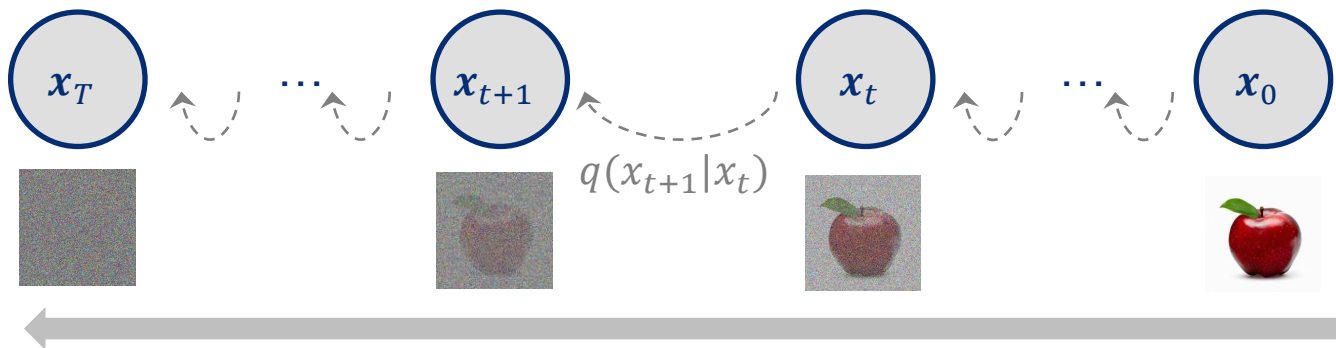
- Motivation: transforms the starting state ( $x_0$ ) into the tractable noise ( $x_i$ )

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- Formally, we call the joint distribution  $q(x_{1:T}|x_0)$  as the **diffusion process**.

# Diffusion/Forward Process (1/3)

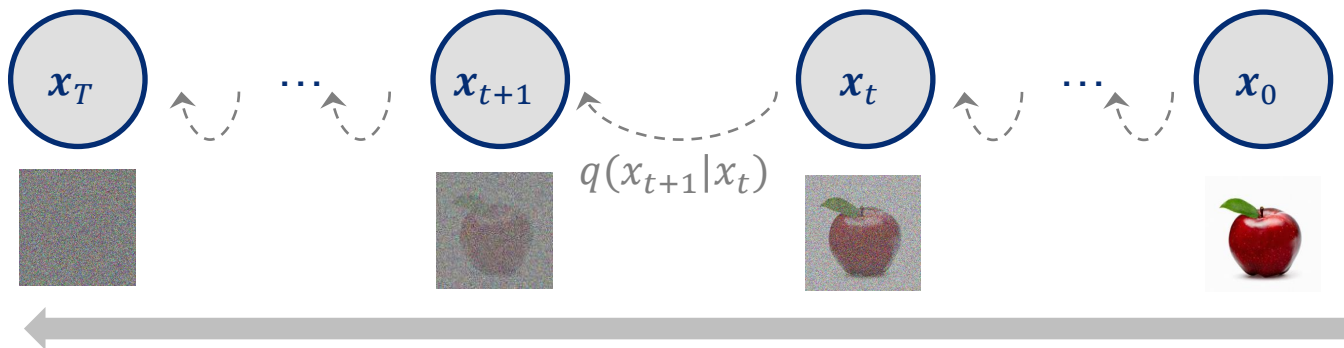


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- Formally, we call the joint distribution  $q(x_{1:T}|x_0)$  as the **diffusion process**.
- In DDPM,  $q(x_{1:T}|x_0)$  is defined as a Markov chain:

$$q(x_{1:T}|x_0) = \prod_{t=1}^T q(x_t|x_{t-1}, x_{t-2}, \dots, x_0)$$

Chain Rule (Probabilistic Properties)

# Diffusion/Forward Process (1/3)



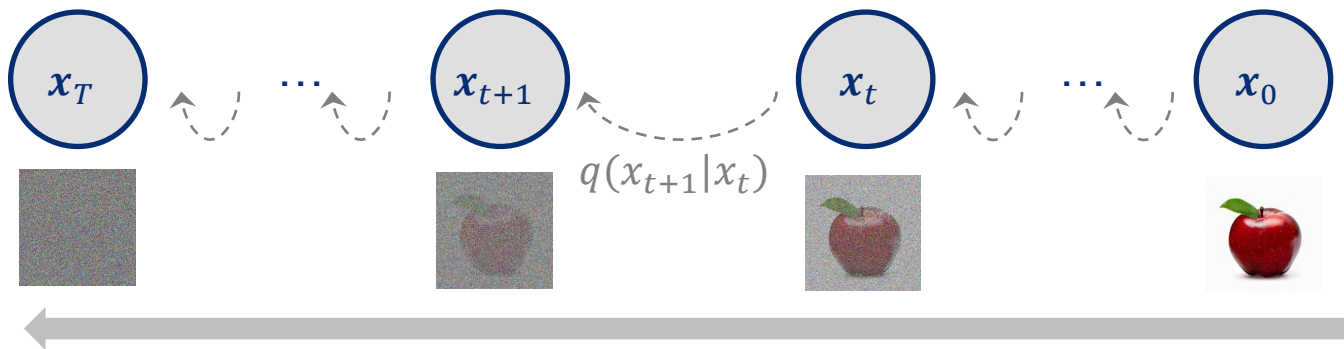
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$$q(x_{1:T}|x_0) = \prod_{t=1}^T \boxed{q(x_t|x_{t-1})}$$

Markov Property ->  
Transition kernel



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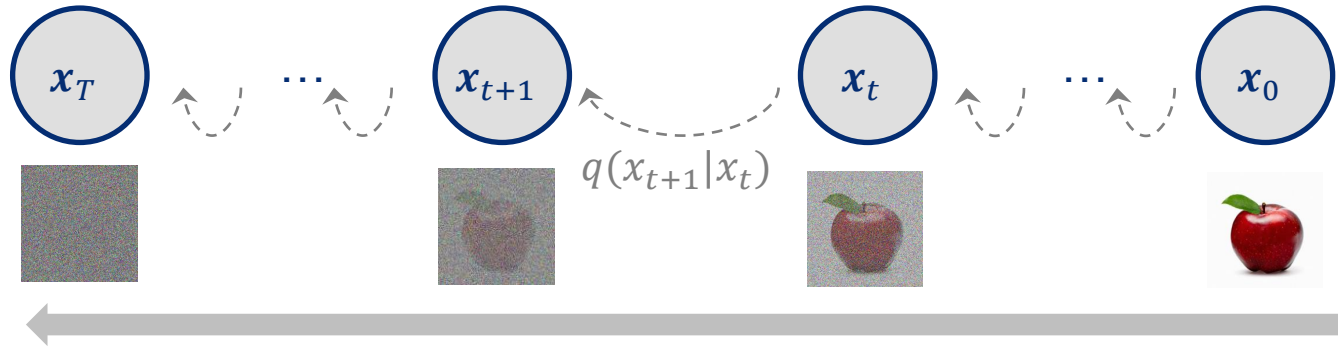
$$q(x_{1:T}|x_0) = \prod_{t=1}^T \boxed{q(x_t|x_{t-1})} \text{ Transaction kernel}$$

- The **transaction kernel** in DDPM employs Gaussian perturbation, i.e.

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

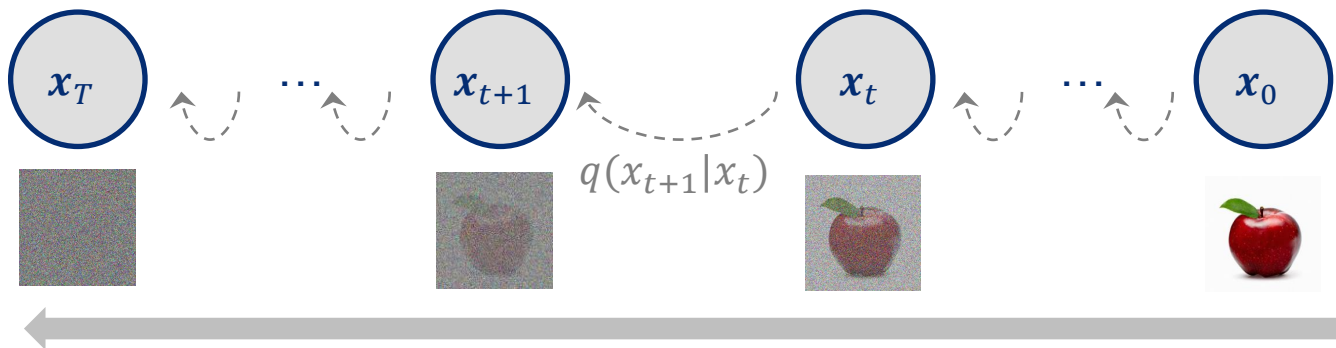


# Diffusion/Forward Process (2/3)



Q: Why Gaussian perturbation i.e.,  $q(x_t|x_{t-1}) = \mathcal{N}(x_t|\sqrt{1-\beta_t}x_{t-1}, \beta_t I)$ ?

## Diffusion/Forward Process (2/3)

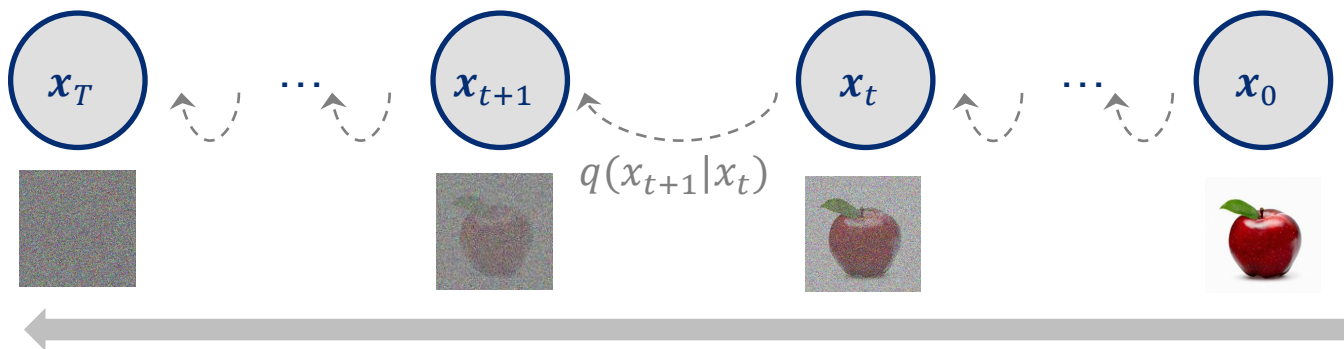


Q: Why Gaussian perturbation i.e.,  $q(x_t|x_{t-1}) = \mathcal{N}(x_t|\sqrt{1-\beta_t}x_{t-1}, \beta_t I)$ ?

A: Composition of Gaussians is still Gaussian

$$q(x_t|x_0) = \mathcal{N}(x_t|\sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_t)I) \quad \text{where} \quad \bar{\alpha}_t = \prod_{s=1}^t(1-\beta_s)$$

## Diffusion/Forward Process (2/3)



Q: Why Gaussian perturbation i.e.,  $q(x_t|x_{t-1}) = \mathcal{N}(x_t|\sqrt{1 - \beta_t}x_{t-1}, \beta_t I)$ ?

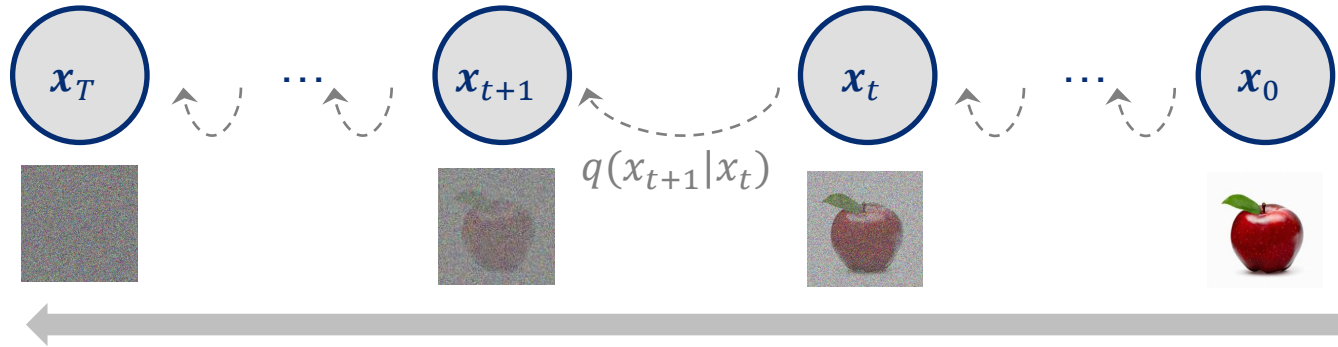
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By choosing  $\beta_t$  properly (e.g., all  $\beta_t < \text{Constant} < 1$ ), we have

$$\lim_{n \rightarrow \infty} \bar{\alpha}_t = 0 \quad \text{and} \quad \lim_{t \rightarrow \infty} q(x_t) = \lim_{t \rightarrow \infty} q(x_t|x_0) = \mathcal{N}(0, I).$$

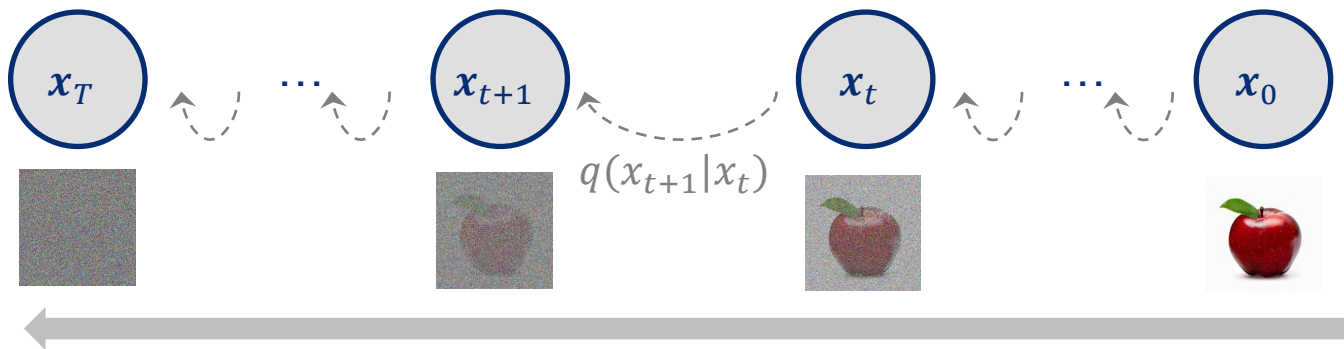
# Diffusion/Forward Process (3/3)



Q: How to sample from  $q(x_t|x_{t-1}) = \mathcal{N}(x_t|\sqrt{1 - \beta_t}x_{t-1}, \beta_t I)$ ?



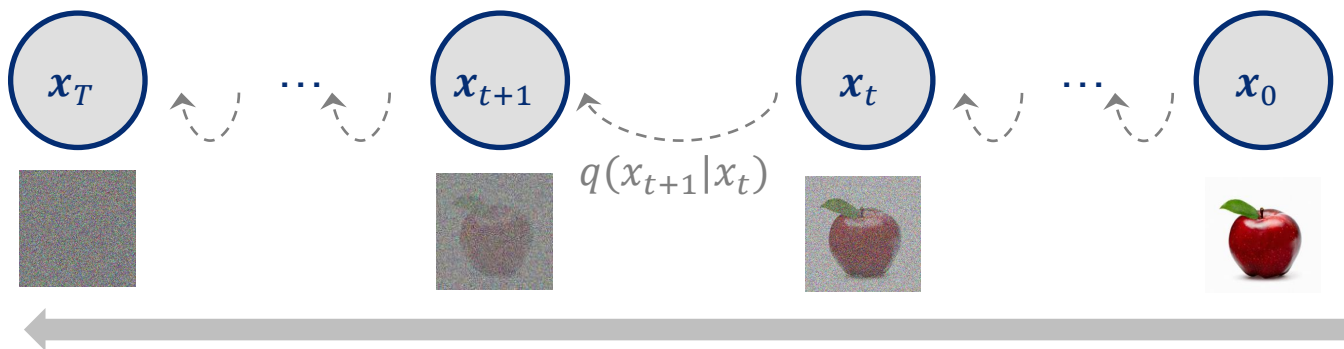
# Diffusion/Forward Process (3/3)



Q: How to sample from  $q(x_t|x_{t-1}) = \mathcal{N}(x_t|\sqrt{1 - \beta_t}x_{t-1}, \beta_t I)$ ?

A:  $x_t = \sqrt{1 - \beta_t}x_{t-1} + \beta_t \cdot \epsilon_{t-1}$  where  $\epsilon_{t-1} \sim \mathcal{N}(0, I)$ .

# Diffusion/Forward Process (3/3)

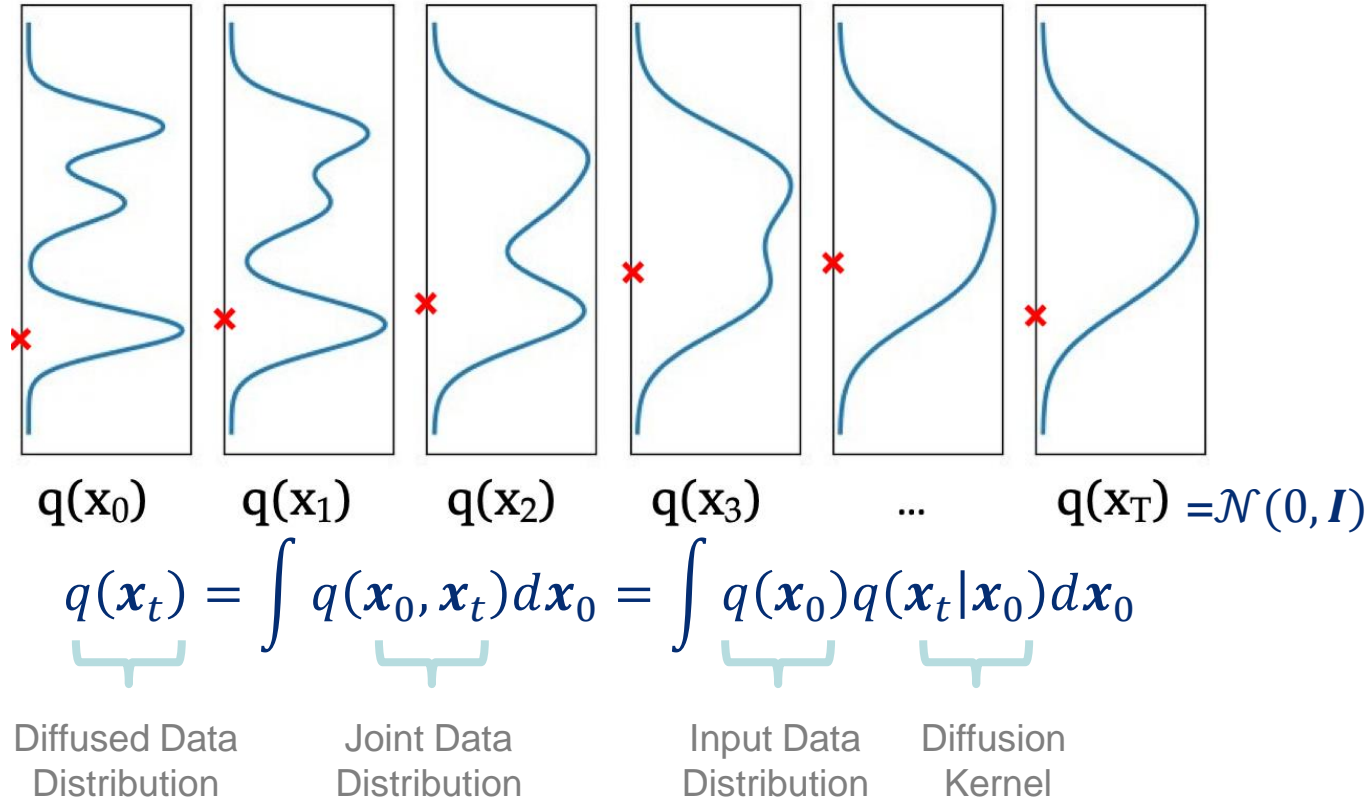


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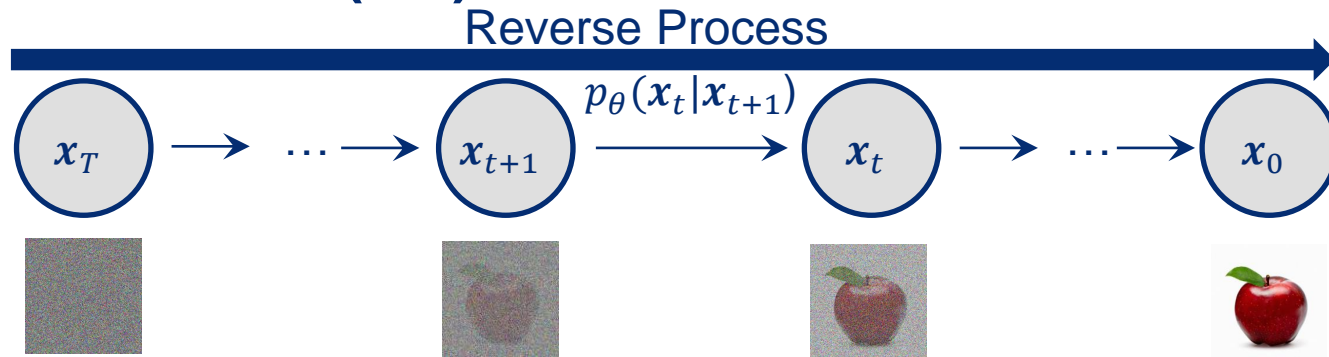
A:  $x_t = \sqrt{1 - \beta_t}x_{t-1} + \beta_t \cdot \epsilon_{t-1}$  where  $\epsilon_{t-1} \sim \mathcal{N}(0, I)$ .

Similarly,  $q(x_t|x_0) = \mathcal{N}(x_t|\sqrt{\bar{\alpha}_t}x_0, (1 - \bar{\alpha}_t)I)$  yields  $x_t = \sqrt{\bar{\alpha}_t}x_0 + (1 - \bar{\alpha}_t) \cdot \epsilon$ , where  $\epsilon \sim \mathcal{N}(0, I)$ .

# What Happen in the Diffusion/Forward Process?

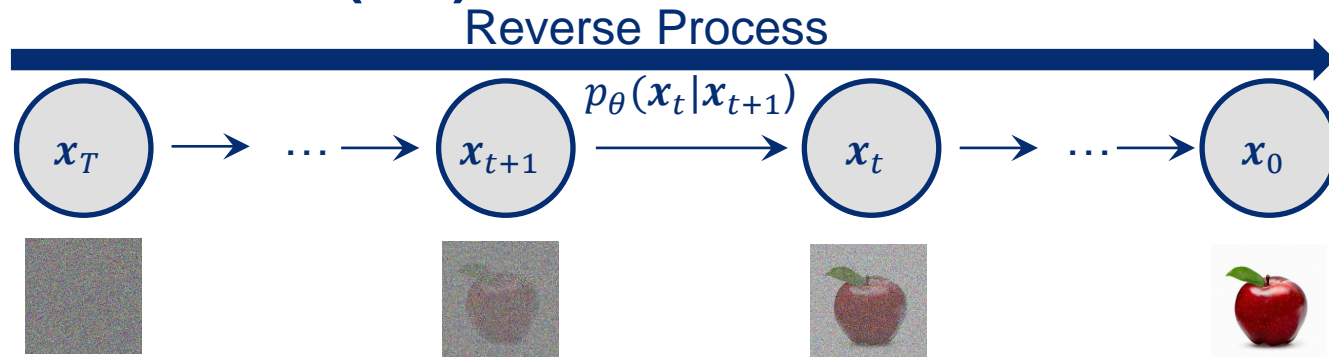


# Reverse Process (1/2)



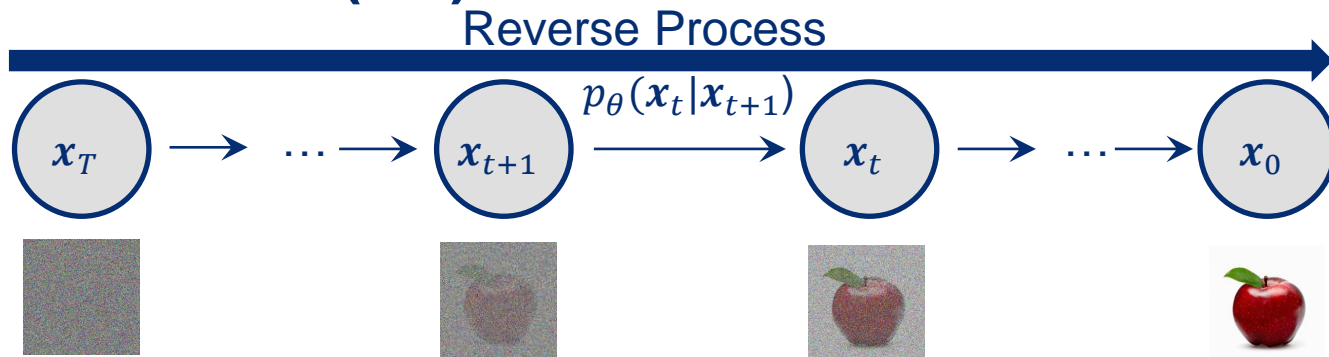
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# Reverse Process (1/2)



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- Formally, we term the joint distribution  $p_\theta(x_{0:T})$  as the **reverse process**.

# Reverse Process (1/2)

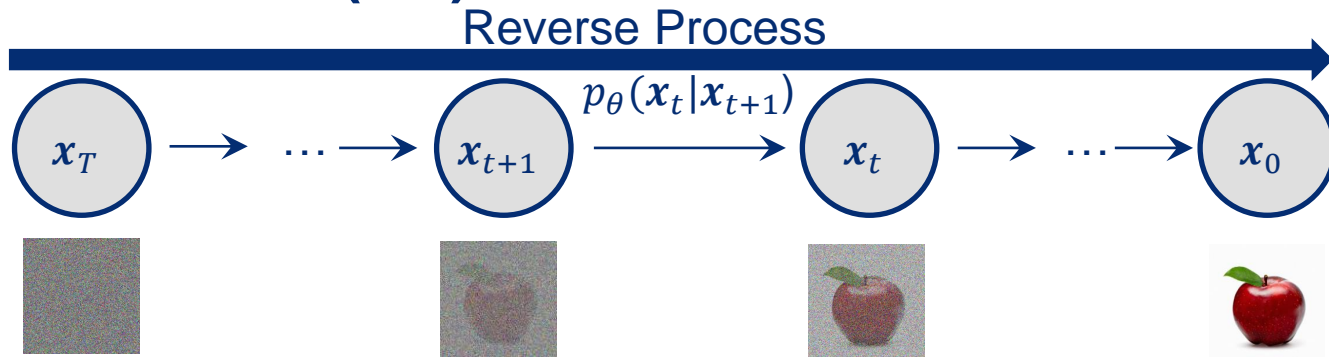


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- Formally, we term the joint distribution  $p_\theta(x_{0:T})$  as the **reverse process**.
- In DDPM,  $p_\theta(x_{0:T})$  is also a Markov chain, i.e.

$$p_\theta(x_{0:T}) = p_\theta(x_T) \prod_{t=1}^T p_\theta(x_{t-1} | x_t).$$



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- Each factor  $p_\theta(x_{t-1} | x_t)$  learns to approximate unknown  $q(x_{t-1} | x_t)$  by:

$$p_\theta(x_{t-1} | x_t) = \mathcal{N}(x_{t-1} | \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$$

$\mu_\theta$  is learnable mapping (e.g., U-Net).

$\Sigma_\theta$  can be learnable, but simply set to  $\sigma_t I$



## Reverse Process (2/2)

- However,  $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$  is not identifiable
- $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$  is identifiable, using the Bayesian Rule:

$$\begin{aligned} q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) &= q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0) \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} \\ &\propto \exp \left( -\frac{1}{2} \left( \frac{(\mathbf{x}_t - \sqrt{\alpha_t} \mathbf{x}_{t-1})^2}{\beta_t} + \frac{(\mathbf{x}_{t-1} - \sqrt{\bar{\alpha}_{t-1}} \mathbf{x}_0)^2}{1 - \bar{\alpha}_{t-1}} - \frac{(\mathbf{x}_t - \sqrt{\alpha_t} \mathbf{x}_0)^2}{1 - \bar{\alpha}_t} \right) \right) \\ &= \exp \left( -\frac{1}{2} \left( \left( \frac{\alpha_t}{\beta_t} + \frac{1}{1 - \bar{\alpha}_{t-1}} \right) \mathbf{x}_{t-1}^2 - \left( \frac{2\sqrt{\alpha_t}}{\beta_t} \mathbf{x}_t + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1 - \bar{\alpha}_{t-1}} \mathbf{x}_0 \right) \mathbf{x}_{t-1} + C(\mathbf{x}_t, \mathbf{x}_0) \right) \right) \end{aligned}$$

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 \end{aligned}$$

- In brief, we have  $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}|\widetilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \widetilde{\beta}_t \mathbf{I})$  with

$$\widetilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\bar{\alpha}_{t-1}} \beta_t}{1 - \bar{\alpha}_t} \mathbf{x}_0 + \frac{\sqrt{\alpha_t} (1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \mathbf{x}_t \text{ and } \widetilde{\beta}_t = \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t} \beta_t$$

# Training Objective (1/2)

- To approximate  $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$  with  $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ , we define the loss to be the KL-divergence between them *i.e.*,  $D_{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))$ , which can be simplified to:

$$\mathbb{E}_{\mathbf{x}_t \sim q} \left[ \frac{1}{2\sigma_t^2} \|\widetilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \boldsymbol{\varepsilon}) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, t)\|^2 \right]$$

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- It means that  $\boldsymbol{\mu}_\theta(\mathbf{x}_t, t)$  tries to predict  $\widetilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \boldsymbol{\varepsilon}) = \frac{1}{\sqrt{\alpha_t}} (\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\alpha_t}} \boldsymbol{\varepsilon})$ .

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- We come to the parametrization  $\boldsymbol{\mu}_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{\alpha_t}} (\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\alpha_t}} \boldsymbol{\varepsilon}_\theta(\mathbf{x}_t, t))$  where  $\boldsymbol{\varepsilon}_\theta(\mathbf{x}_t, t)$  intends to predict  $\boldsymbol{\varepsilon}$  from  $\mathbf{x}_t$ .

# Training Objective (1/2)

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- It leads the loss function to be

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

Known weights



## Training Objective (2/2)

- To simplify the formulation, we can re-weight  $L_t = \mathbb{E}_{x_0, \epsilon} \left[ \frac{\beta_t^2}{2\sigma_t^2 \alpha_t (1 - \bar{\alpha}_t)} \|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)\|^2 \right]$ , which is empirically found beneficial to the sample quality

$$\mathbb{E}_{x_0, \epsilon} \|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)\|^2$$

- where  $t$  is uniform between 1 and  $T$ .

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

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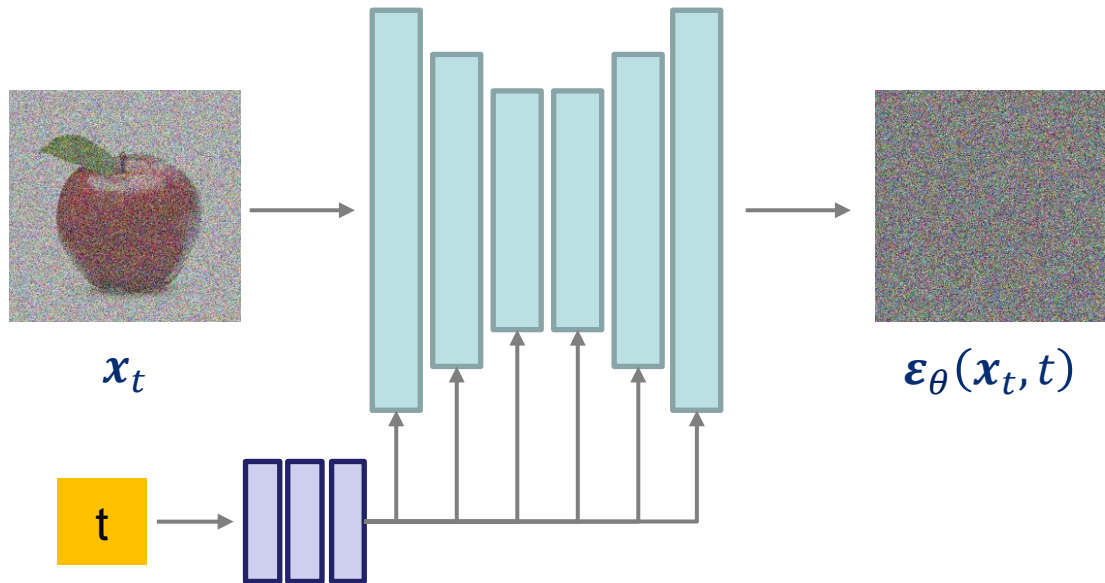
## Algorithm 1 Training

---

- 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
-

# Denoising Network $\varepsilon_{\theta}(x_t, t)$

U-Net with ResNet blocks + self-attention layers + time embedding



- Time Representation: Sinusoidal Positional Embeddings

MLP

- Time embeddings are fed to the residual blocks using either simple spatial addition or using adaptive group normalization layers

# Sampling Process

- **Goal** Generate a sample  $\widehat{x}_0$  from the Gaussian  $x_T$ .
- **Limitation** **Slow**. Take **20 hours** to sample 50k images of size  $32 \times 32$  on a NVIDIA 2080Ti (vs. a GAN takes less than **1 min**)

---

## Algorithm 2 Sampling

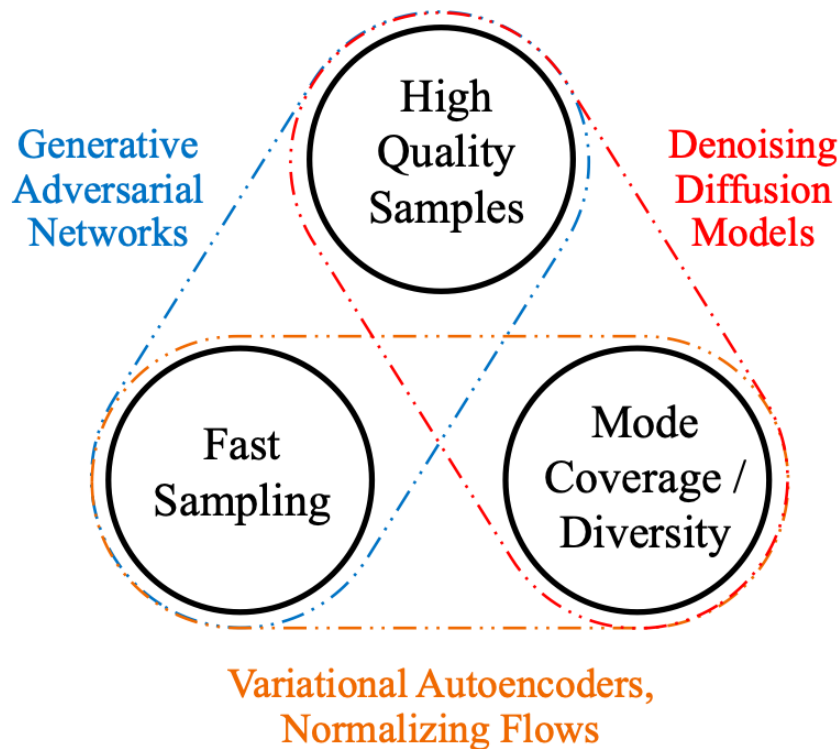
---

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



Unconditional CIFAR10 progressive generation

# Comparisons with Other Generative Model



[Tackling the Generative Learning Trilemma with Denoising Diffusion GANs](#) ICLR 2022

Intro Diffusion Models

# Conditional Diffusion Model



# Applications of Conditional Diffusion Models

## Text-to-Image Generation

“A teddy bear on a skateboard in times square”

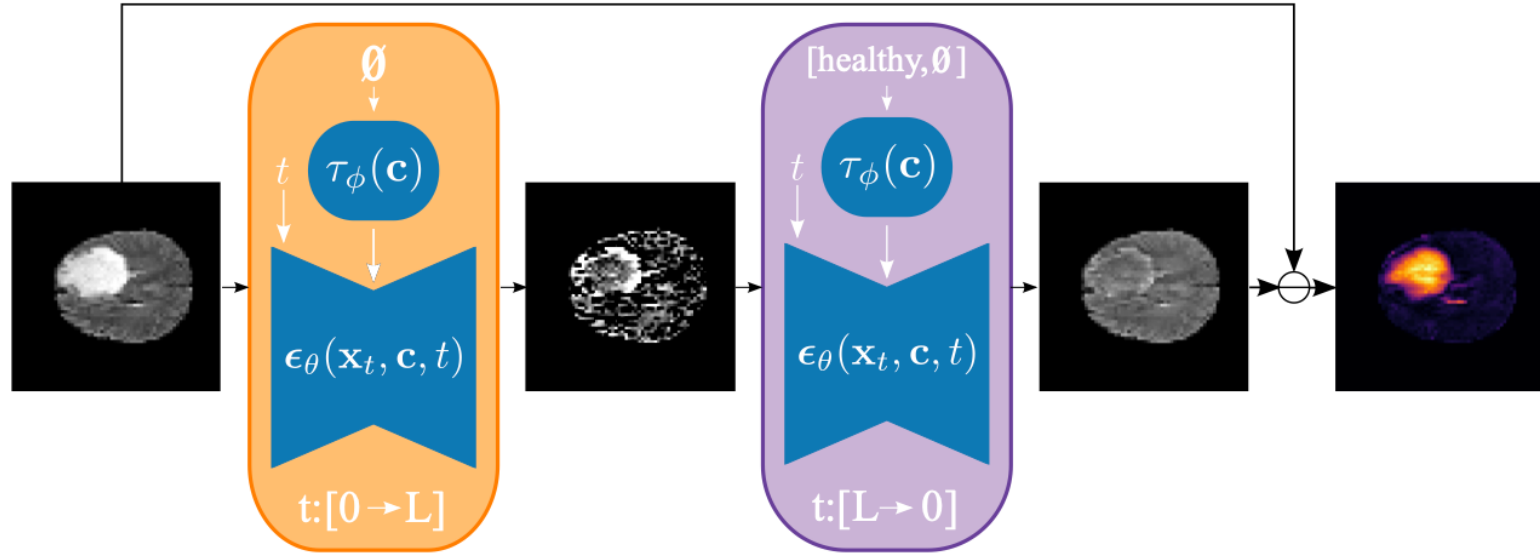


<https://openai.com/product/dall-e-2>



# Applications of Conditional Diffusion Models

## Counterfactual Generation



[What is Healthy? Generative Counterfactual Diffusion for Lesion Localization](#) MICCAI/W 2022

# Applications of Conditional Diffusion Models

## Image Inpainting

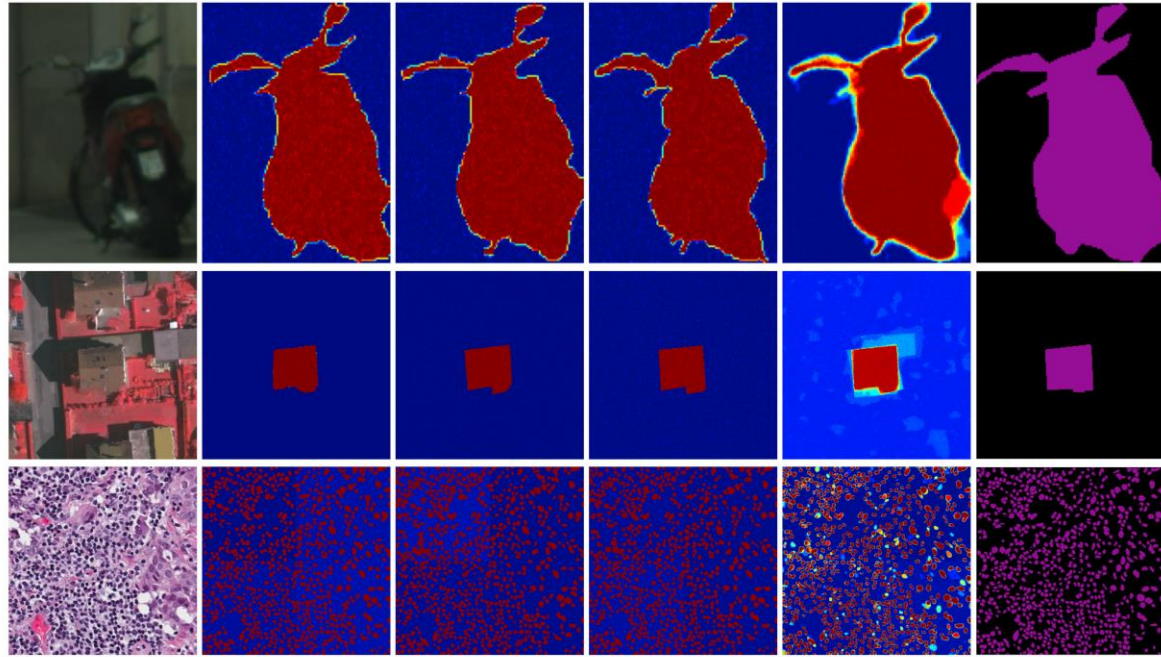


Randomness

[RePaint: Inpainting using Denoising Diffusion Probabilistic Models](#), CVPR 2022

# Applications of Conditional Diffusion Models

## Image Segmentation



Input

Multiple runs on the  
same input

Averaged Ground  
Truth

# Include Condition to Reverse Process

- Conditional Reverse Process:

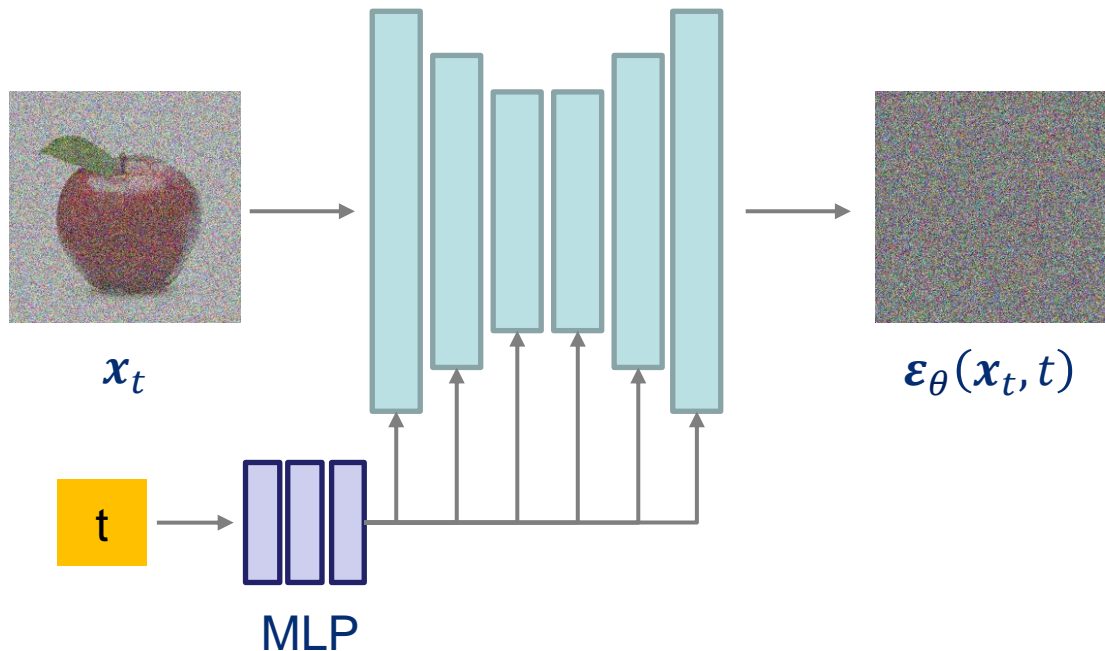
$$p_{\theta}(x_{0:T}|\mathbf{c}) = p_{\theta}(x_T) \prod_{t=1}^T p_{\theta}(x_{t-1}|x_t, \mathbf{c})$$
$$p_{\theta}(x_{t-1}|x_t, \mathbf{c}) = \mathcal{N}(x_{t-1} | \mu_{\theta}(x_t, t, \mathbf{c}), \Sigma_{\theta}(x_t, t, \mathbf{c}))$$

Impose Conditions onto the Denoising UNet

- Scalar Conditioning (Representations):** encode scalar as a vector embedding, simple spatial addition or adaptive group normalization layers.
- Image Conditioning:** channel-wise concatenation of the conditional image.
- Text Conditioning:** single vector embedding – spatial addition or adaptive group norm / a seq of vector embeddings - cross-attention.

# Conditional Denoising Network $\varepsilon_{\theta}(x_t, t, c)$

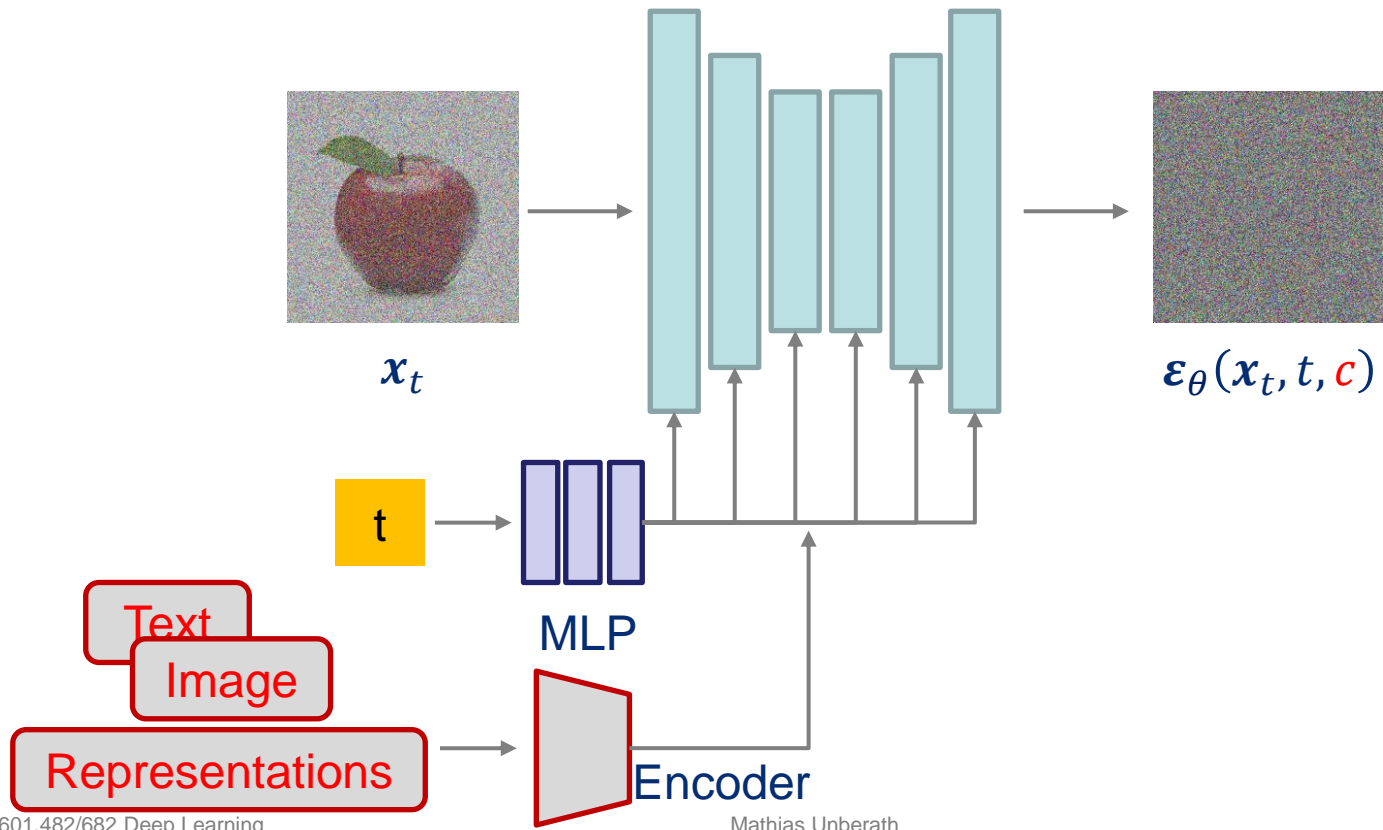
U-Net with ResNet blocks + self-attention layers + time embedding





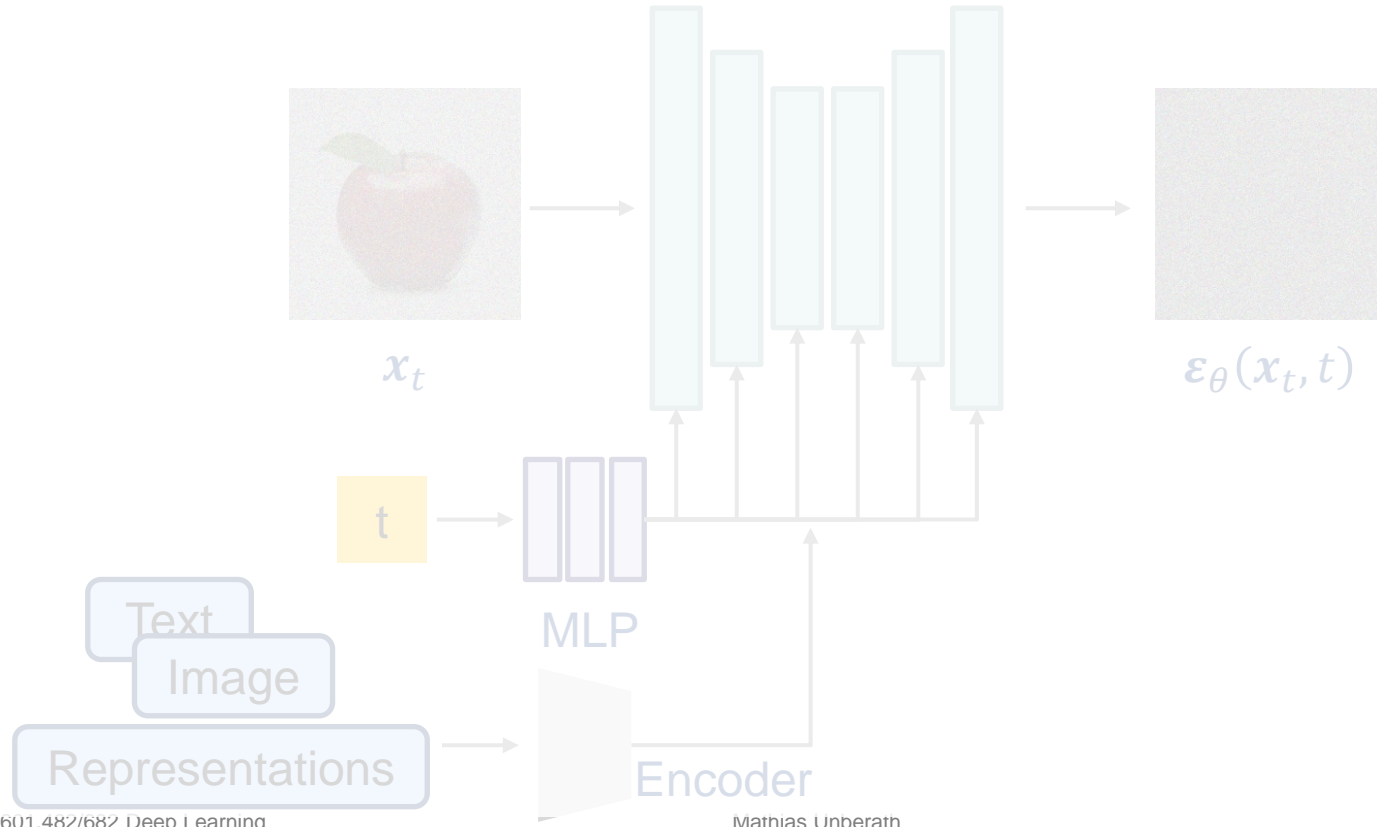
# Conditional Denoising Network $\varepsilon_{\theta}(x_t, t, c)$

U-Net with ResNet blocks + self-attention layers + time embedding



# Limitations of the Pixel-wise Denoising

U-Net with ResNet blocks + self-attention layers + time embedding

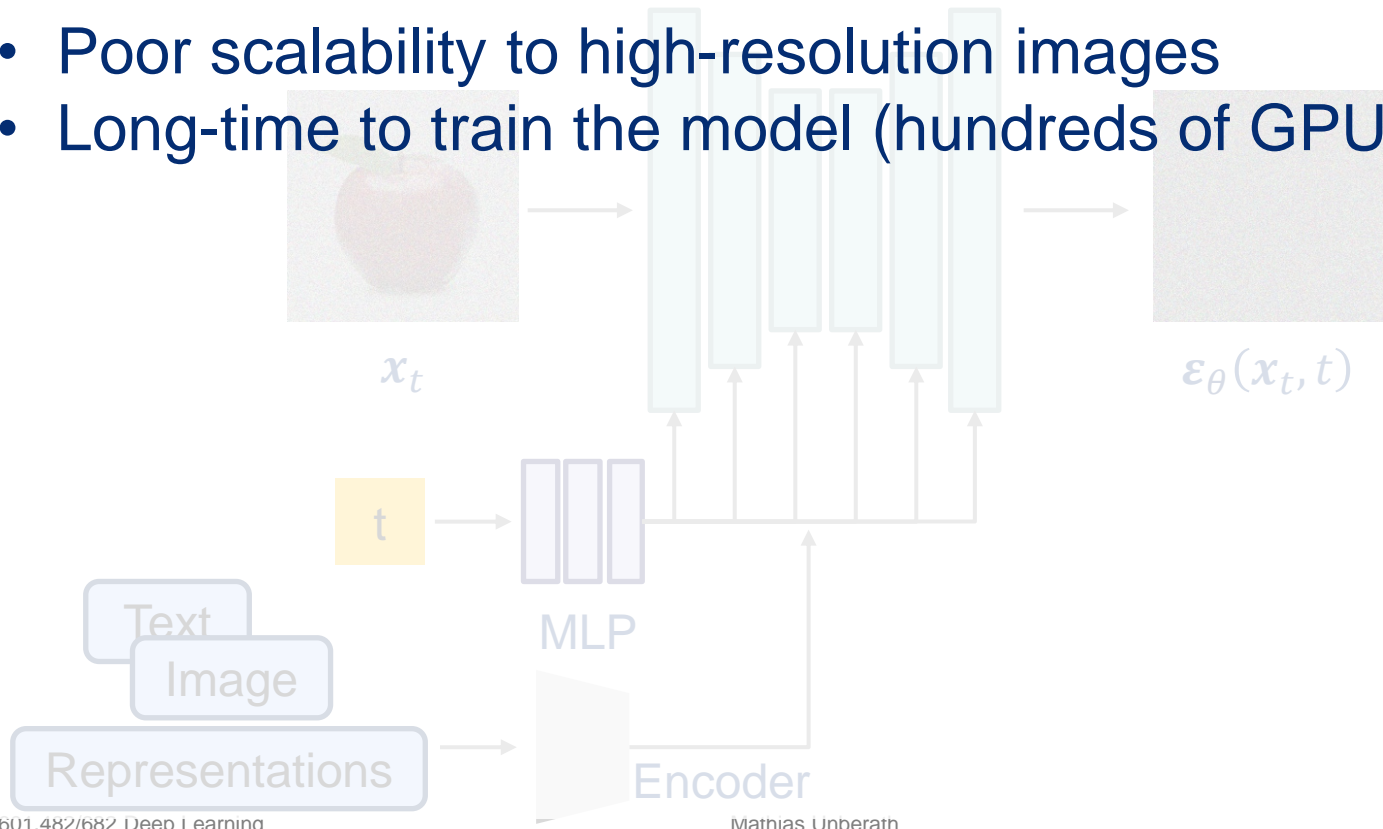




# Limitations of the Pixel-wise Denoising

U-Net with ResNet blocks + self-attention layers + time embedding

- Poor scalability to high-resolution images
- Long-time to train the model (hundreds of GPU days)

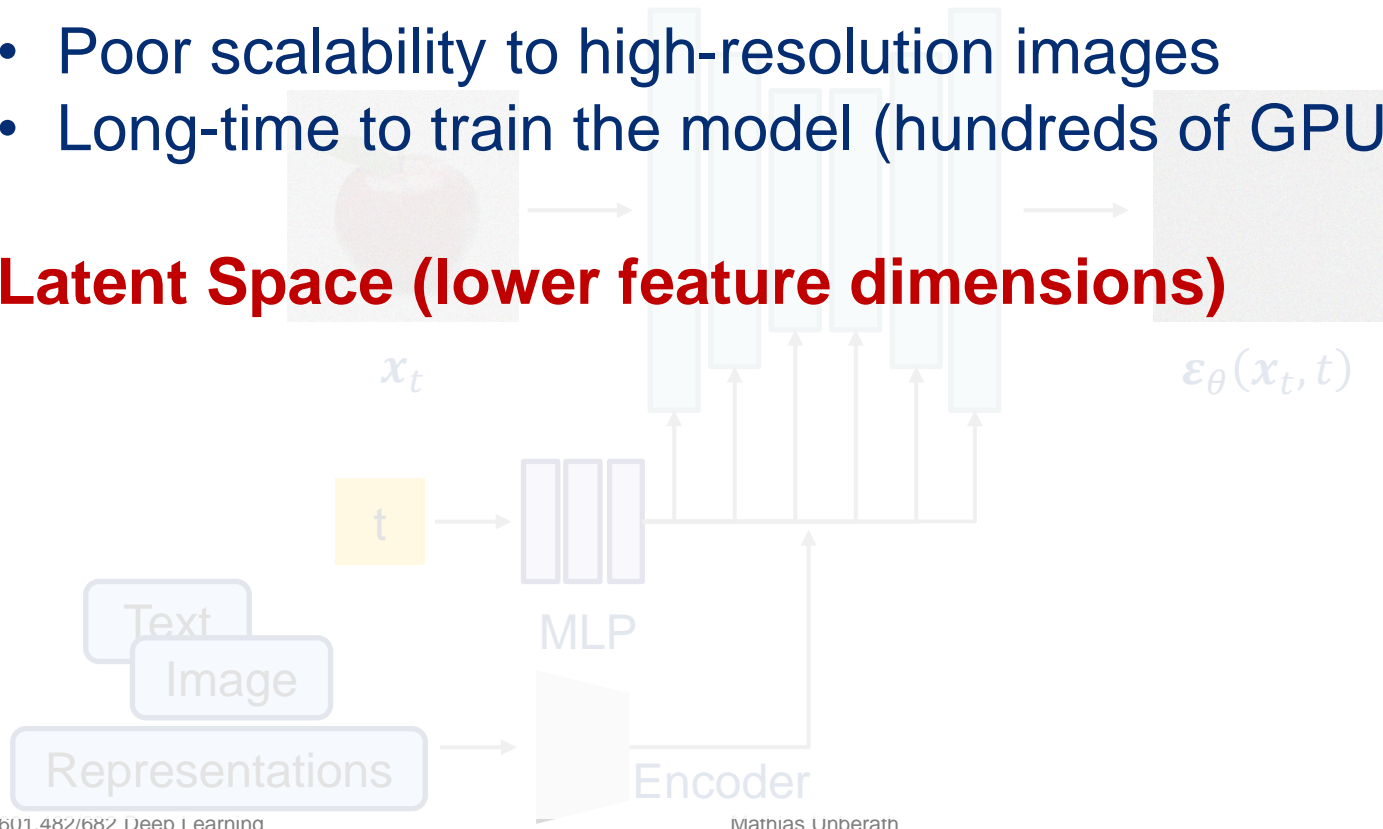


# Limitations of the Pixel-wise Denoising

U-Net with ResNet blocks + self-attention layers + time embedding

- Poor scalability to high-resolution images
- Long-time to train the model (hundreds of GPU days)

**Latent Space (lower feature dimensions)**



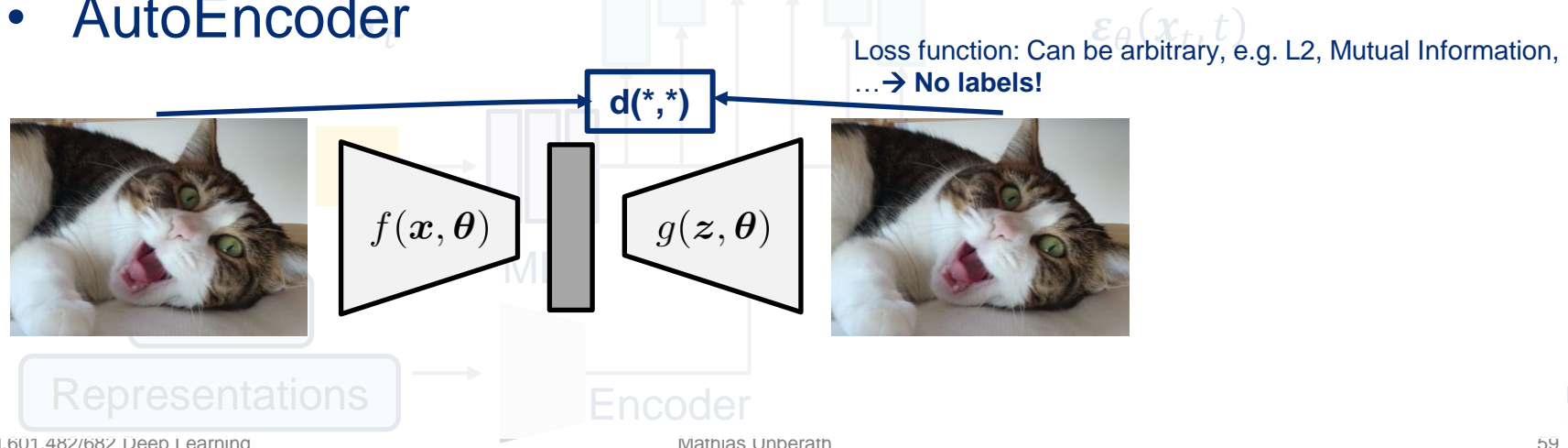
# Limitations of the Pixel-wise Denoising

U-Net with ResNet blocks + self-attention layers + time embedding

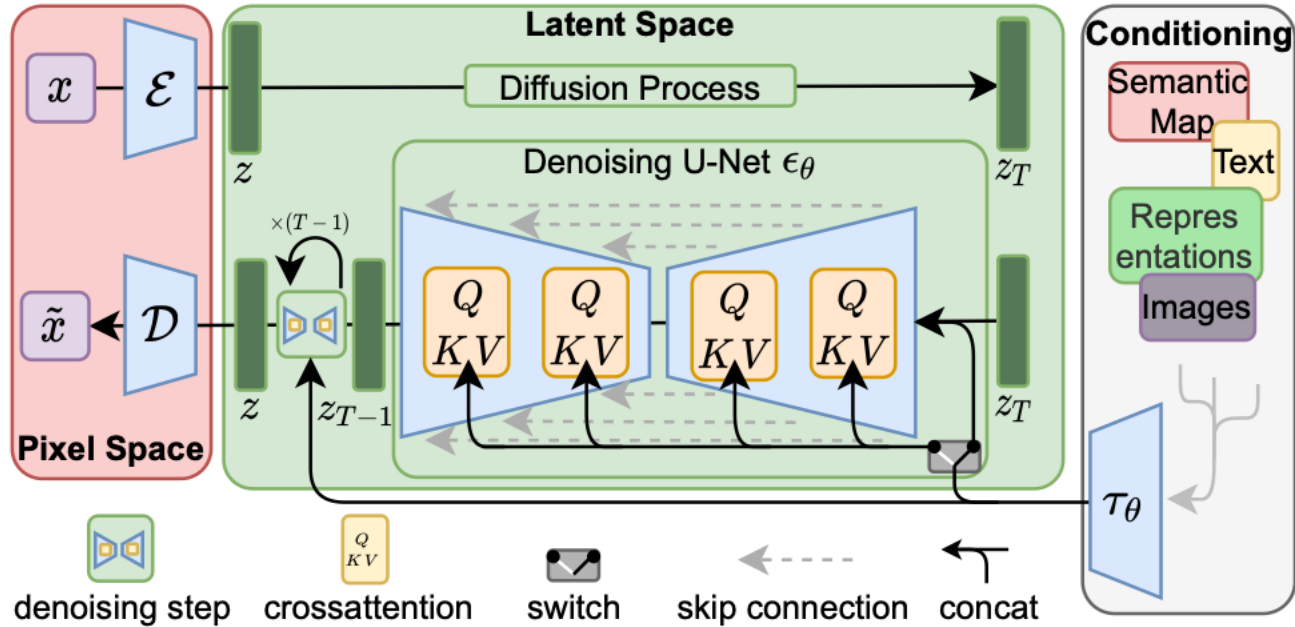
- Poor scalability to high-resolution images
- Long-time to train the model (hundreds of GPU days)

## Latent Space (lower feature dimensions)

- AutoEncoder

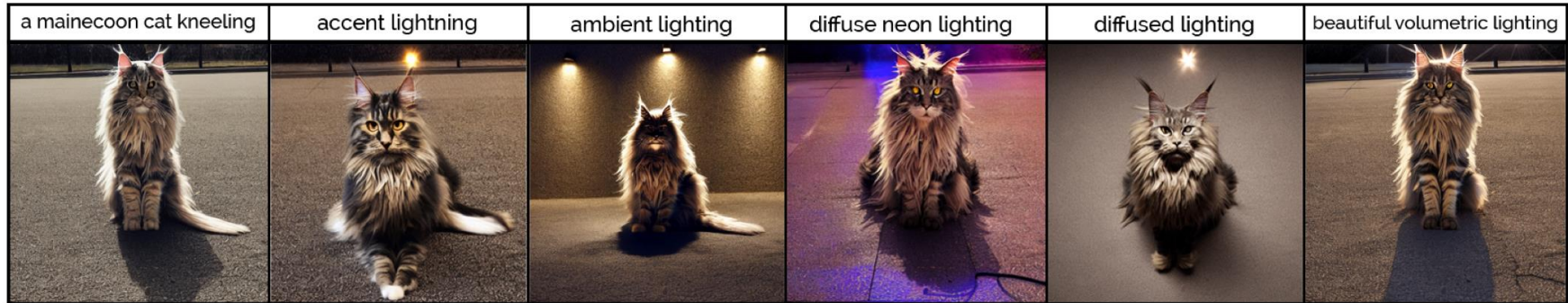


# Laten Diffusion Model



[High-Resolution Image Synthesis with Latent Diffusion Models](#) CVPR 2022

# The Power of Prompt Engineering in Diffusion Model



Adding 'Lighting' Words

<https://arxiv.org/pdf/2211.15462.pdf>

atmospheric lighting	back light	beautiful lighting	volumetric lighting
			
casting lighting	cinema lighting	dark shadows	diffuse lighting
			
diffuse neon lighting	dramatic cinematic lighting	dynamic volumetric lighting	eerie lighting
			

# Stable Diffusion Prompts

The Stable Diffusion prompts search engine.

Explore millions of AI generated images and create collections of prompts. Search generative visuals for everyone by AI artists everywhere in our 12 million prompts database.

Create better prompts. Generative visuals for everyone. By AI artists everywhere.

🔍 Search prompts...

Search

<https://stablediffusionweb.com/prompts>

Intro Diffusion Models

**Questions?**

