

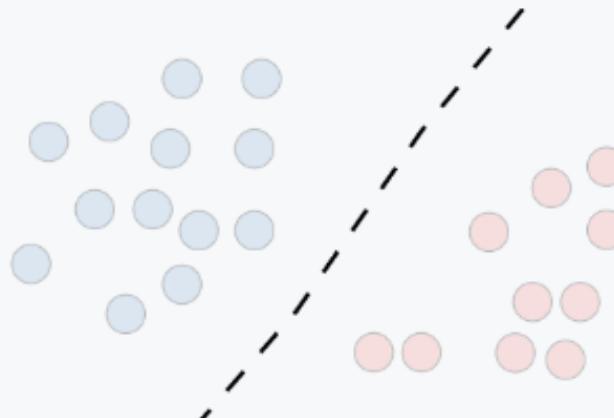
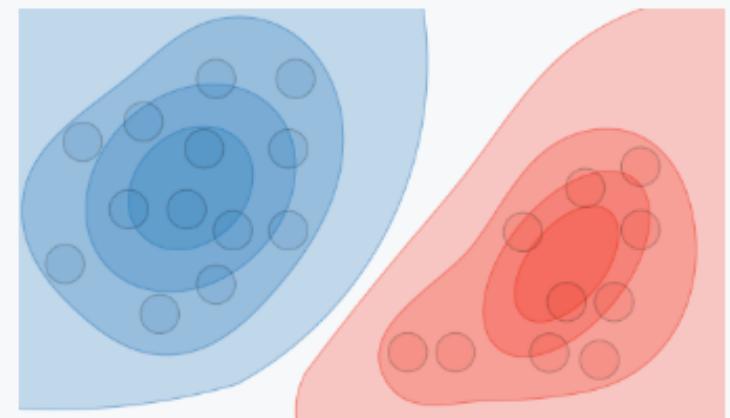
# Deep Learning Diffusion

Hao Chen

Spring 2025

# Generative vs. Discriminative

- Generative models learn the data distribution

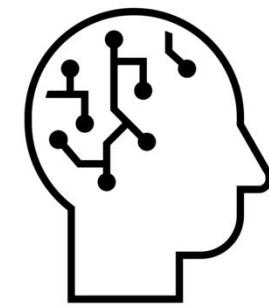
	Discriminative model	Generative model
Goal	Directly estimate $P(y x)$	Estimate $P(x y)$ to then deduce $P(y x)$
What's learned	Decision boundary	Probability distributions of the data
Illustration		

# Generative Models

- Learning to generate data



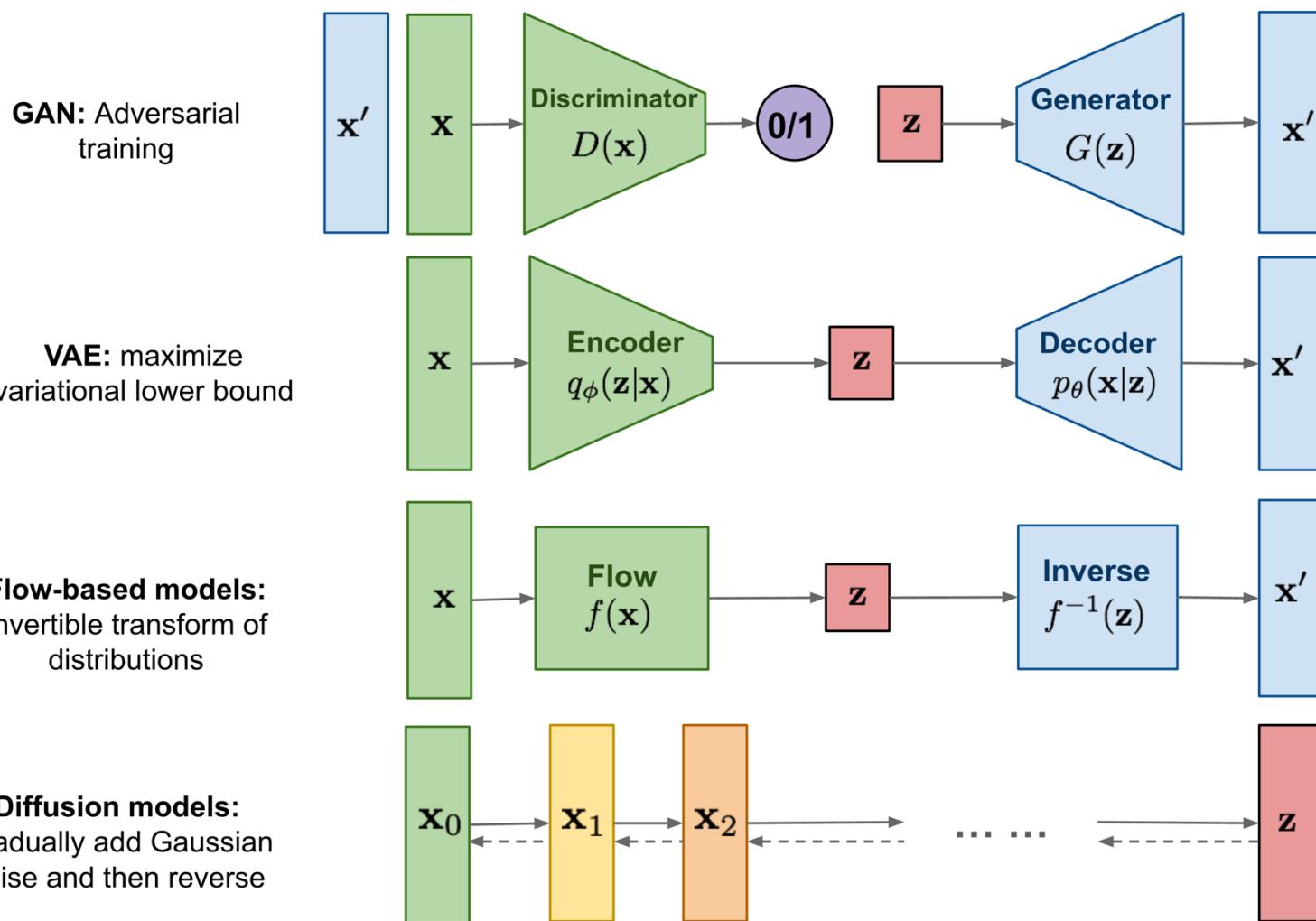
Samples from a Data Distribution



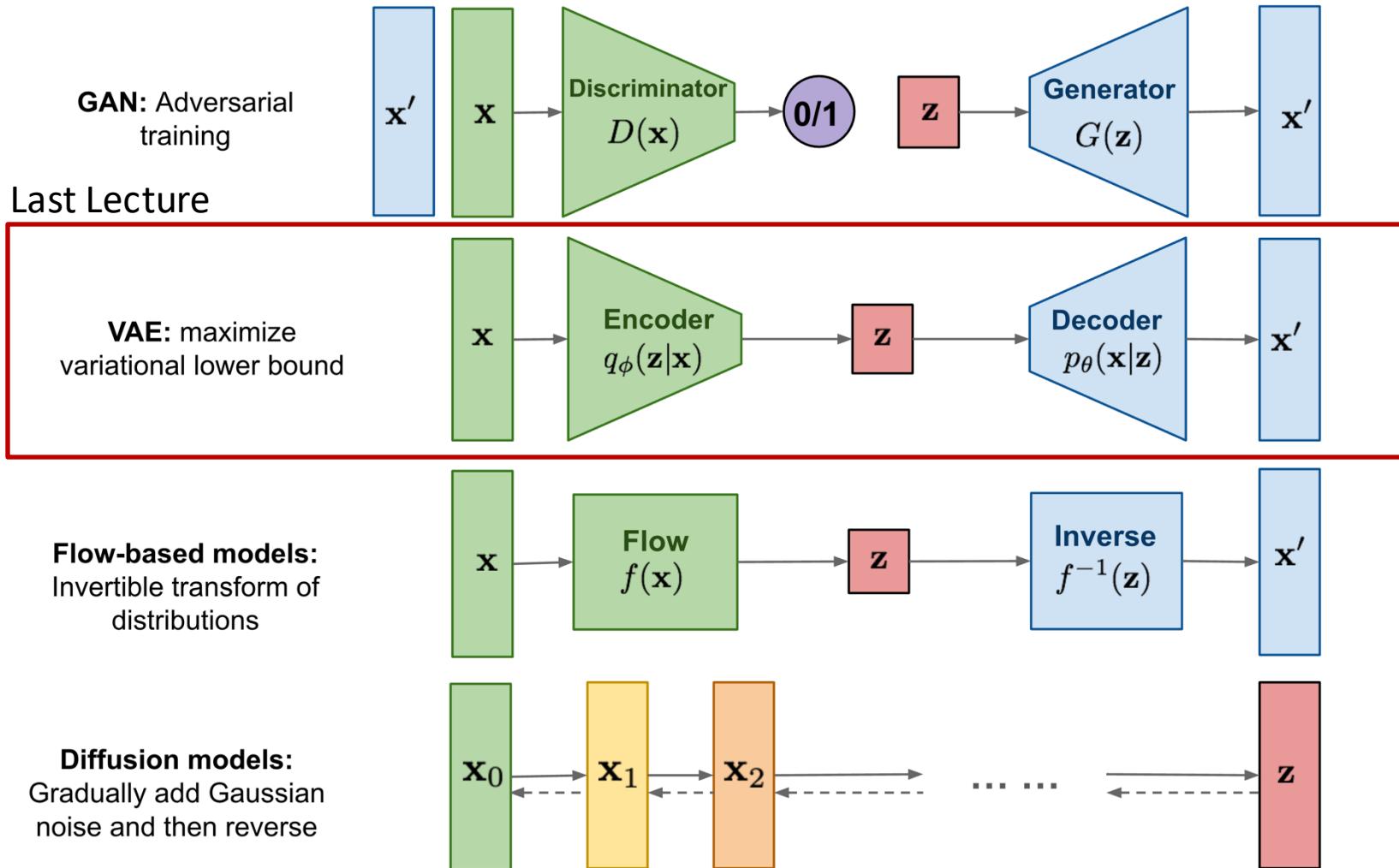
Neural Network



# Generative Models

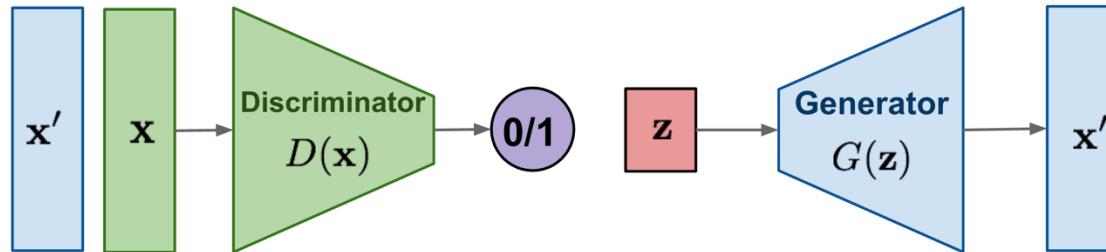


# Generative Models

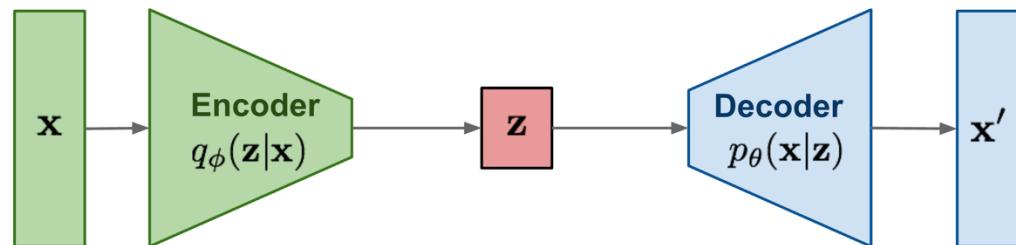


# Generative Models

**GAN:** Adversarial training

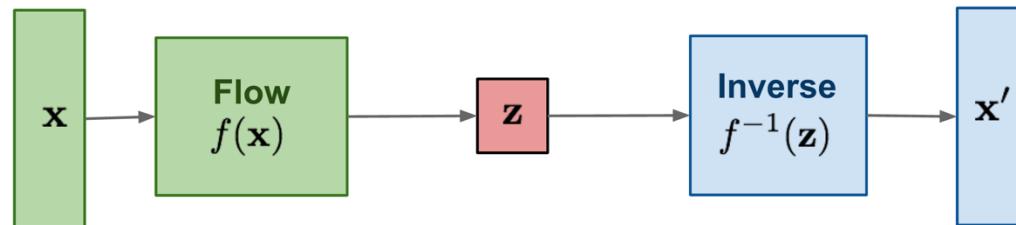


**VAE:** maximize variational lower bound

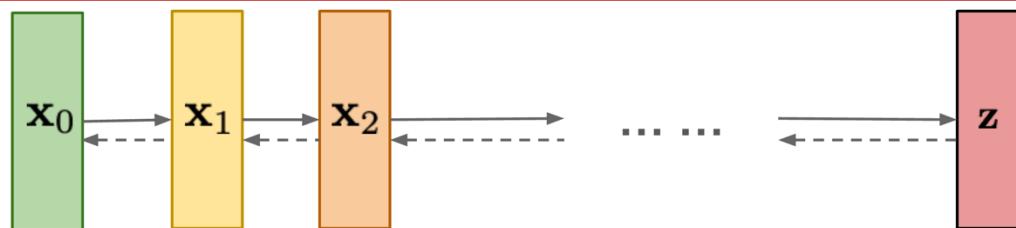


**Flow-based models:**  
Invertible transform of  
distributions

This Lecture



**Diffusion models:**  
Gradually add Gaussian  
noise and then reverse



# A Fast-Evolving Field

VAEs, 2013



GANs, 2014



PixelCNN, 2016



BigGAN, 2019



Imagen, 2022



SORA 2024



# A Fast-Evolving Field

VAEs, 2013



## Transfer between Modalities:

Suppose we directly model  
 $p(\text{text, pixels, sound})$   
with one big autoregressive transformer.

### Pros:

- image generation augmentation
- next level text rendering
- native in-context learning
- unified post-training analysis

### Cons:

- varying bit-rate of different modalities
- Compute not adaptive

## Fixes:

- = model compressed representations
- + compose autoregressive prior with a powerful decoder



Best of 8

[Read more](#)

SORA 2024



# Content

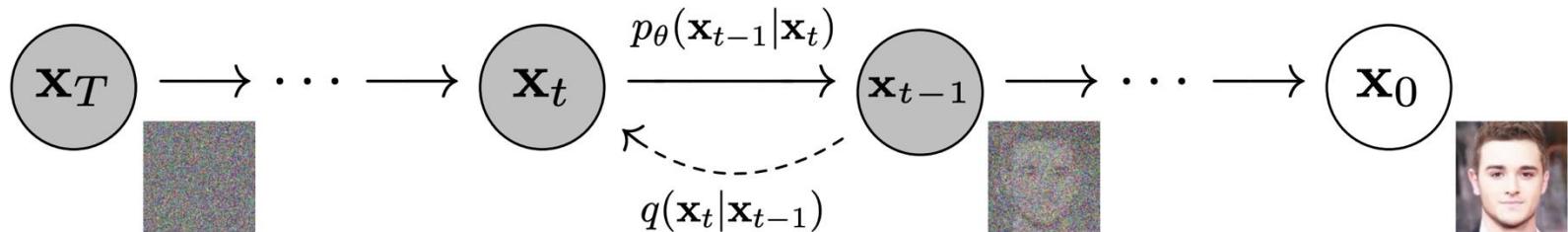
- Denoising Diffusion Model Basics
- Diffusion Models from Stochastic Differential Equations and Score Matching Perspective
- Denoising Diffusion Implicit Model (DDIM)
- Conditional Diffusion Models
- Applications of Diffusion Models

# Content

- Diffusion Model Basics
  - Diffusion Models as Stacking VAEs
  - Diffusion Models: Forward, Reverse, Training, Sampling
- Diffusion Models from Stochastic Differential Equations and Score Matching Perspective
- Denoising Diffusion Implicit Model (DDIM)
- Conditional Diffusion Models
- Applications of Diffusion Models

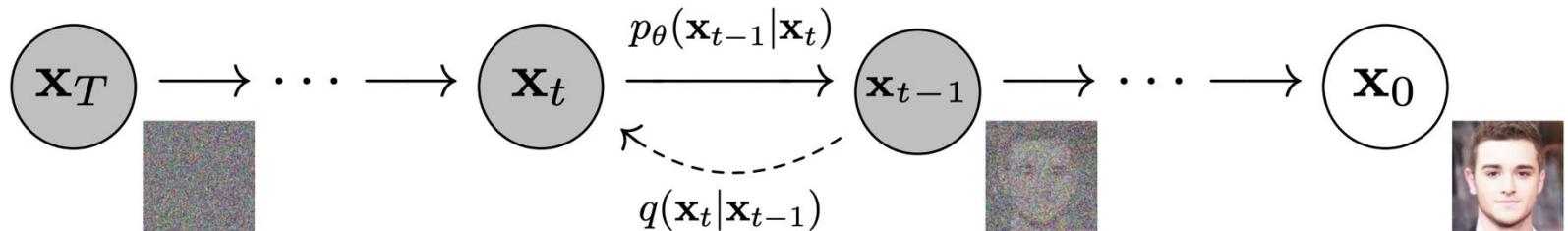
# Denoising Diffusion Models

- what we often see about diffusion models



# Denoising Diffusion Models

- what we often see about diffusion models



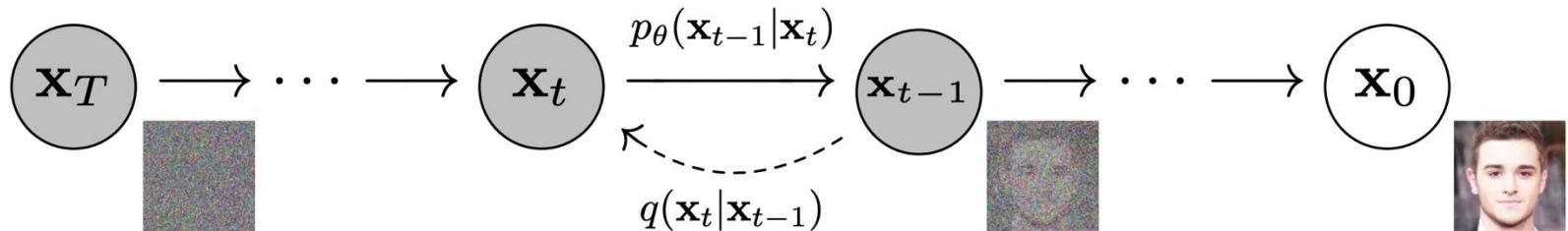
$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N} \left( \mathbf{x}_t; \sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I} \right)$$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{(1 - \bar{\alpha}_t)} \epsilon$$

Forward diffusion process

# Denoising Diffusion Models

- what we often see about diffusion models



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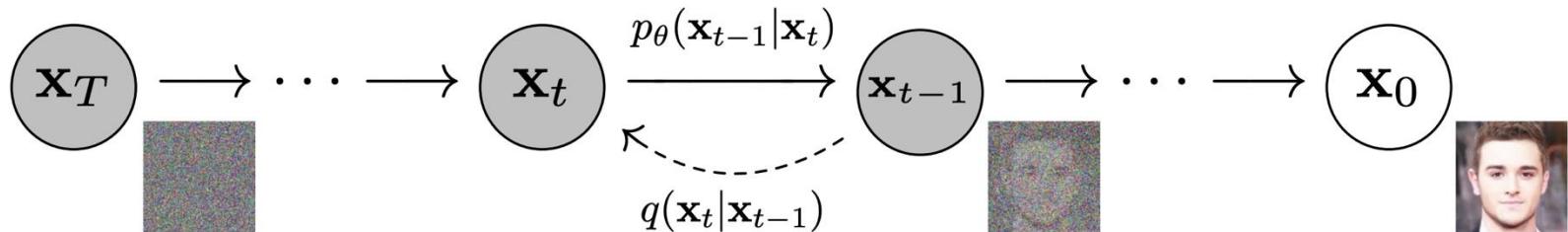
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Forward diffusion process

Reverse denoising process

# Denoising Diffusion Models

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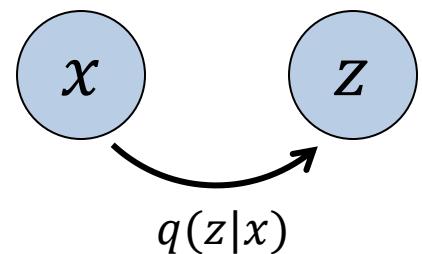
- this lecture: denoising diffusion is a stack of VAEs

# Recap: Variational Autoencoders

- VAEs: a likelihood-based generative model

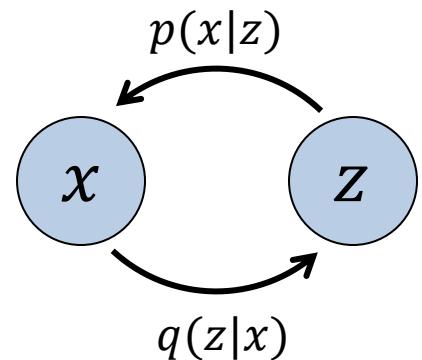
# Recap: Variational Autoencoders

- VAEs: a likelihood-based generative model
- **Encoder**: an inference model that approximates the posterior  $q(z|x)$



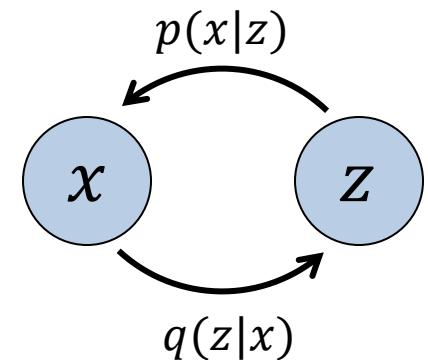
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- VAEs: a likelihood-based generative model
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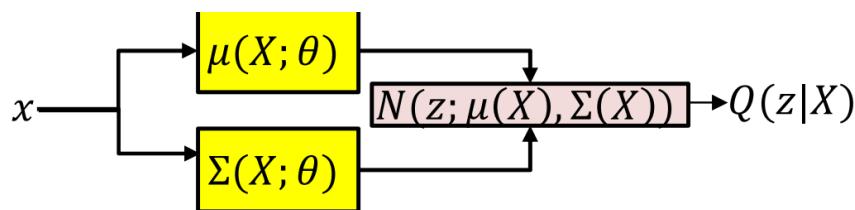
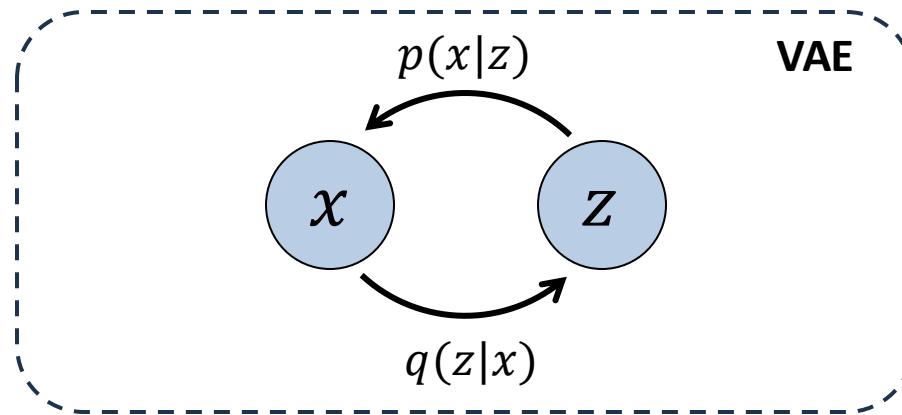
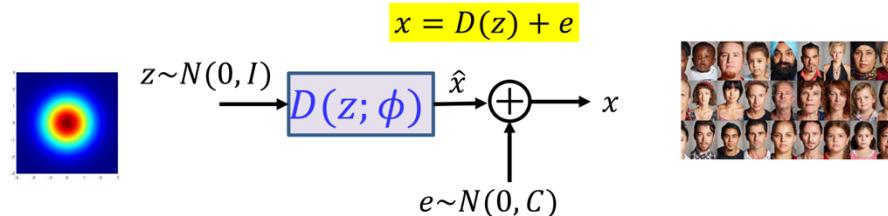
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- VAEs: a likelihood-based generative model
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- **Decoder**: a generative model that transforms a Gaussian variable  $z$  to real data
- **Training**: maximize the ELBO



# Recap: Variational Autoencoders

**Decoder:** transforms a Gaussian variable to real data



**Encoder:** an inference model approximates the posterior, i.e. Gaussian

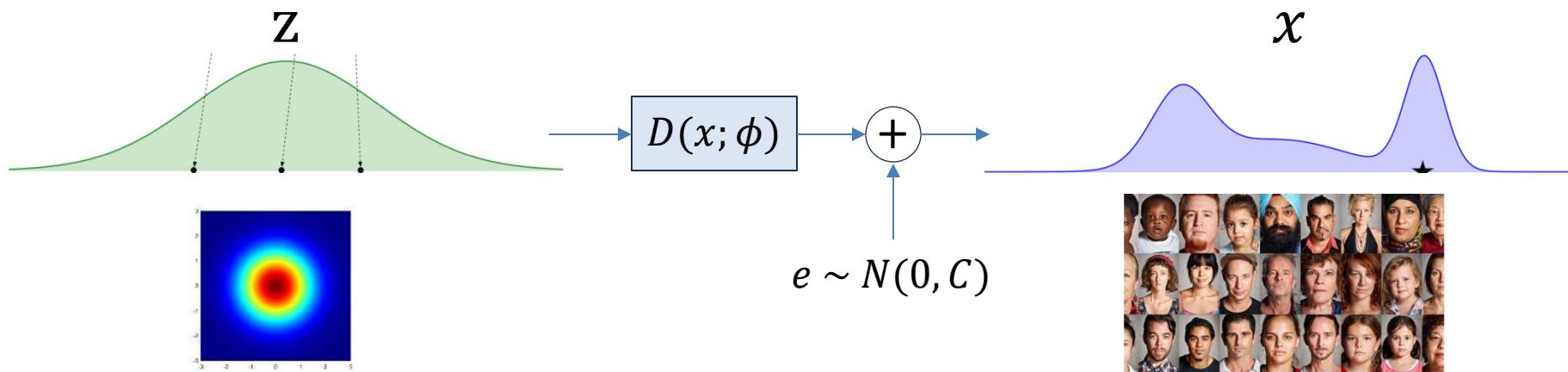
# VAEs are good, but...

- Blurry results



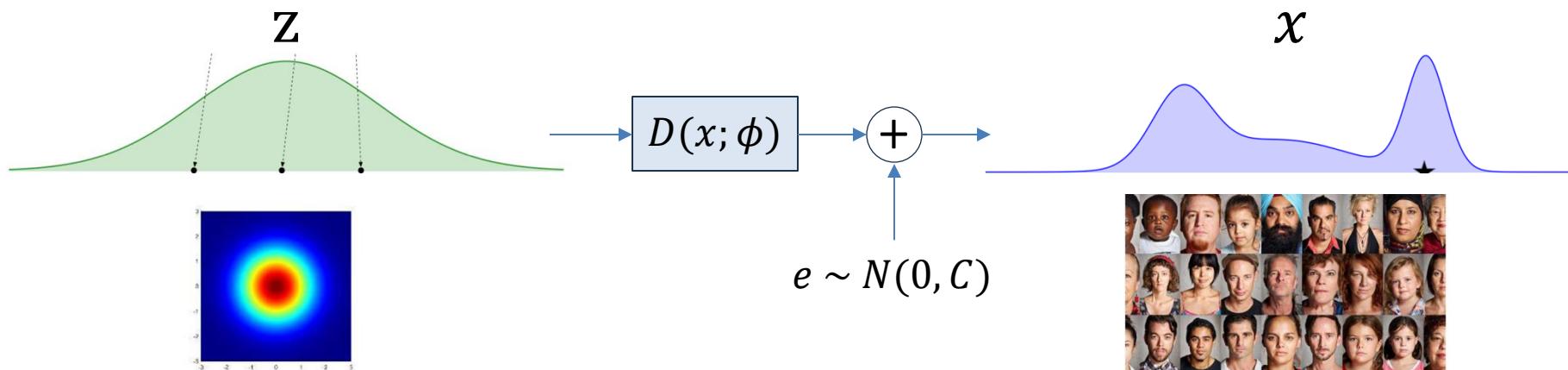
# Limitations of VAEs

- Decoder must transform a standard Gaussian all the way to the target distribution in **one-step**



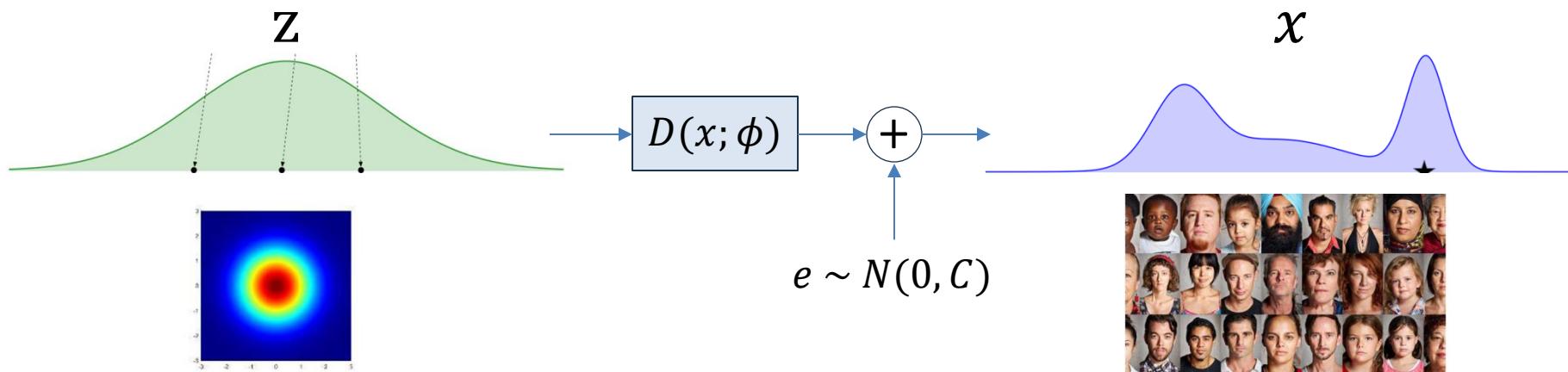
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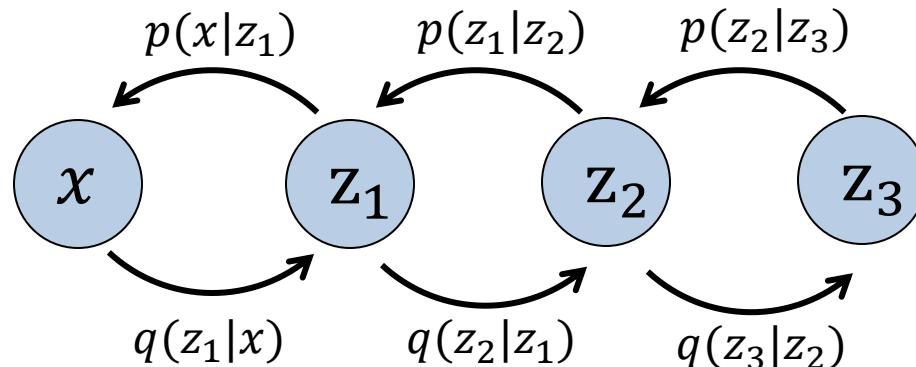
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- Solution: have some intermediate latent variables to reduce the gap of each step

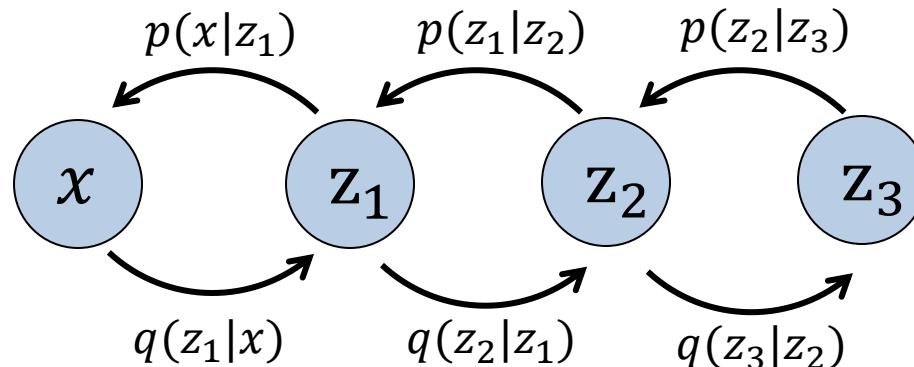
# Hierarchical VAEs

- Hierarchical VAEs – Stacking VAEs on top of each other



# Hierarchical VAEs

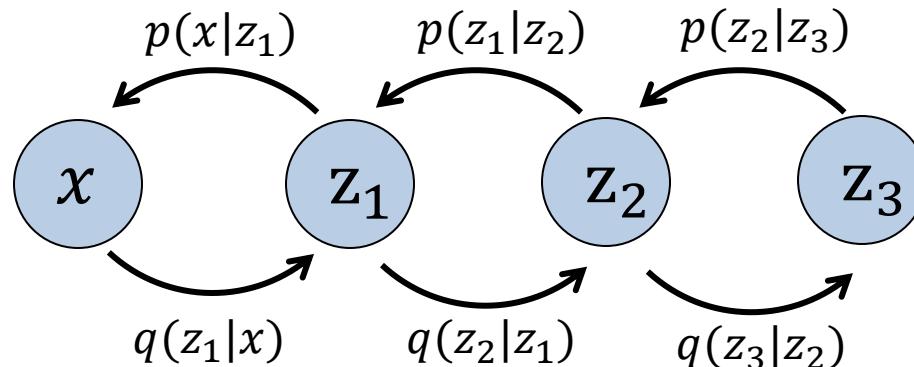
- Hierarchical VAEs – Stacking VAEs on top of each other
  - Multiple ( $T$ ) intermediate latent
  - Joint distribution  $p(\mathbf{x}, \mathbf{z}_{1:T}) = p(\mathbf{z}_T)p_{\boldsymbol{\theta}}(\mathbf{x} | \mathbf{z}_1) \prod_{t=2}^T p_{\boldsymbol{\theta}}(\mathbf{z}_{t-1} | \mathbf{z}_t)$



# Hierarchical VAEs

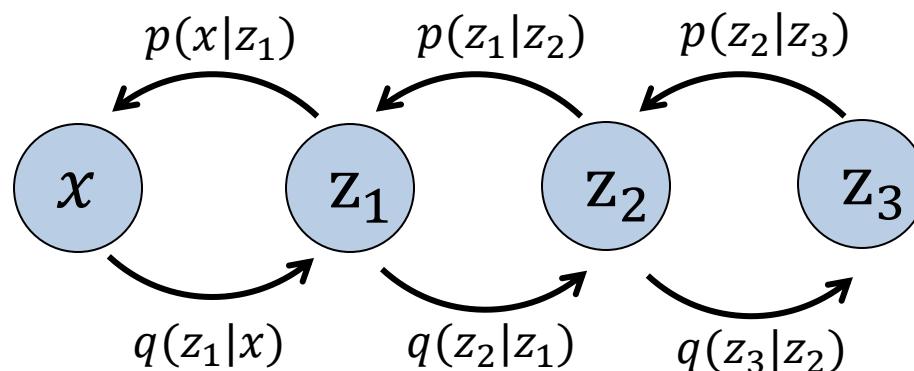
- Hierarchical VAEs – Stacking VAEs on top of each other
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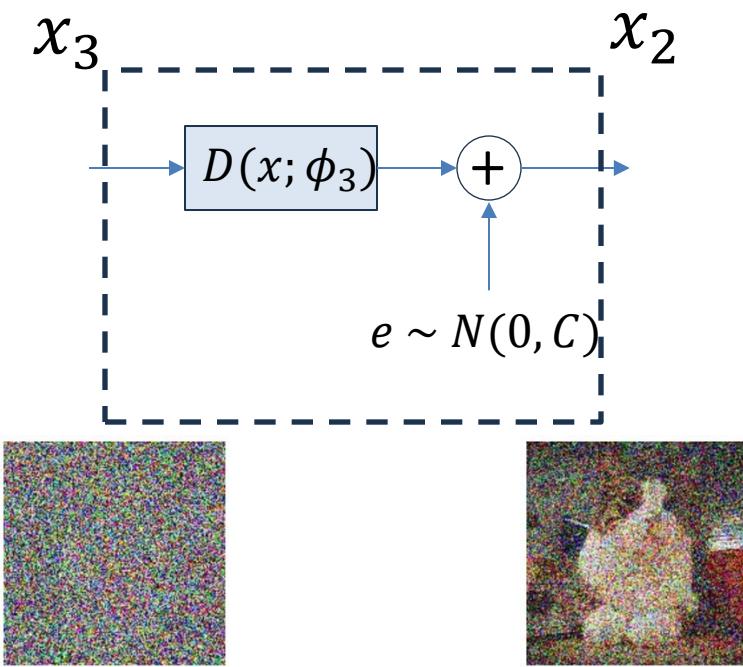
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- Better likelihood achieved!



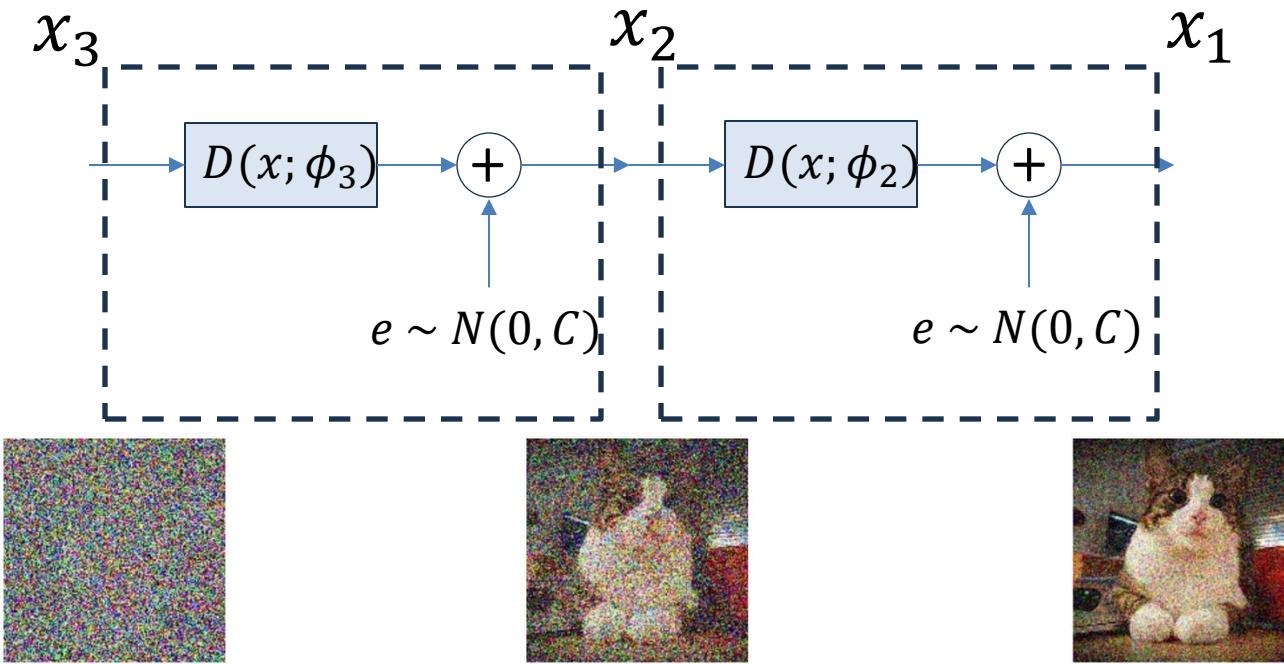
# Stacking VAEs

- Each step, the decoder removes part of the noise



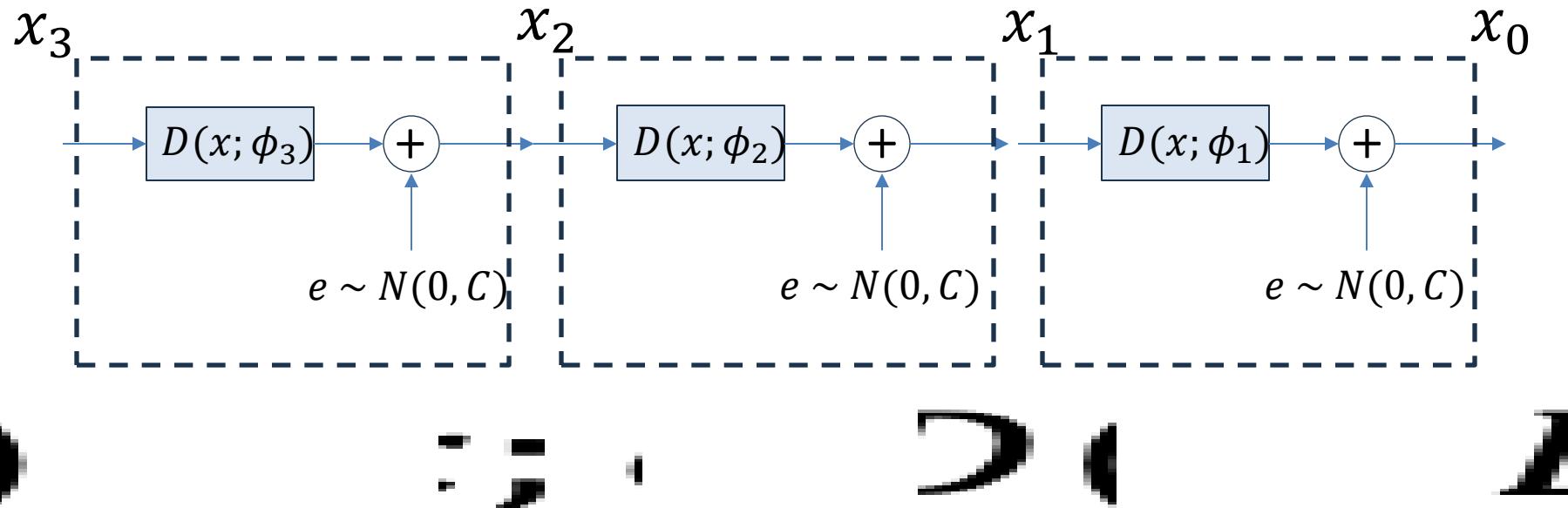
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- Provides a seed model closer to final distribution



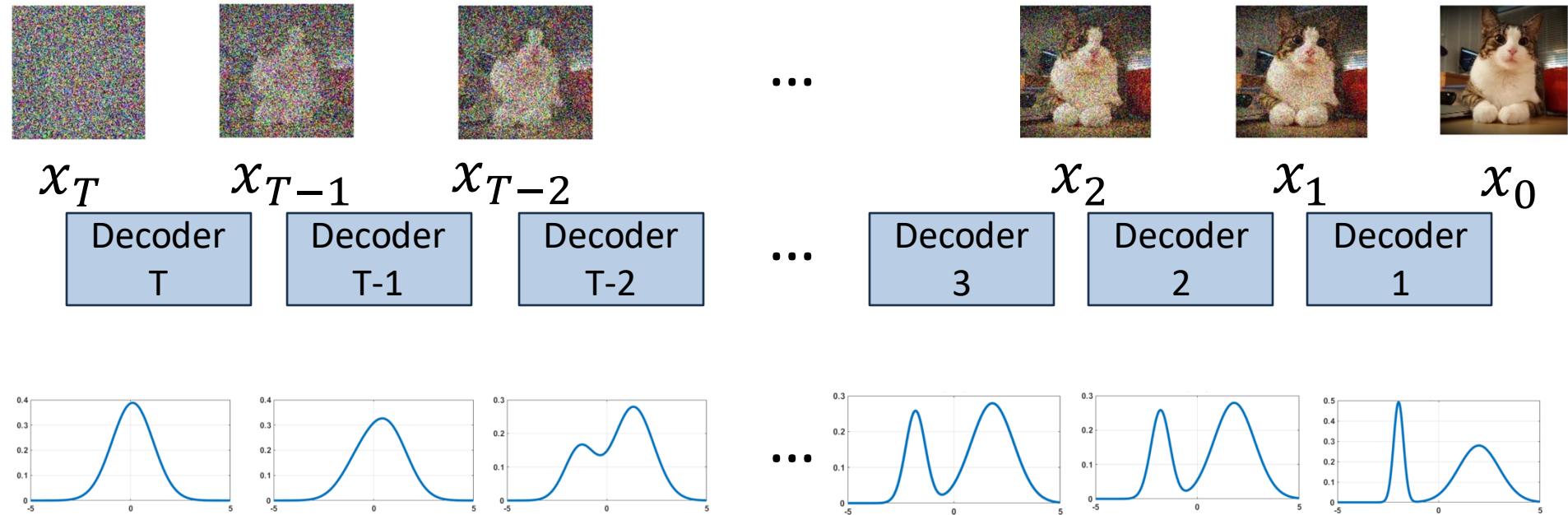
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# Stacking VAEs

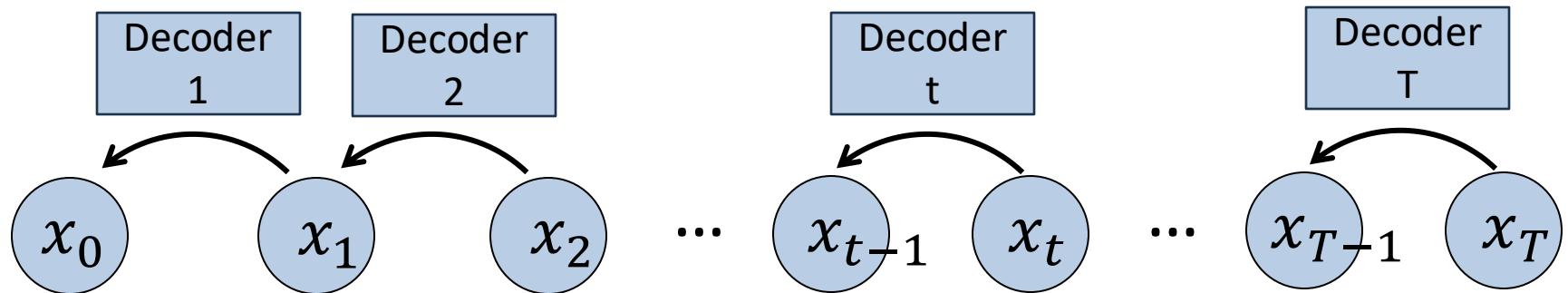
- We can have many many steps (in total T)...
- Each step incrementally recovers the final distribution



- Looks familiar?

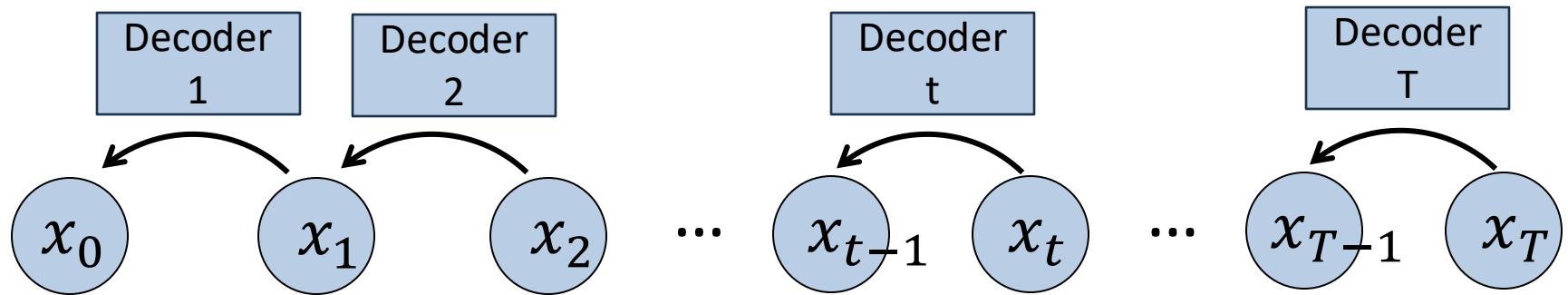
# Diffusion Models are Stacking VAEs

- Diffusion models are special cases of Stacking VAEs



# Diffusion Models are Stacking VAEs

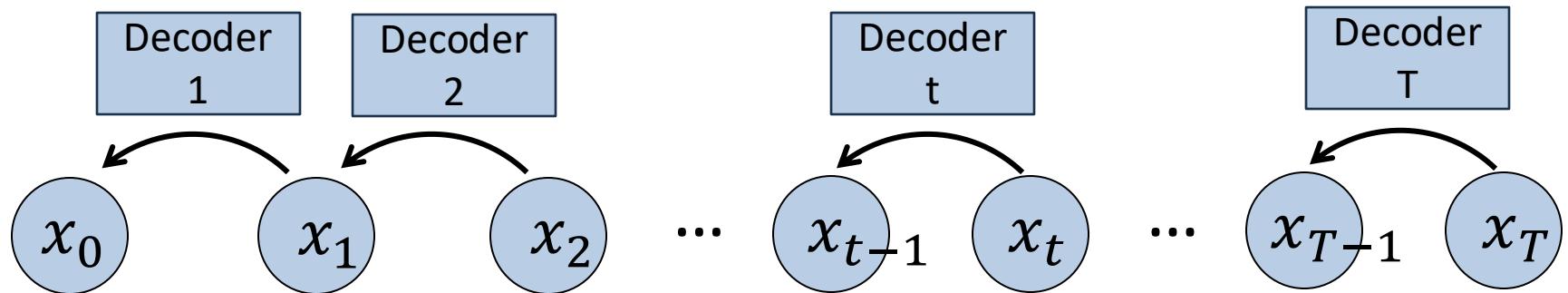
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# Diffusion Models are Stacking VAEs

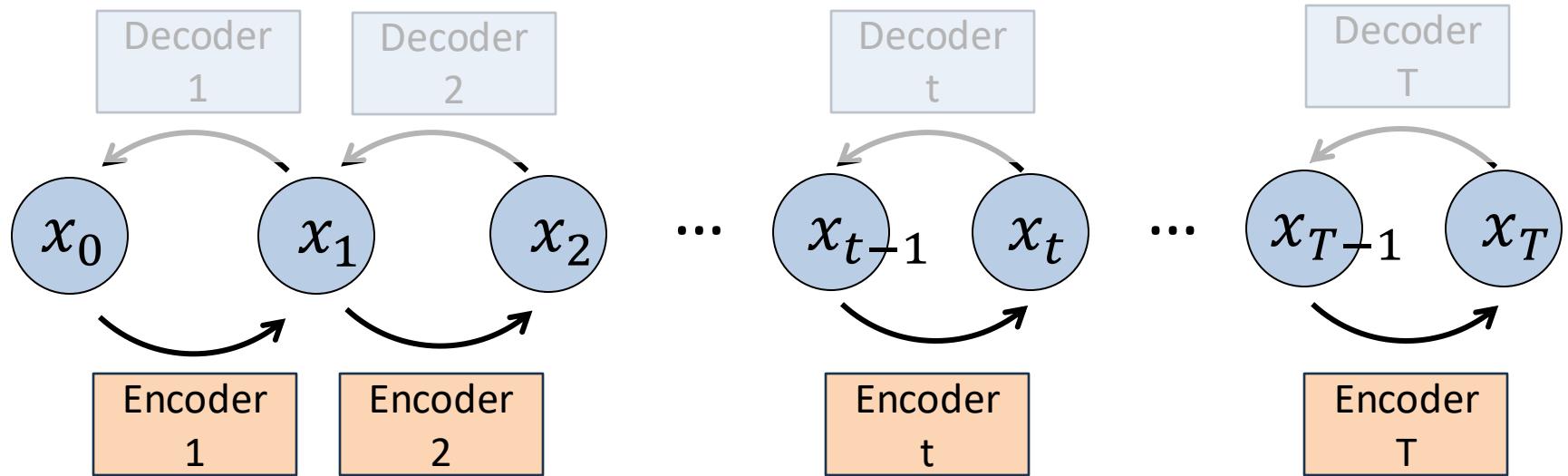
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- The reverse denoising process is the stack of decoders
- What about encoders?

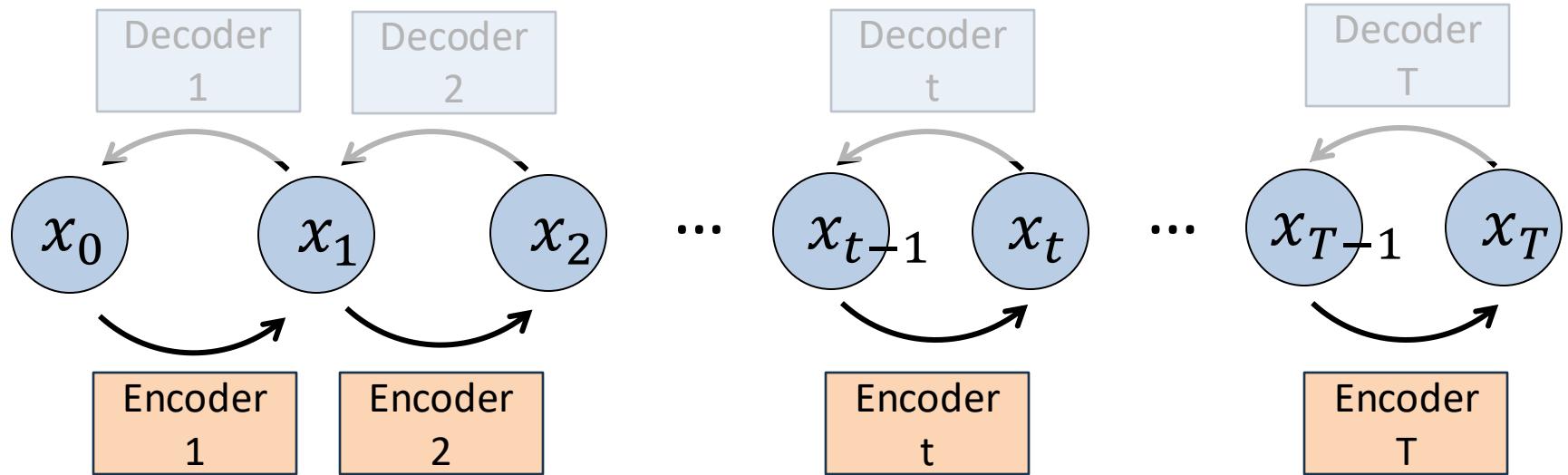
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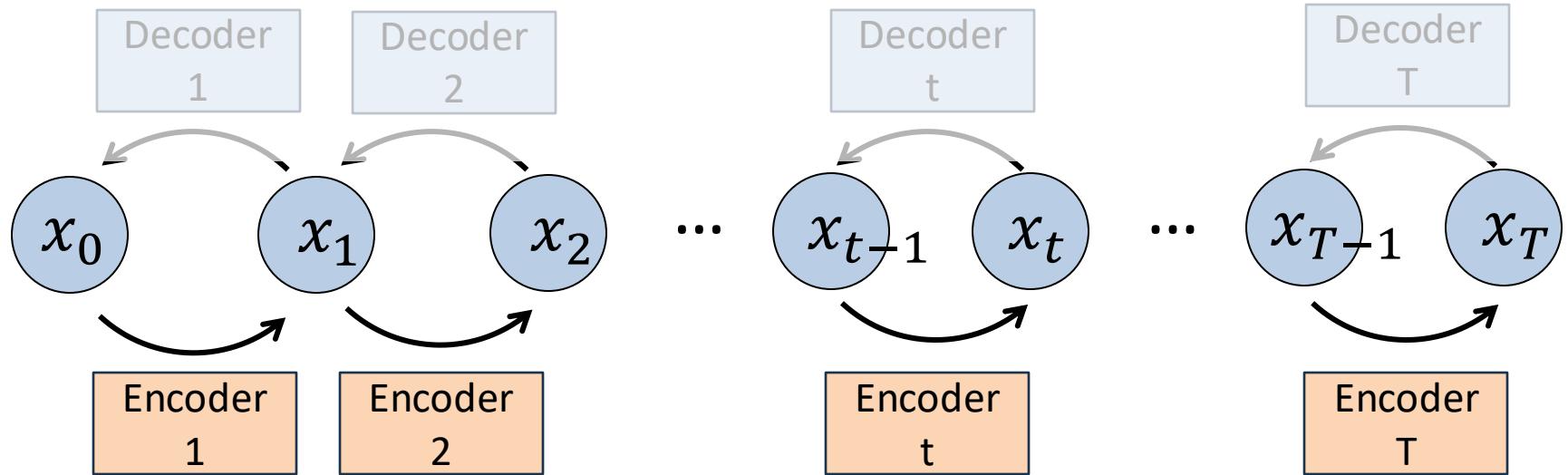
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- In VAEs, encoders are learned with KL-divergence between the posterior and the prior
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# Diffusion Models are Stacking VAEs

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- In VAEs, encoders are learned with KL-divergence between the posterior and the prior
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- Diffusion models use **fixed inference encoders**

# Poll 1

Diffusion Models' reverse process is the stack of

- VAE encoders
- VAE decoders

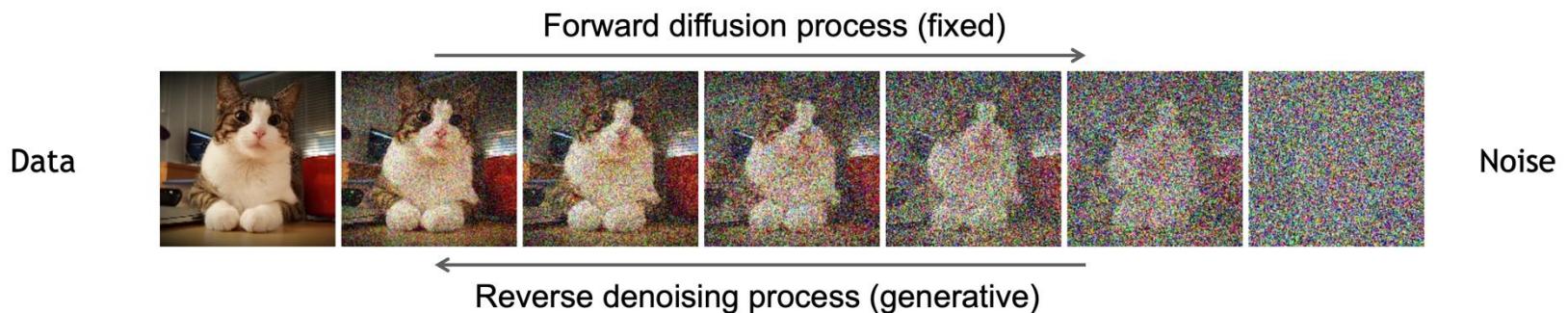
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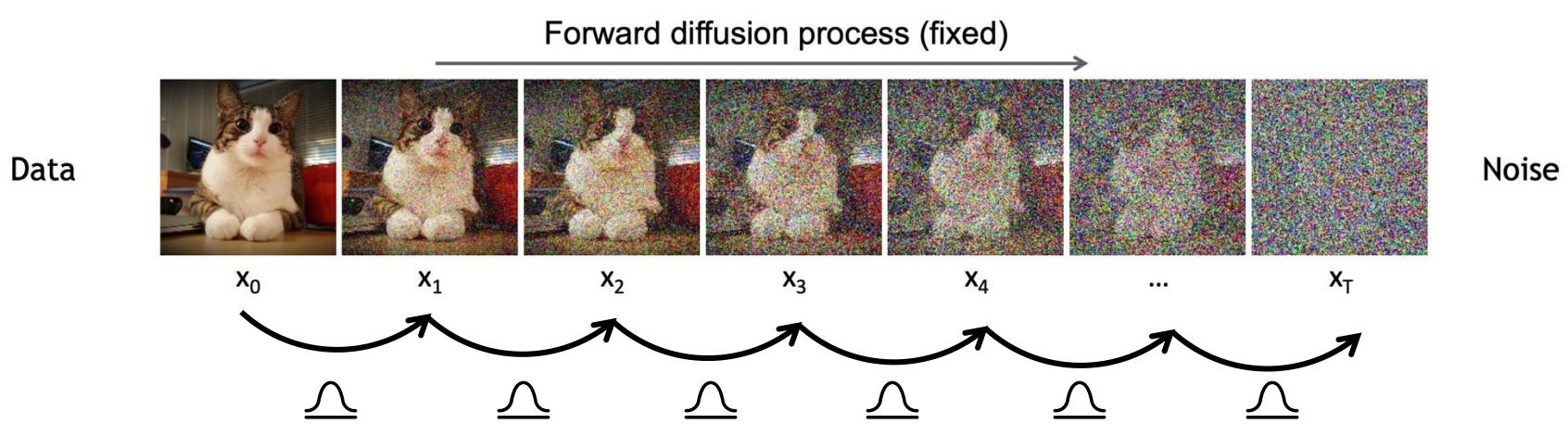
# Denoising Diffusion Models

- Diffusion models have two processes
- **Forward diffusion process** gradually adds noise to input
- **Reverse denoising process** learns to generate data by denoising



# Forward Diffusion Process

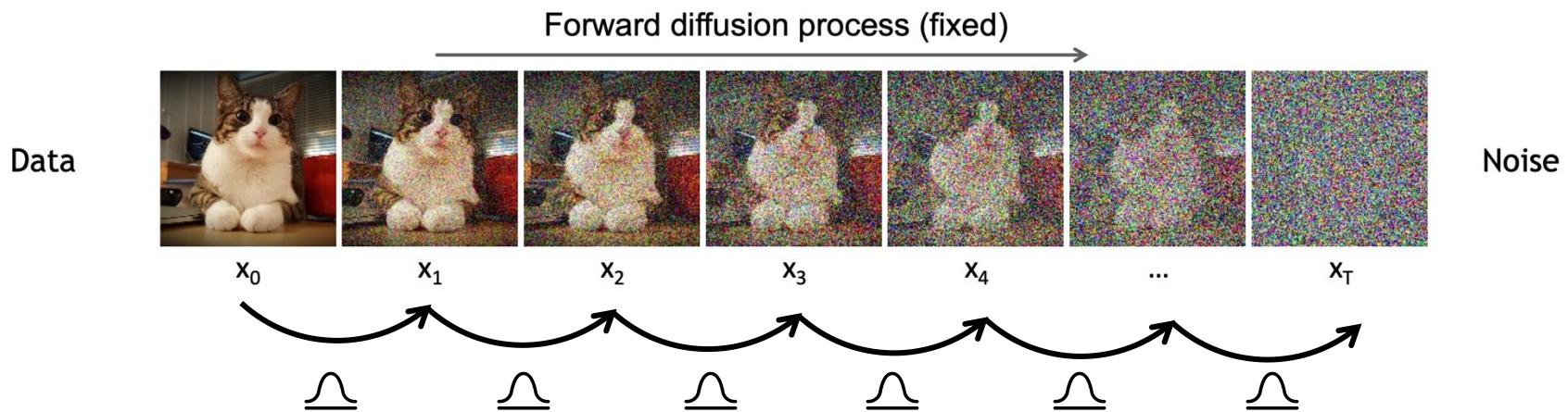
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# Forward Diffusion Process

- Forward diffusion process is stacking **fixed** VAE encoders
    - gradually adding Gaussian noise according to schedule  $\beta_t$

$$q(\mathbf{x}_t \mid \mathbf{x}_{t-1}) = \mathcal{N} \left( \mathbf{x}_t; \sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I} \right)$$

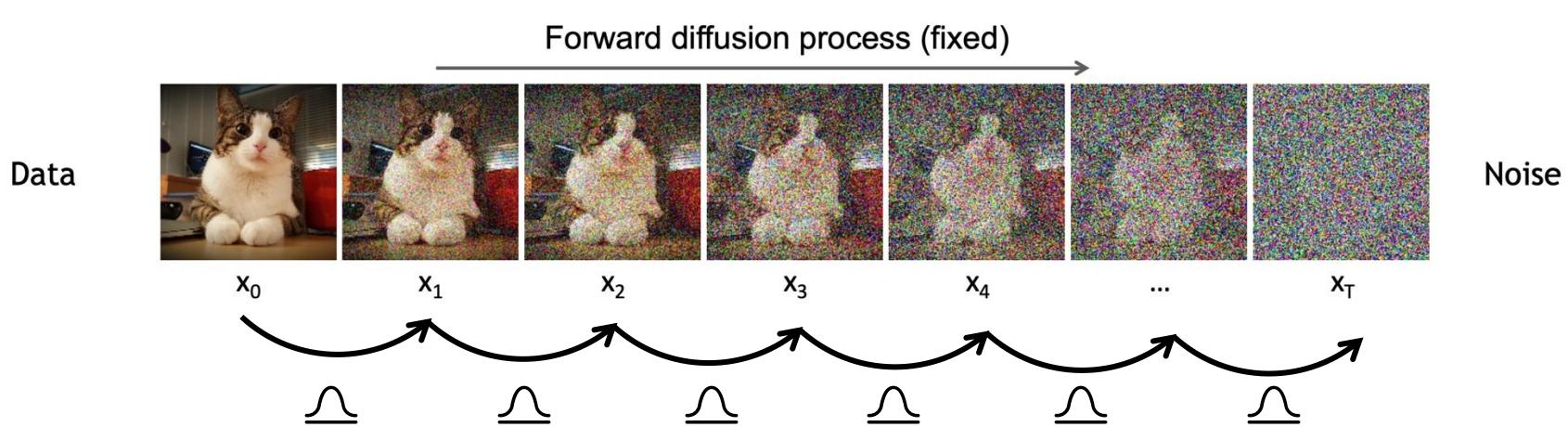


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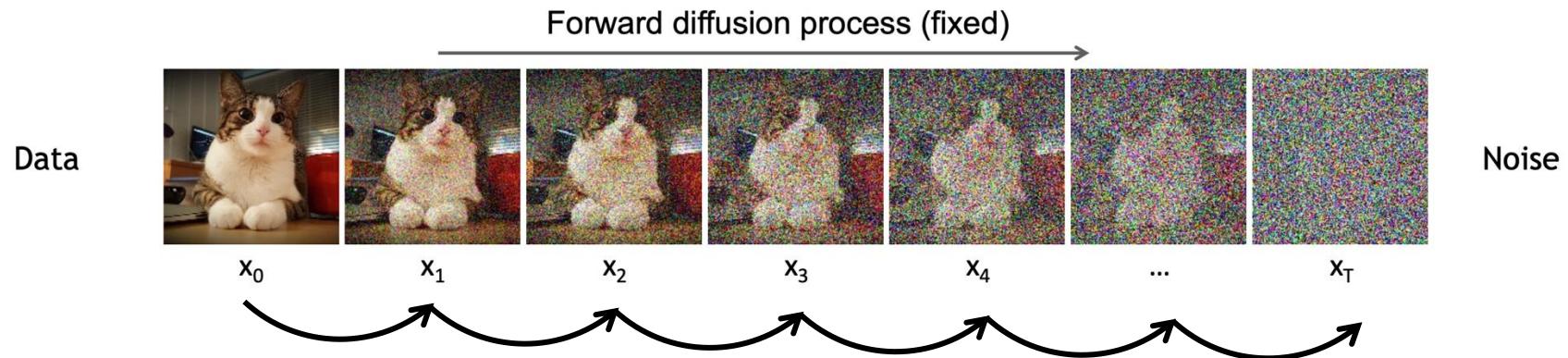
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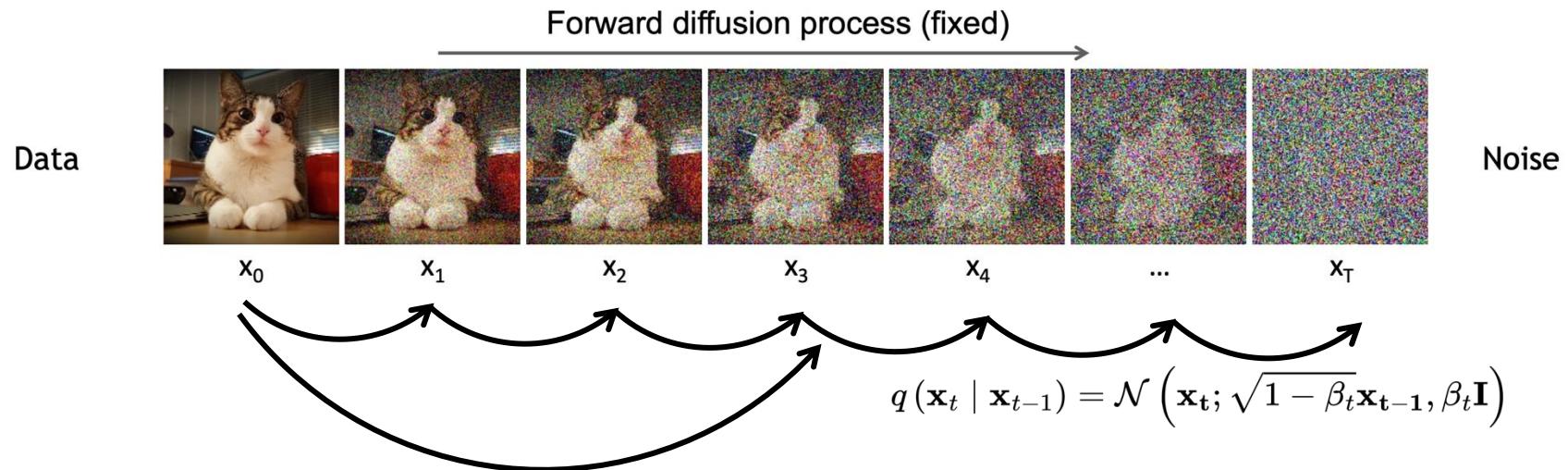
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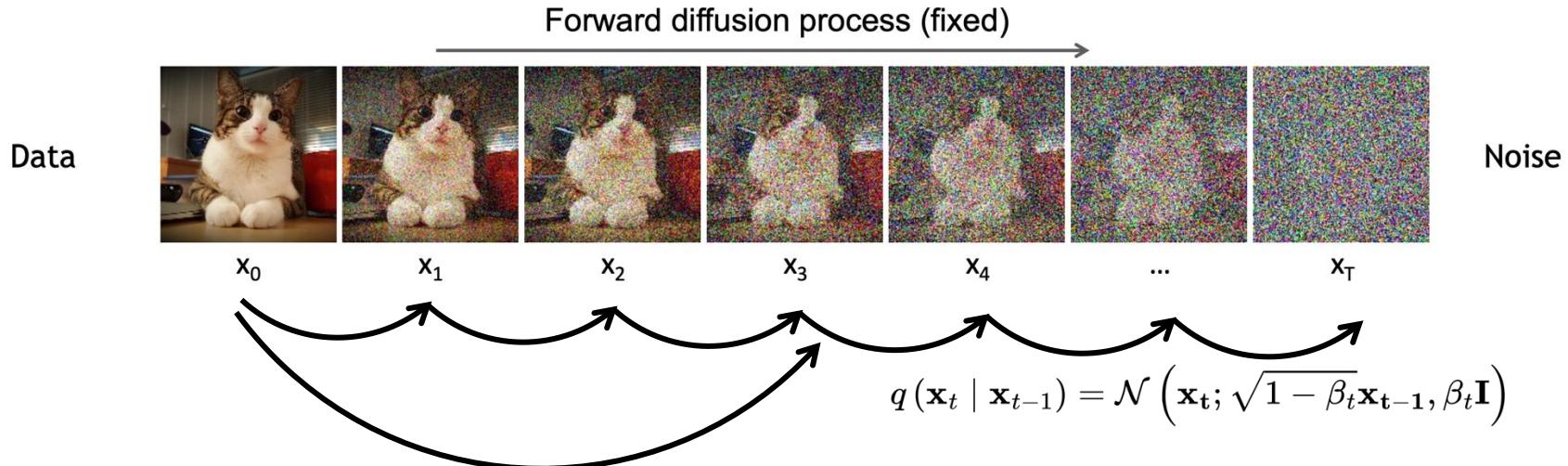
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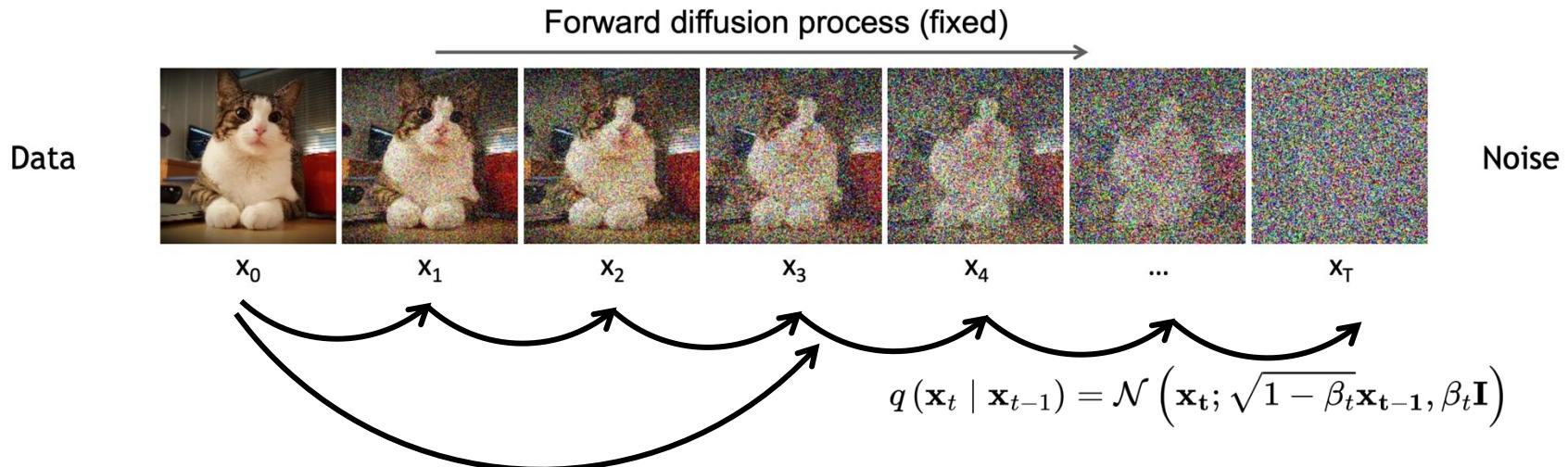


- The forward process allows sampling of  $x_t$  at arbitrary timestep  $t$  in closed form:

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$$q(\mathbf{x}_T | \mathbf{x}_0) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$$

# Reverse Denoising Process

- Generation process
  - Sample  $\mathbf{x}_T \sim \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$
  - Iteratively sample  $\mathbf{x}_{t-1} \sim q(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$

# Reverse Denoising Process

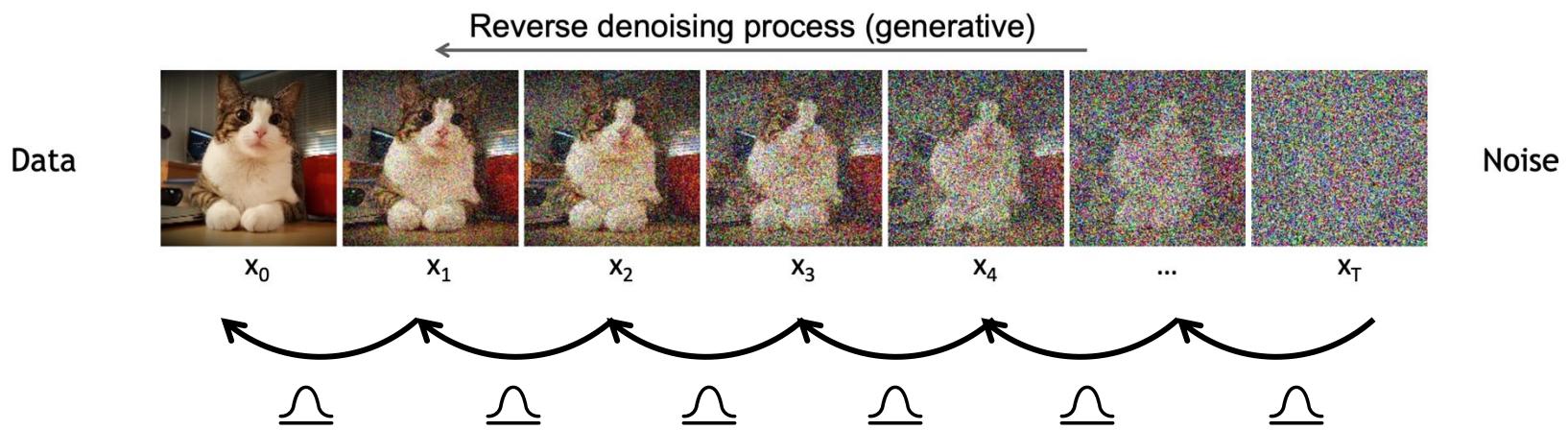
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  - Generation process
    - Sample
    - Iteratively sample
  - not directly tractable
  - But can be estimated with a Gaussian distribution if  $\beta_t$  is small at each step
    - The purpose of our stack of VAE decoders!
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# Reverse Denoising Process

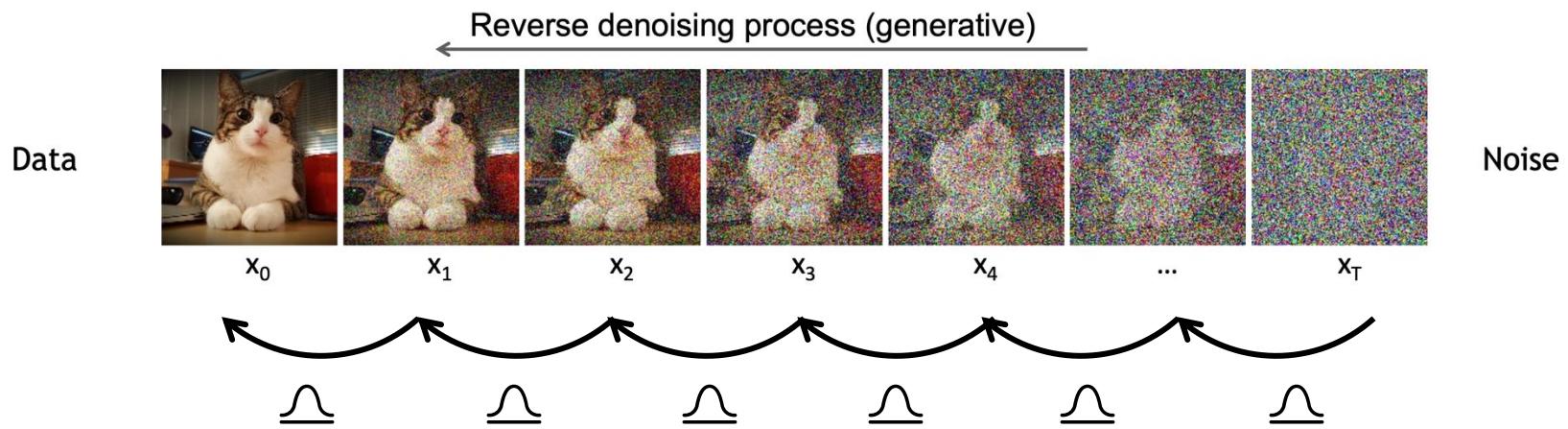
- Reverse diffusion process is stacking **learnable** VAE decoders



# Reverse Denoising Process

- Reverse diffusion process is stacking **learnable** VAE decoders
    - Predicting the mean and std of added Gaussian Noise

$$\begin{aligned} p(\mathbf{x}_T) &= \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}) & p_\theta(\mathbf{x}_{0:T}) &= p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t) \\ p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t) &= \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \sigma_t^2 \mathbf{I}) \end{aligned}$$



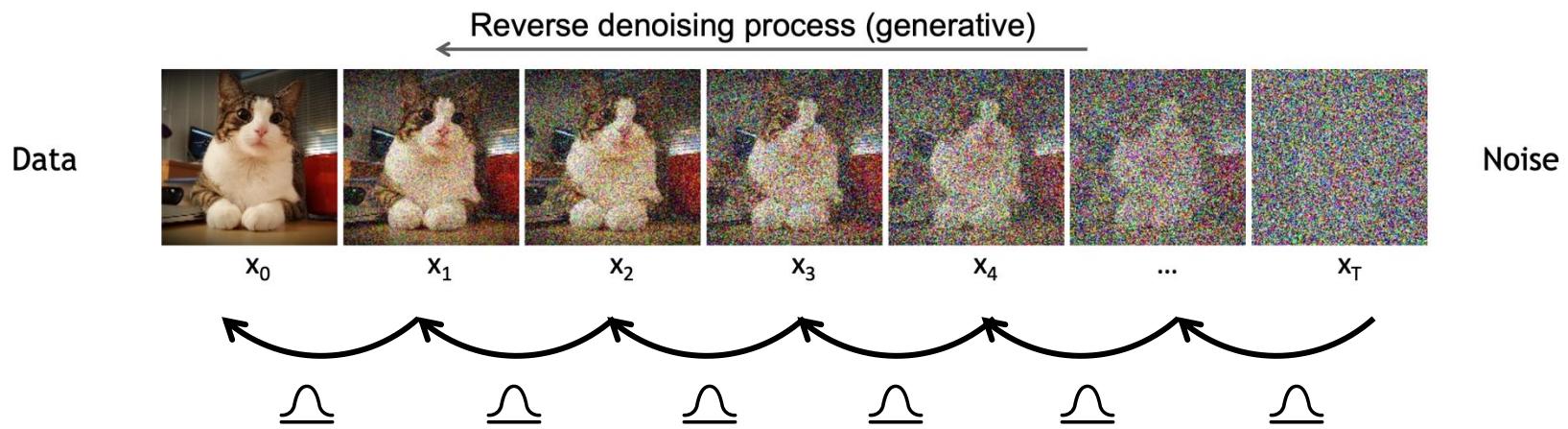
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$$p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$$

$$p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)$$

$$p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \sigma_t^2 \mathbf{I})$$



# Reverse Denoising Process

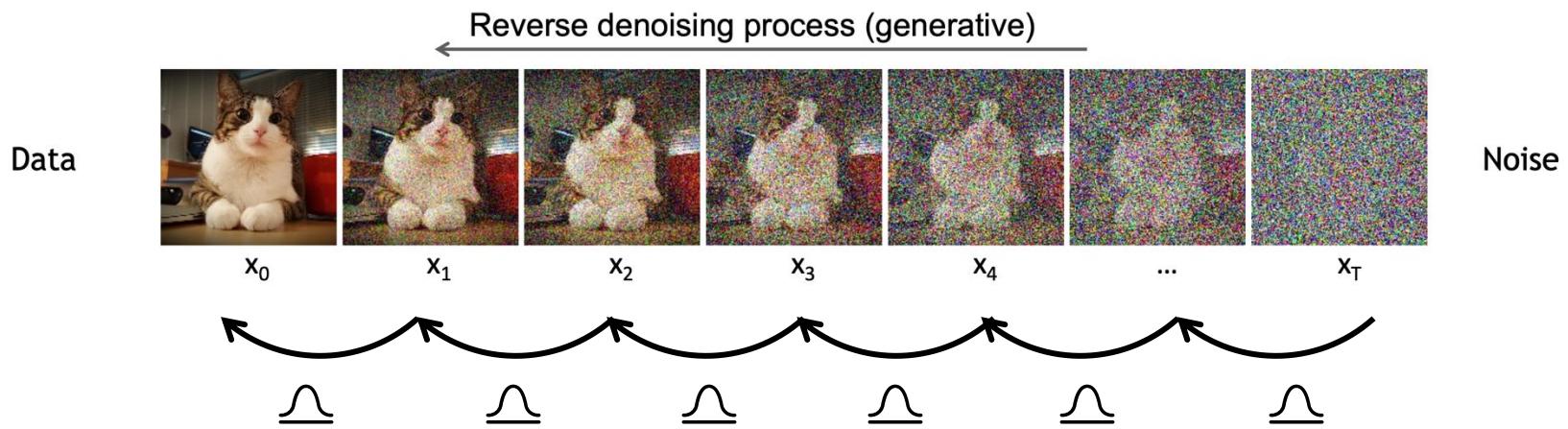
- Reverse diffusion process is stacking **learnable** VAE decoders
  - Predicting the mean and std of added Gaussian Noise

$$p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}) \quad p_{\theta}(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^T p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t)$$

$$p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_{\theta}(\mathbf{x}_t, t), \sigma_t^2 \mathbf{I})$$



**Trainable Network, Shared Across All Timesteps**



# Learning the Denoising Model

- Denoising models are trained with variational upper bound (negative ELBO), as VAEs

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

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- which derives to:

$$L = \mathbb{E}_q \underbrace{[D_{\text{KL}}(q(\mathbf{x}_T | \mathbf{x}_0) \| p(\mathbf{x}_T))]}_{L_T} + \sum_{t>1} \underbrace{D_{\text{KL}}(q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) \| p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t))}_{L_{t-1}} \underbrace{-\log p_\theta(\mathbf{x}_0 | \mathbf{x}_1)}_{L_0}$$

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constant Scaling

- tractable posterior distribution (closed-form)

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) = \mathcal{N} \left( \mathbf{x}_{t-1}; \tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I} \right)$$

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

# Learning the Denoising Model

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

- which derives to:

$$L = \underbrace{\mathbb{E}_q [D_{\text{KL}}(q(\mathbf{x}_T | \mathbf{x}_0) \| p(\mathbf{x}_T))]}_{L_T \text{ constant}} + \sum_{t>1} \underbrace{D_{\text{KL}}(q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) \| p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t))}_{L_{t-1}} \underbrace{-\log p_\theta(\mathbf{x}_0 | \mathbf{x}_1)}_{L_0 \text{ Scaling}}$$

# Learning the Denoising Model

- Denoising models are trained with variational upper bound (negative ELBO), as VAEs

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

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$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}\left(\mathbf{x}_{t-1}; \tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}\right)$$

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

# Parameterizing the Denoising Model

- KL divergence has a simple form between Gaussians

$$L_{t-1} = D_{\text{KL}}(q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) \| p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)) = \mathbb{E}_q \left[ \frac{1}{2\sigma_t^2} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_\theta(\mathbf{x}_t, t)\|^2 \right] + C$$

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- Recall that:  $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{(1 - \bar{\alpha}_t)} \epsilon$

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{1 - \beta_t}} \left( \mathbf{x}_t - \frac{\beta_t}{\sqrt{1 - \bar{\alpha}_t}} \epsilon \right)$$

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- Trainable network predicts the noise mean

$$\mu_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{1 - \beta_t}} \left( \mathbf{x}_t - \frac{\beta_t}{\sqrt{1 - \bar{\alpha}_t}} \boxed{\epsilon_\theta(\mathbf{x}_t, t)} \right)$$

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- Final Objective

$$L_{t-1} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[ \frac{\beta_t^2}{2\sigma_t^2 (1 - \beta_t) (1 - \bar{\alpha}_t)} \|\epsilon - \epsilon_\theta(\underbrace{\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon}_{\mathbf{x}_t}, t)\|^2 \right] + C$$

64

# Simplified Training Objective

$$L_{t-1} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[ \underbrace{\frac{\beta_t^2}{2\sigma_t^2 (1 - \beta_t) (1 - \bar{\alpha}_t)}}_{\lambda_t} \left\| \epsilon - \epsilon_\theta \left( \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t \right) \right\|^2 \right]$$

- $\lambda_t$  ensures the weighting for correct maximum likelihood estimation
- In DDPM, this is further simplified to:

$$L_{\text{simple}} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), t \sim \mathcal{U}(1, T)} [\|\underbrace{\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)}_{\mathbf{x}_t}\|^2]$$

# Summary: Training and Sampling

---

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

6: until converged
```

---

---

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

5: end for
6: return  $\mathbf{x}_0$ 
```

---

# Summary: Noise Schedule

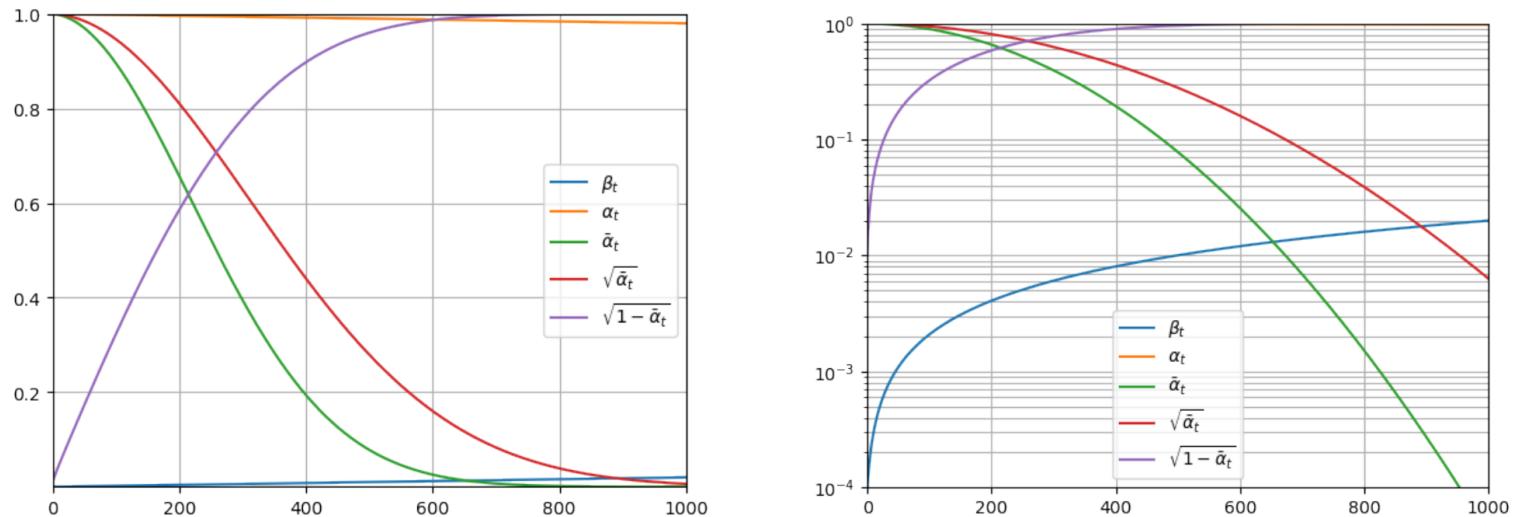
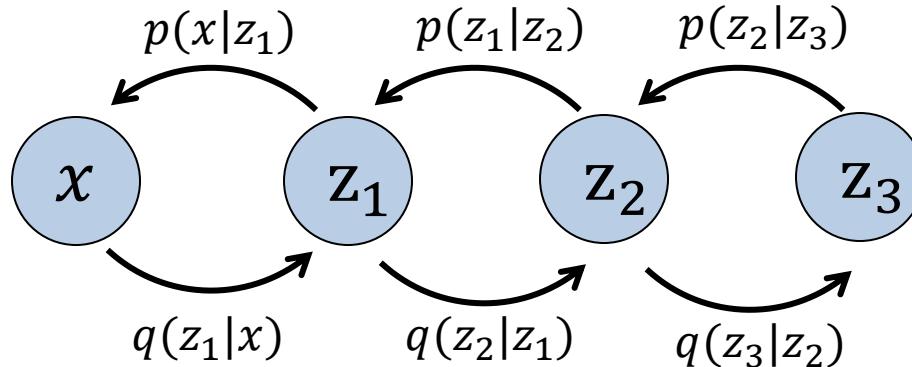


Figure 2: Parameter values for  $\beta = [10^{-4}, 0.02]$  over 1000 time steps  $t$  using a linear schedule. The information in the two figures are the same, but the right-hand side uses log-scale on the  $y$ -axis to show the speed of which  $\bar{\alpha}_t$  goes towards zero.

# Connection with Hierarchical VAEs

- Diffusion models are special case of Hierarchical VAEs
  - Fixed inference models in forward process
  - Latent variables have same dimension as data
  - ELBO is decomposed to each timestep: faster to train
  - Model is trained with some weighting of ELBO



# Poll 2

What's the neural network predicting in diffusion models at  $x_t$

- Mean of added Gaussian noise
- The denoised latent  $x_{\{t-1\}}$
- Std of the added Gaussian noise
- The added Gaussian noise  $\epsilon_{\{t-1\}}$

# Poll 2

What's the neural network predicting in diffusion models at  $x_t$

- Mean of added Gaussian noise
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# Content

- Diffusion Model Basics
  - Diffusion Models as Stacking VAEs
  - Diffusion Models: Forward, Reverse, Training, Sampling
- Diffusion Models from Stochastic Differential Equations and Score Matching Perspective
- Classifier-Free Guidance for Conditional Models
- Applications of Diffusion Models

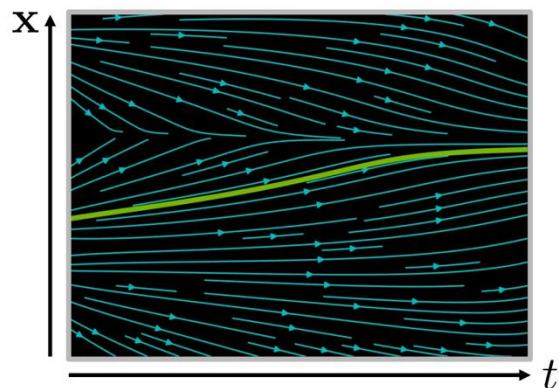
# Why SDEs?

- A unified framework for interpreting diffusion models and score-based generation models
  - Variants of diffusion-based and flow-based models

# Ordinary Differential Equations

Ordinary Differential Equation (ODE):

$$\frac{dx}{dt} = f(x, t) \text{ or } dx = f(x, t)dt$$



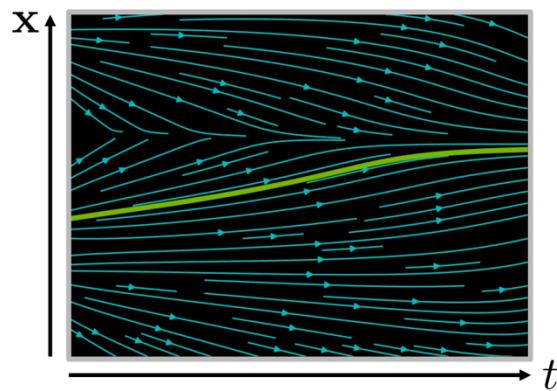
Analytical Solution:  $x(t) = x(0) + \int_0^t f(x, \tau)d\tau$

Iterative Numerical  
Solve:  $x(t + \Delta t) \approx x(t) + f(x(t), t)\Delta t$

# Stochastic Differential Equations

Ordinary Differential Equation (ODE):

$$\frac{dx}{dt} = f(x, t) \text{ or } dx = f(x, t)dt$$



Analytical Solution:

$$x(t) = x(0) + \int_0^t f(x, \tau)d\tau$$

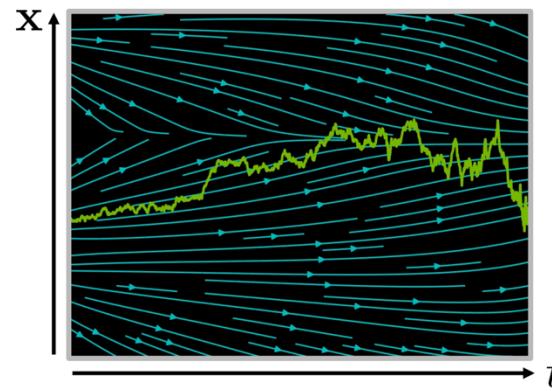
Iterative Numerical

$$x(t + \Delta t) \approx x(t) + f(x(t), t)\Delta t$$

Stochastic Differential Equation (SDE):

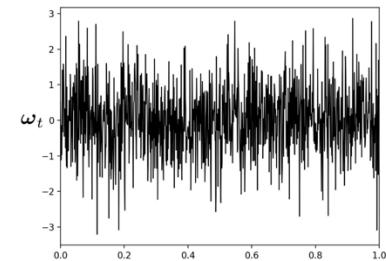
$$\frac{dx}{dt} = \underbrace{f(x, t)}_{\text{drift coefficient}} + \underbrace{\sigma(x, t)\omega_t}_{\text{diffusion coefficient}}$$

$$(dx = f(x, t)dt + \sigma(x, t)d\omega_t)$$



$$x(t + \Delta t) \approx x(t) + f(x(t), t)\Delta t + \sigma(x(t), t)\sqrt{\Delta t} \mathcal{N}(\mathbf{0}, \mathbf{I})$$

Wiener Process  
(Gaussian White Noise)



# Score Matching

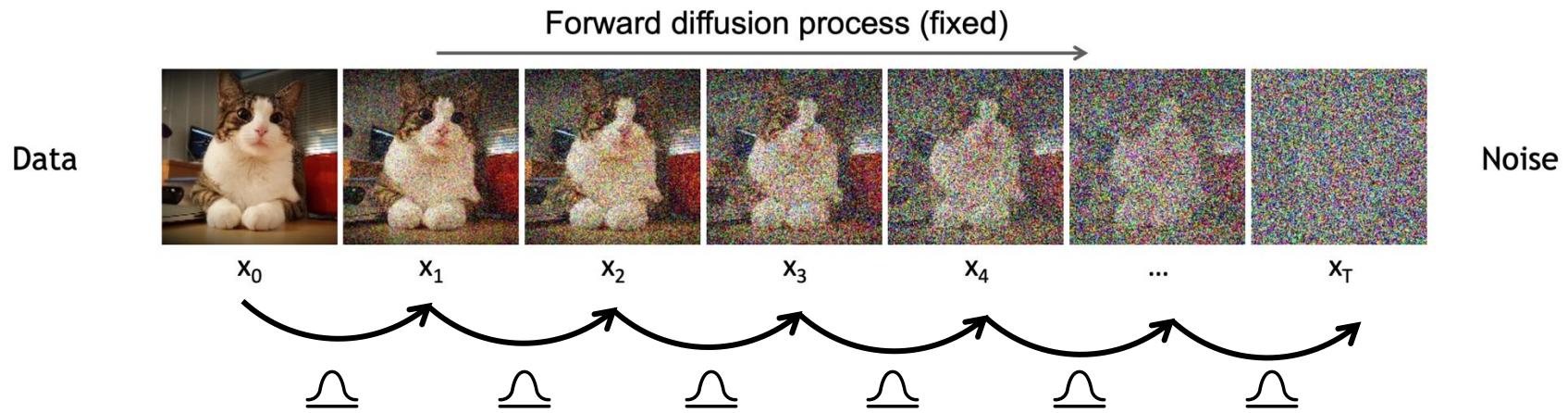
- General form of probability density function

$$p_\theta(\mathbf{x}) = \frac{e^{-f_\theta(\mathbf{x})}}{Z_\theta}$$

- Maximizing the log-likelihood requires us to know  $Z_\theta$ 
  - Often intractable
- Instead, we can model the score function

$$\nabla_{\mathbf{x}} \log p(\mathbf{x})$$

# Forward Diffusion Process as SDEs

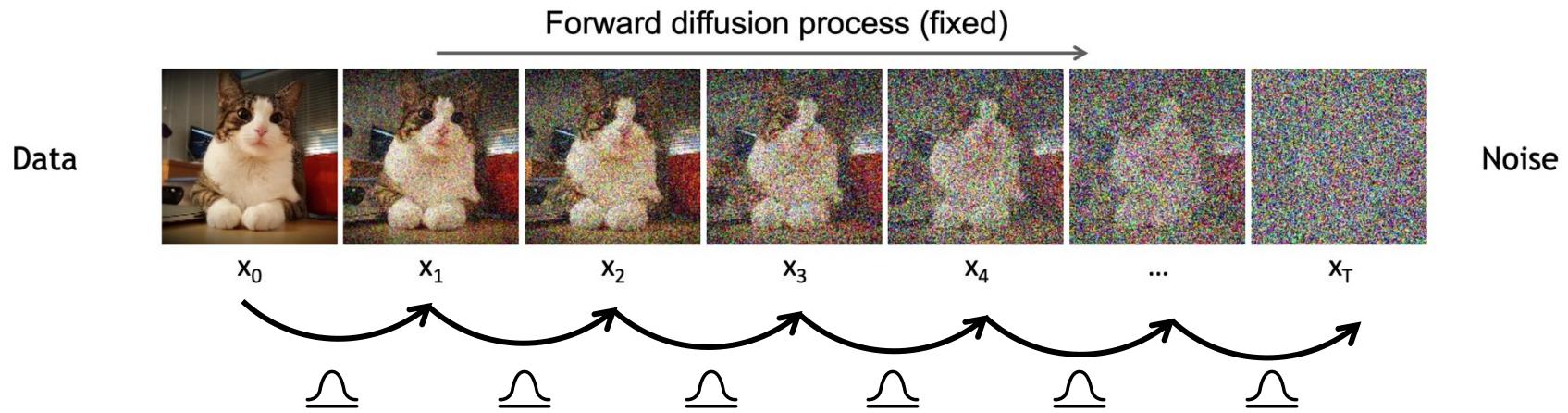


- Consider a forward process with many many small steps (continuous time)

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N} \left( \mathbf{x}_t; \sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I} \right)$$

$$\mathbf{x}_t = \sqrt{1 - \beta_t} \mathbf{x}_{t-1} + \sqrt{\beta_t} \mathcal{N}(\mathbf{0}, \mathbf{I})$$

# Forward Diffusion Process as SDEs



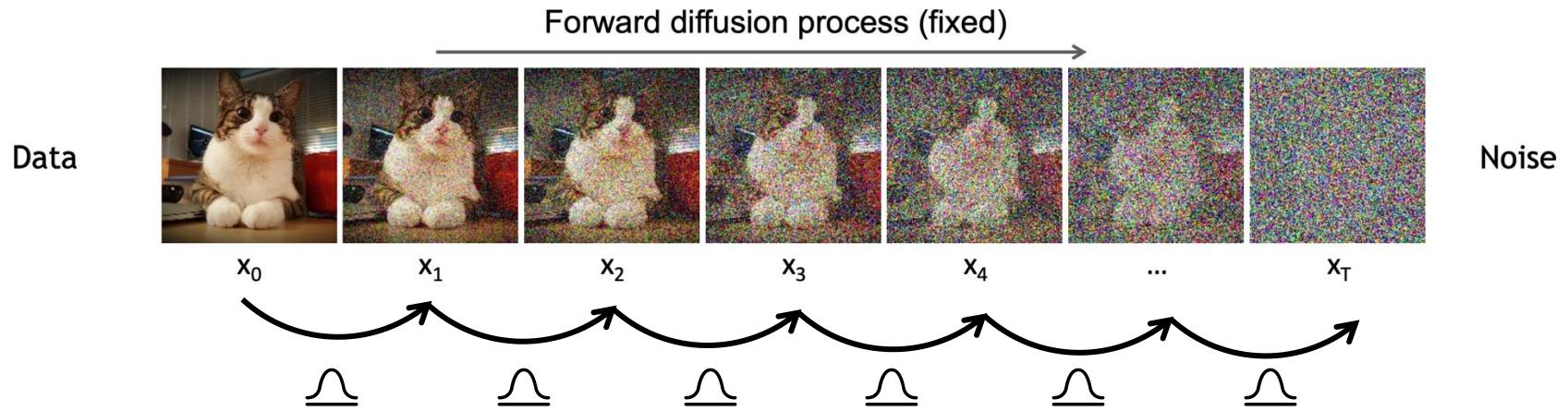
- Consider a forward process with many many small steps

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I})$$

$$\begin{aligned}\mathbf{x}_t &= \sqrt{1 - \beta_t} \mathbf{x}_{t-1} + \sqrt{\beta_t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \\ &= \sqrt{1 - \beta(t)\Delta t} \mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad (\beta_t := \beta(t)\Delta t)\end{aligned}$$

Allows different size along t      Step size

# Forward Diffusion Process as SDEs

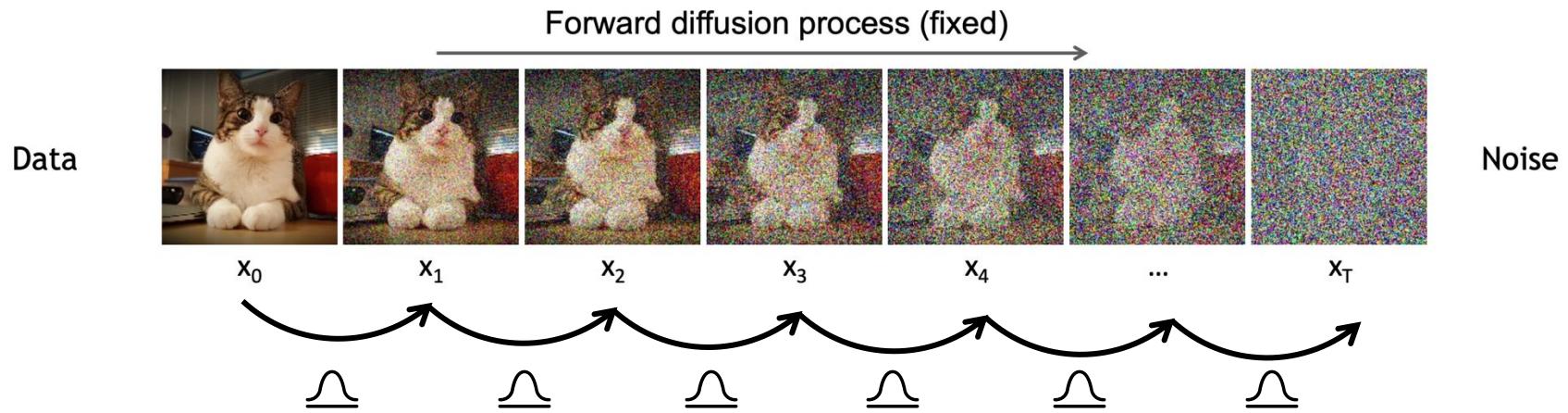


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$$\begin{aligned}\mathbf{x}_t &= \sqrt{1 - \beta_t} \mathbf{x}_{t-1} + \sqrt{\beta_t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \\ &= \sqrt{1 - \beta(t)\Delta t} \mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad (\beta_t := \beta(t)\Delta t) \\ &\approx \mathbf{x}_{t-1} - \frac{\beta(t)\Delta t}{2} \mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad \text{Taylor expansion}\end{aligned}$$

# Forward Diffusion Process as SDEs



- An iterative update that can be viewed as SDEs

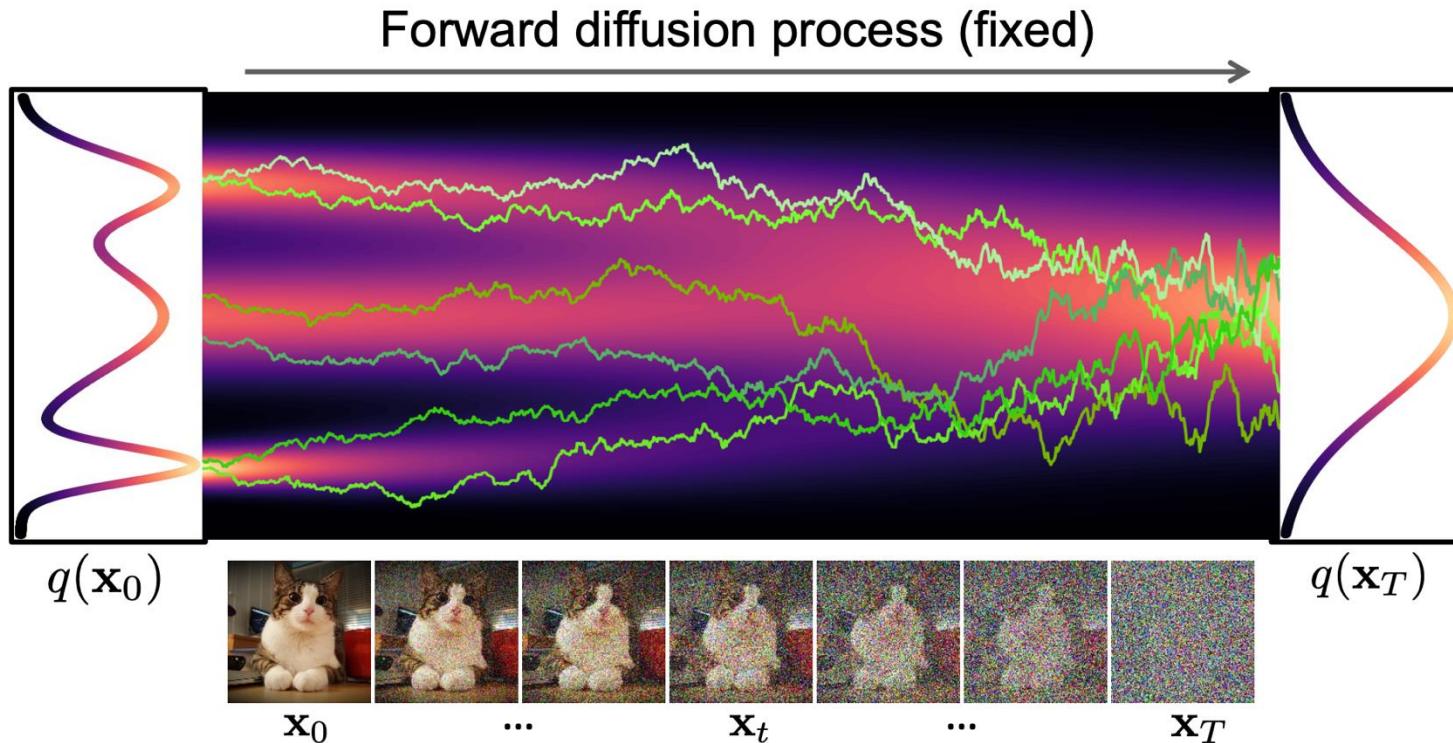
$$\mathbf{x}_t \approx \mathbf{x}_{t-1} - \frac{\beta(t)\Delta t}{2} \mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t} \mathcal{N}(\mathbf{0}, \mathbf{I})$$



$$d\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t dt + \sqrt{\beta(t)}d\omega_t$$

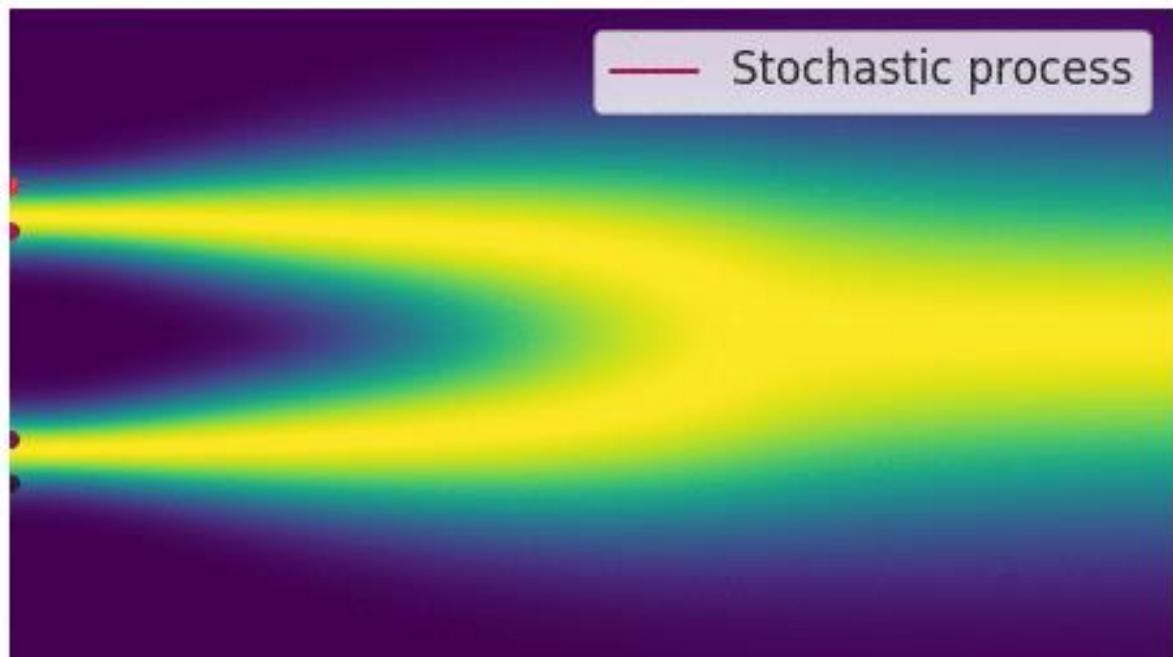
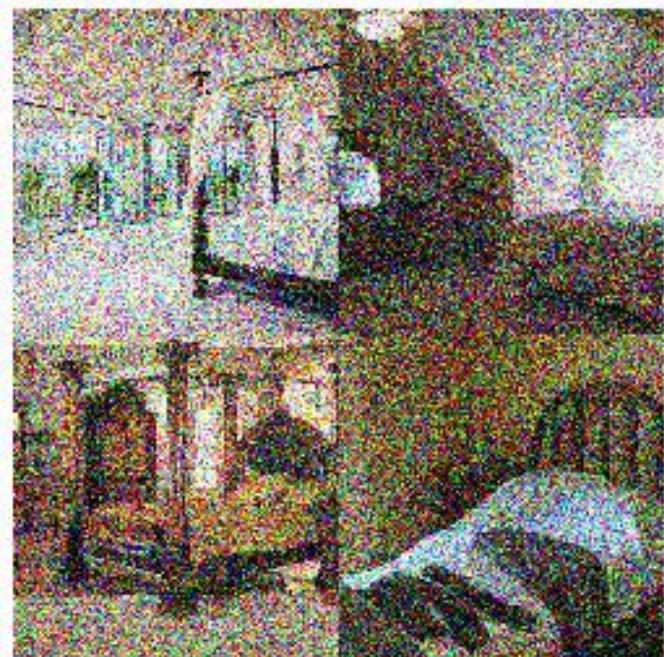
Stochastic Differential Equation (SDE)

# Forward Diffusion Process as SDEs

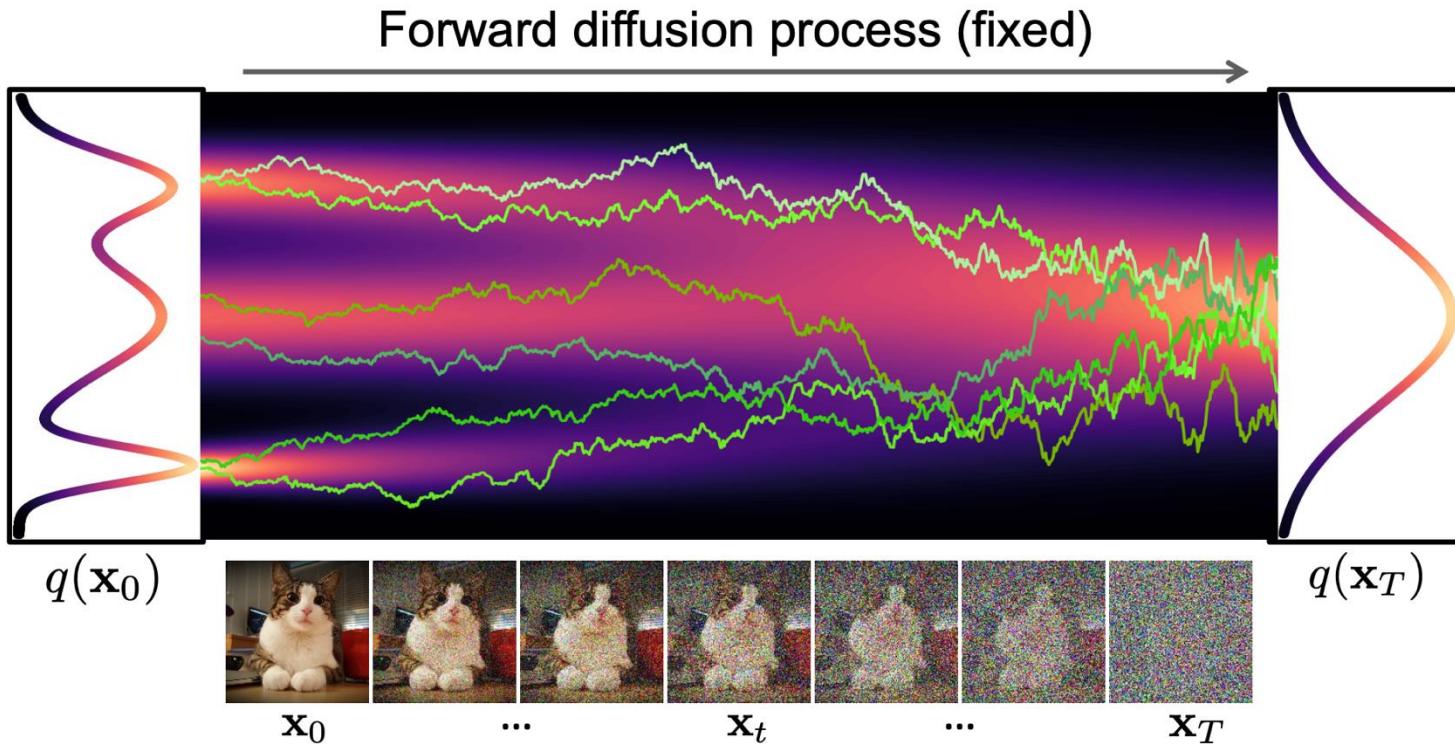


$$d\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t dt + \sqrt{\beta(t)}d\omega_t$$

Drift Term                      Diffusion Term  
(Pulls toward the mode)    (Injects Noise)

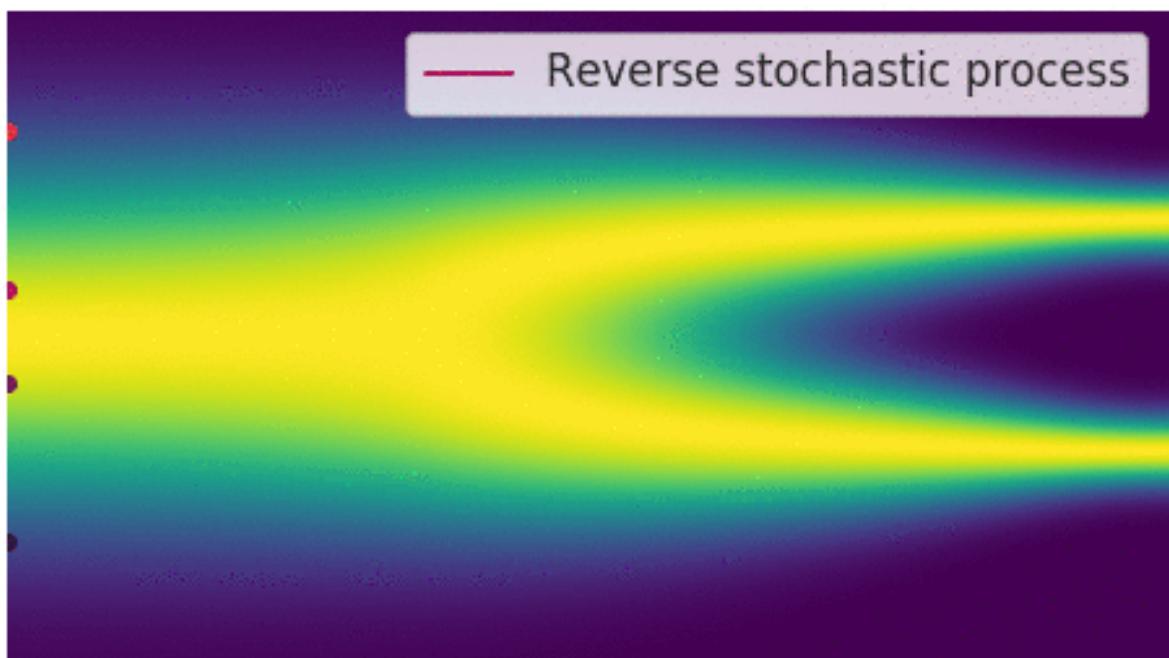


# Generative Reverse SDEs

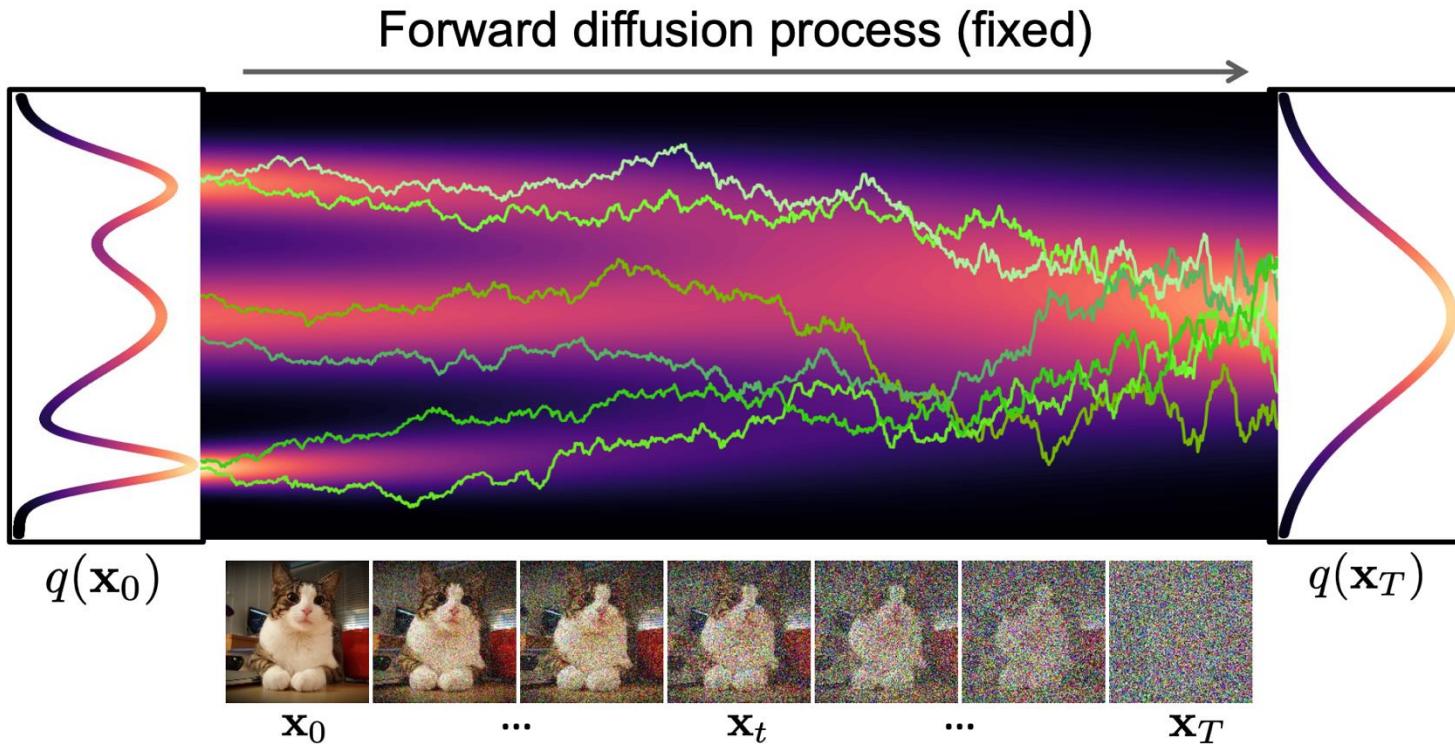


- The forward SDE has a reverse form:

$$d\mathbf{x}_t = \left[ -\frac{1}{2}\beta(t)\mathbf{x}_t - \beta(t)\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t) \right] dt + \sqrt{\beta(t)} d\bar{\omega}_t$$



# Generative Reverse SDEs



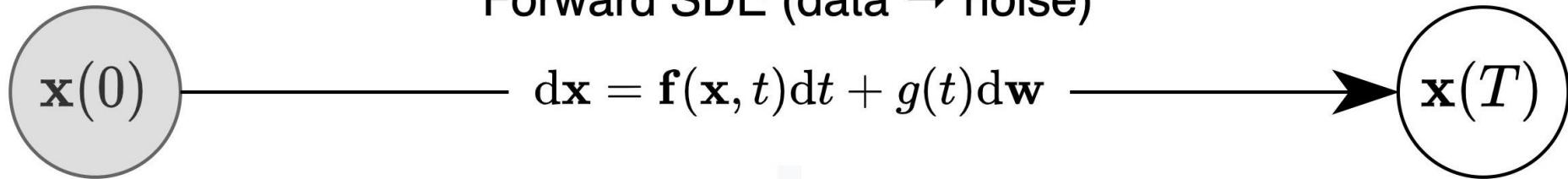
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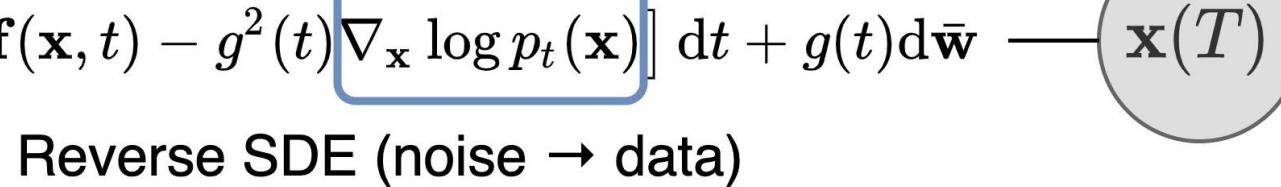
Score function  
How to get it?

# Denoising Score Matching

Forward SDE (data → noise)

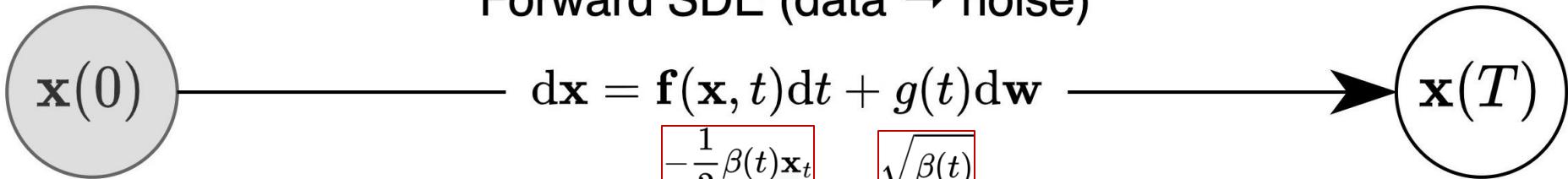


score function

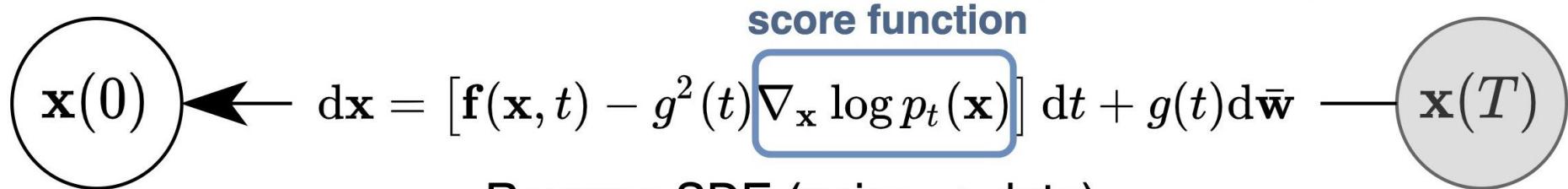


# Denoising Score Matching

Forward SDE (data → noise)



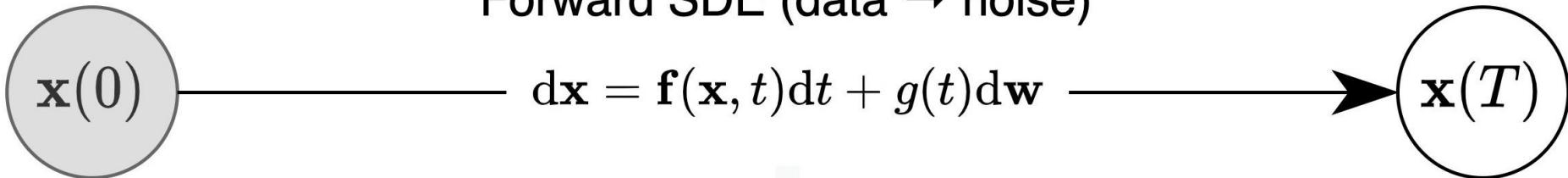
score function



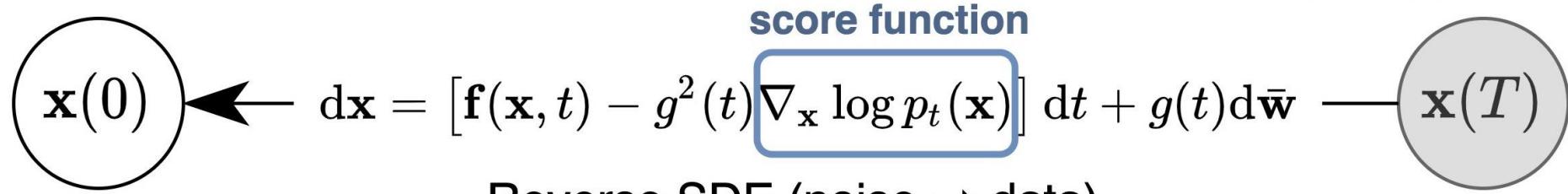
$$d\mathbf{x}_t = \left[ -\frac{1}{2}\beta(t)\mathbf{x}_t - \beta(t)\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t) \right] dt + \sqrt{\beta(t)}d\bar{\omega}_t$$

# Denoising Score Matching

Forward SDE (data → noise)



score function



Reverse SDE (noise → data)

$$\min_{\theta} \underbrace{\mathbb{E}_{t \sim \mathcal{U}(0,T)} \underbrace{\mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \underbrace{\mathbb{E}_{\mathbf{x}_t \sim q_t(\mathbf{x}_t | \mathbf{x}_0)}}_{\text{diffused data sample}}} _{\text{diffusion time } t} \cdot \underbrace{\tilde{w}(t) \cdot}_{\text{weighting function}} \underbrace{\|\mathbf{s}_{\theta}(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t | \mathbf{x}_0)\|_2^2}_{\text{score of diffused data sample}}$$

Looks similar?

# Denoising Score Matching

- Denoising score matching objective

$$\min_{\theta} \underbrace{\mathbb{E}_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\mathbf{x}_t \sim q_t(\mathbf{x}_t | \mathbf{x}_0)}}_{\begin{array}{c} \text{diffusion} \\ \text{time } t \\ \text{sample } \mathbf{x}_0 \end{array}} \underbrace{\tilde{w}(t) \cdot}_{\begin{array}{c} \text{weighting} \\ \text{function} \end{array}} \underbrace{\|\mathbf{s}_{\theta}(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t | \mathbf{x}_0)\|_2^2}_{\begin{array}{c} \text{neural} \\ \text{network} \\ \text{score of diffused} \\ \text{data sample} \end{array}}$$

- Re-parametrized sampling:

$$\mathbf{x}_t = \alpha_t \mathbf{x}_0 + \sigma_t \boldsymbol{\epsilon} \quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

- Score function:

$$\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t | \mathbf{x}_0) = -\nabla_{\mathbf{x}_t} \frac{(\mathbf{x}_t - \alpha_t \mathbf{x}_0)^2}{2\sigma_t^2} = -\frac{\mathbf{x}_t - \alpha_t \mathbf{x}_0}{\sigma_t^2} = -\frac{\alpha_t \mathbf{x}_0 + \sigma_t \boldsymbol{\epsilon} - \alpha_t \mathbf{x}_0}{\sigma_t^2} = -\frac{\boldsymbol{\epsilon}}{\sigma_t}$$

- Denoising network:

$$\mathbf{s}_{\theta}(\mathbf{x}_t, t) := -\frac{\boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t)}{\sigma_t}$$

- Final objective:

$$\min_{\theta} \mathbb{E}_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \hat{w}(t) \cdot \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t)\|_2^2 \quad \hat{w}(t) = \frac{\tilde{w}(t)}{\sigma_t}$$

# Weighted Diffusion Objective

- Denoising score matching objective with loss weighting

$$\min_{\theta} \mathbb{E}_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \frac{\lambda(t)}{\sigma_t^2} \|\epsilon - \epsilon_{\theta}(\mathbf{x}_t, t)\|_2^2$$

- Loss weights trade-off between
  - good perceptual quality:  $\lambda(t) = \sigma_t^2$
  - maximum likelihood:  $\lambda(t) = \beta(t)$
- More complicated model parametrization and loss weighting leads to different diffusion model variants in the literature!

# Poll 3

The drift term of SDE in the forward process of diffusion models

- Pulls the data towards the uni-gaussian mode
- Adds random gaussian noise

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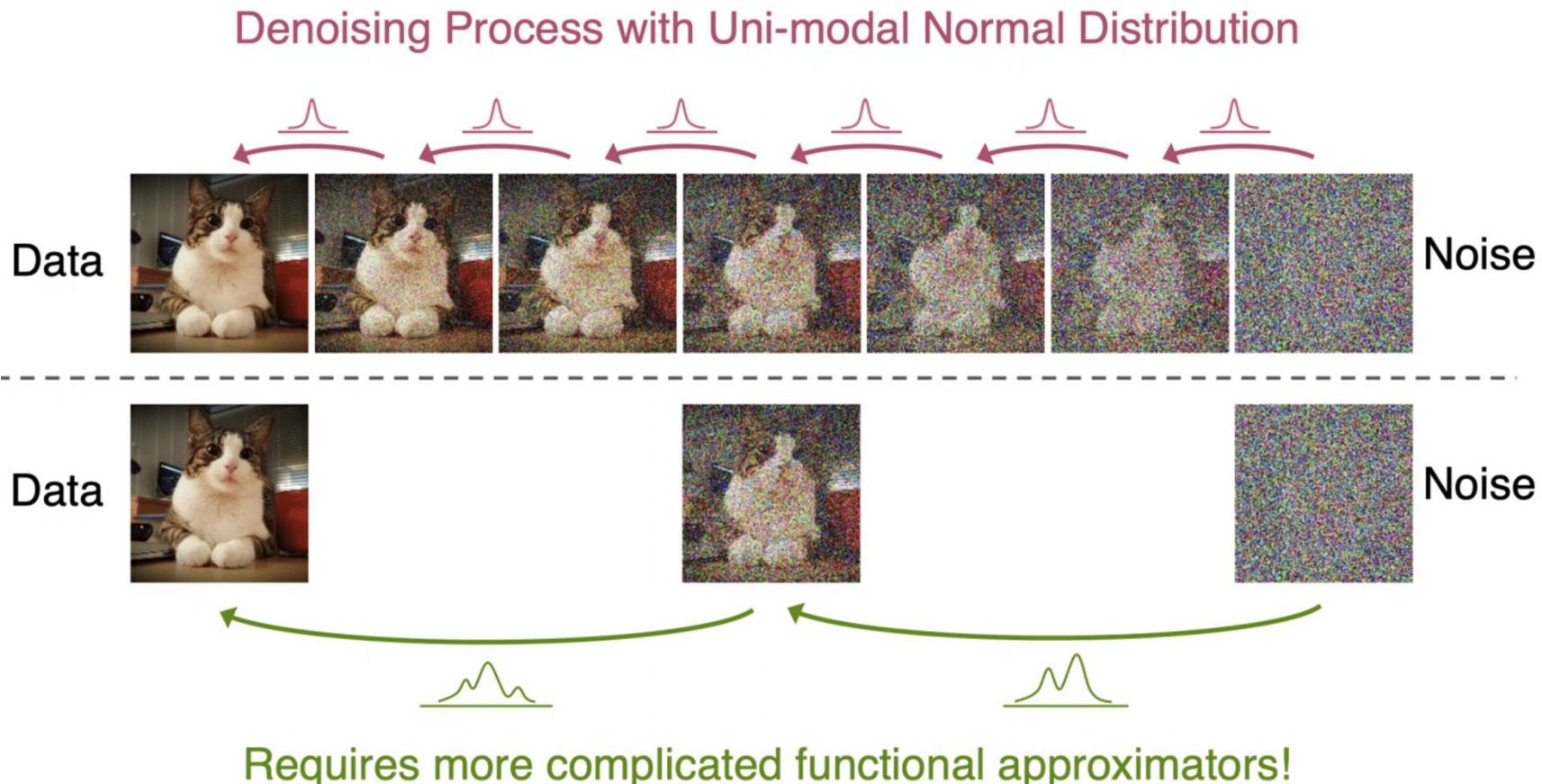
# Content

- Diffusion Model Basics
- Diffusion Models from Stochastic Differential Equations and Score Matching Perspective
- Denoising Diffusion Implicit Model (DDIM)
- Conditional Diffusion Models
- Applications of Diffusion Models

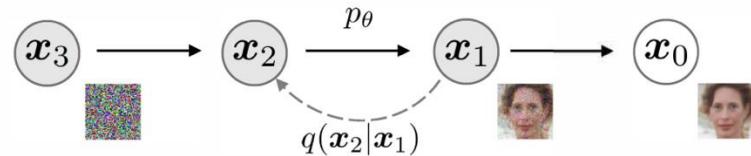
# Many Steps in Diffusion

- Slow in generation
- In Training, we randomly sample one time step
- But in inference, we must transit from  $T$  to 0
  - 1000 steps
  - extremely slow for raw images/signals

# Can we do generation with less steps?



# DDPM

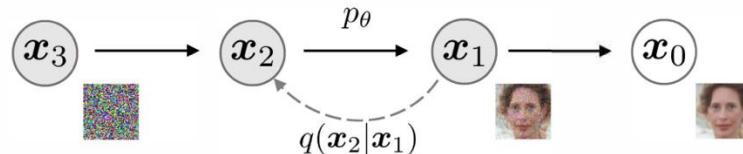


$$q(\mathbf{x}_t \mid \mathbf{x}_{t-1}) = \mathcal{N} \left( \mathbf{x}_t; \sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I} \right)$$

$$q(\mathbf{x}_t \mid \mathbf{x}_0) = \mathcal{N} \left( \mathbf{x}_t; \sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I} \right)$$

$$L_{\text{simple}} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), t \sim \mathcal{U}(1, T)} [\|\epsilon - \epsilon_\theta(\underbrace{\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)}_{\mathbf{x}_t}\|^2]$$

# DDPM



Only depends on previous step

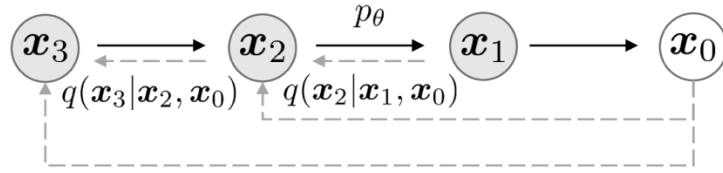
$$q(\mathbf{x}_t \mid \mathbf{x}_{t-1}) = \mathcal{N} \left( \mathbf{x}_t; \sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I} \right)$$

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$$L_{\text{simple}} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), t \sim \mathcal{U}(1, T)} [\|\underbrace{\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)}_{\mathbf{x}_t}\|^2]$$

Only used during training

# DDIM



$$q_\sigma(\mathbf{x}_{1:T} \mid \mathbf{x}_0) := q_\sigma(\mathbf{x}_T \mid \mathbf{x}_0) \prod_{t=2}^T q_\sigma(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$$

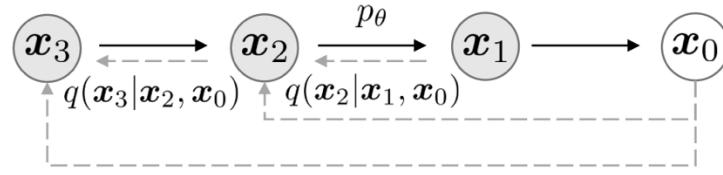
$$q_\sigma(\mathbf{x}_T \mid \mathbf{x}_0) = \mathcal{N}(\sqrt{\alpha_T} \mathbf{x}_0, (1 - \alpha_T) \mathbf{I})$$

$$q_\sigma(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}\left(\sqrt{\alpha_{t-1}} \mathbf{x}_0 + \sqrt{1 - \alpha_{t-1} - \sigma_t^2} \cdot \frac{\mathbf{x}_t - \sqrt{\alpha_t} \mathbf{x}_0}{\sqrt{1 - \alpha_t}}, \sigma_t^2 \mathbf{I}\right)$$

- A Non-Markovian Forward Process

$$q_\sigma(\mathbf{x}_t \mid \mathbf{x}_{t-1}, \mathbf{x}_0) = \frac{q_\sigma(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) q_\sigma(\mathbf{x}_t \mid \mathbf{x}_0)}{q_\sigma(\mathbf{x}_{t-1} \mid \mathbf{x}_0)}$$

# DDIM



- Backward process

$$p_\theta^{(t)}(\mathbf{x}_{t-1} | \mathbf{x}_t) = \begin{cases} \mathcal{N}\left(f_\theta^{(1)}(\mathbf{x}_1), \sigma_1^2 \mathbf{I}\right) & \text{if } t = 1 \\ q_\sigma\left(\mathbf{x}_{t-1} | \mathbf{x}_t, f_\theta^{(t)}(\mathbf{x}_t)\right) & \text{otherwise,} \end{cases}$$
$$f_\theta^{(t)}(\mathbf{x}_t) := \left(\mathbf{x}_t - \sqrt{1 - \alpha_t} \cdot \epsilon_\theta^{(t)}(\mathbf{x}_t)\right) / \sqrt{\alpha_t}$$

# DDPM vs DDIM

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## Algorithm DDPM Sampling

---

```
 $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
for all  $t$  from  $T$  to 1 do
     $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
     $\mu \leftarrow \frac{1}{\sqrt{\alpha_t}} (\mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \epsilon_\theta(\mathbf{x}_t, t))$ 
     $\mathbf{x}_{t-1} \leftarrow \mu + \sigma_t \epsilon$  Stochastic
end for
return  $\mathbf{x}_0$ 
```

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## Algorithm DDIM Sampling

---

```
 $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
for all  $t$  from  $T$  to 1 do
     $\bar{\epsilon} \leftarrow \epsilon_\theta(\mathbf{x}_t, t)$ 
     $\bar{\mathbf{x}}_0 \leftarrow \frac{\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t} \bar{\epsilon}}{\sqrt{\bar{\alpha}_t}}$  Estimate  $\mathbf{x}_0$ 
     $\mathbf{x}_{t-1} \leftarrow \sqrt{\bar{\alpha}_{t-1}} \bar{\mathbf{x}}_0 + \sqrt{1 - \bar{\alpha}_{t-1}} \bar{\epsilon}$ 
end for
return  $\mathbf{x}_0$ 
```

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# DDIM with Fewer Steps Sampling

## DDIM

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**Algorithm** Original DDIM Sampling

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```
xT ~  $\mathcal{N}(\mathbf{0}, \mathbf{I})$ 
for all t from T to 1 do
     $\bar{\epsilon}$  ←  $\epsilon_{\theta}(\mathbf{x}_t, t)$ 
     $\bar{\mathbf{x}}_0$  ←  $\frac{\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t} \bar{\epsilon}}{\sqrt{\bar{\alpha}_t}}$ 
     $\mathbf{x}_{t-1}$  ←  $\sqrt{\bar{\alpha}_{t-1}} \bar{\mathbf{x}}_0 + \sqrt{1 - \bar{\alpha}_{t-1}} \bar{\epsilon}$ 
end for
return  $\mathbf{x}_0$ 
```

---

Increasing  
Sub-sequence

$[1, \dots, T] \Rightarrow [\tau_0 = 0, \dots, \tau_S = T]$   
E.g.,  $\tau = [0, 10, 20, 30, \dots, 1000]$

---

**Algorithm** Fewer-Steps DDIM Sampling

---

```
xT ~  $\mathcal{N}(\mathbf{0}, \mathbf{I})$ 
for all s from S to 1 do
     $t \leftarrow \tau_s$ 
     $t' \leftarrow \tau_{s-1}$ 
     $\bar{\epsilon} \leftarrow \epsilon_{\theta}(\mathbf{x}_t, t)$ 
     $\bar{\mathbf{x}}_0$  ←  $\frac{\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t} \bar{\epsilon}}{\sqrt{\bar{\alpha}_t}}$ 
     $\mathbf{x}_{t'} \leftarrow \sqrt{\bar{\alpha}_{t'}} \bar{\mathbf{x}}_0 + \sqrt{1 - \bar{\alpha}_{t'}} \bar{\epsilon}$ 
end for
return  $\mathbf{x}_0$ 
```

---

# DDIM Results

Table 1: CIFAR10 and CelebA image generation measured in FID.  $\eta = 1.0$  and  $\hat{\sigma}$  are cases of DDPM (although Ho et al. (2020) only considered  $T = 1000$  steps, and  $S < T$  can be seen as simulating DDPMs trained with  $S$  steps), and  $\eta = 0.0$  indicates DDIM.

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

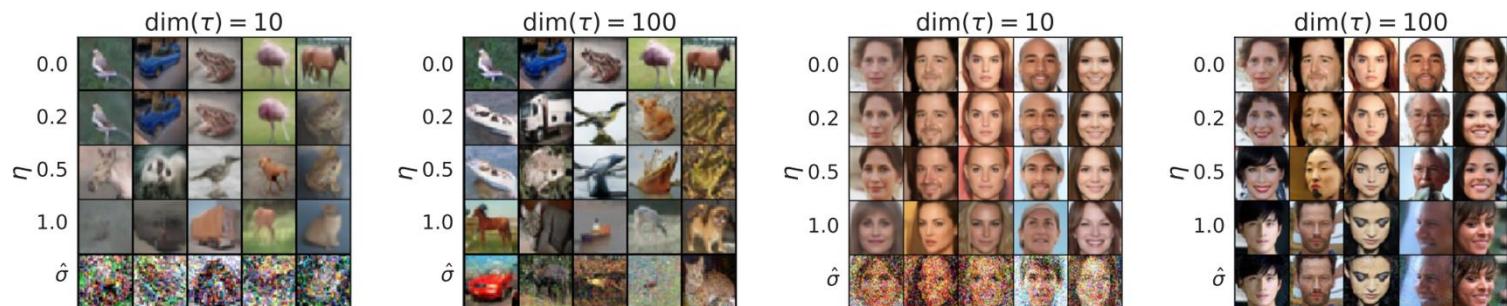


Figure 3: CIFAR10 and CelebA samples with  $\dim(\tau) = 10$  and  $\dim(\tau) = 100$ .

# Poll 4

DDIM differs from the DDPM inference process as:

- DDIM first predicts the noise given time t, then estimate x, and finally get  $x_{\{t-1\}}$ .
- DDIM first predicts the noise given time t, then get  $x_{\{t-1\}}$
- DDIM has a non-markov forward process
- DDIM has a markov forward process

# Poll 4

DDIM differs from the DDPM inference process as:

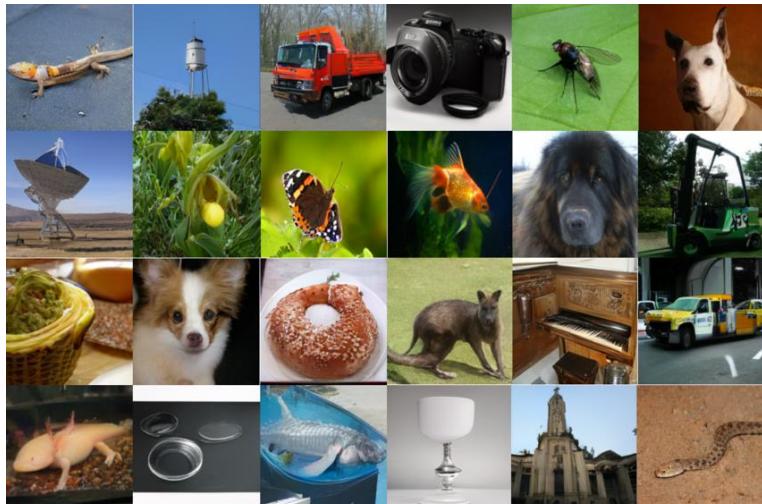
- DDIM first predicts the noise given time t, then estimate x, and finally get  $x_{\{t-1\}}$ .
- DDIM first predicts the noise given time t, then get  $x_{\{t-1\}}$
- **DDIM has a non-markov forward process**
- DDIM has a markov forward process

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# Conditional Diffusion Models

- Un-conditional
  - Conditional



$$p(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^T p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

- Conditional



$$p(\mathbf{x}_{0:T} \mid y) = p(\mathbf{x}_T) \prod_{t=1}^T p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t, y)$$

## More controllable!

# Conditional Score Matching

- Score matching with conditional information

$$\begin{aligned}\nabla \log p(\mathbf{x}_t | y) &= \nabla \log \left( \frac{p(\mathbf{x}_t)p(y | \mathbf{x}_t)}{p(y)} \right) \\ &= \nabla \log p(\mathbf{x}_t) + \nabla \log p(y | \mathbf{x}_t) - \nabla \log p(y) \\ &= \underbrace{\nabla \log p(\mathbf{x}_t)}_{\text{unconditional score}} + \underbrace{\nabla \log p(y | \mathbf{x}_t)}_{\text{adversarial gradient}}\end{aligned}$$

# Classifier Guidance

- Use a discriminative classifier for  $\nabla \log p(y | \mathbf{x}_t)$

$$\nabla \log p(\mathbf{x}_t | y) = \nabla \log p(\mathbf{x}_t) + \gamma \nabla \log p(y | \mathbf{x}_t)$$

- $\gamma$  controls the strength of the condition
- Limitations:
  - Need a separate classifier
  - Conditioning depends on the performance of classifier

# Classifier-Free Guidance

- Score matching with conditional information

$$\nabla \log p(\mathbf{x}_t | y) = \nabla \log p(\mathbf{x}_t) + \gamma \nabla \log p(y | \mathbf{x}_t)$$

$$\nabla \log p(y | \mathbf{x}_t) = \nabla \log p(\mathbf{x}_t | y) - \nabla \log p(\mathbf{x}_t)$$

- Classifier-free guidance

$$\begin{aligned}\nabla \log p(\mathbf{x}_t | y) &= \nabla \log p(\mathbf{x}_t) + \gamma (\nabla \log p(\mathbf{x}_t | y) - \nabla \log p(\mathbf{x}_t)) \\ &= \nabla \log p(\mathbf{x}_t) + \gamma \nabla \log p(\mathbf{x}_t | y) - \gamma \nabla \log p(\mathbf{x}_t) \\ &= \underbrace{\gamma \nabla \log p(\mathbf{x}_t | y)}_{\text{conditional score}} + \underbrace{(1 - \gamma) \nabla \log p(\mathbf{x}_t)}_{\text{unconditional score}}\end{aligned}$$

# Training of Classifier-Free Guidance

- For conditional embeddings
  - Randomly drop  $p$  original conditionals with an additional unconditional class

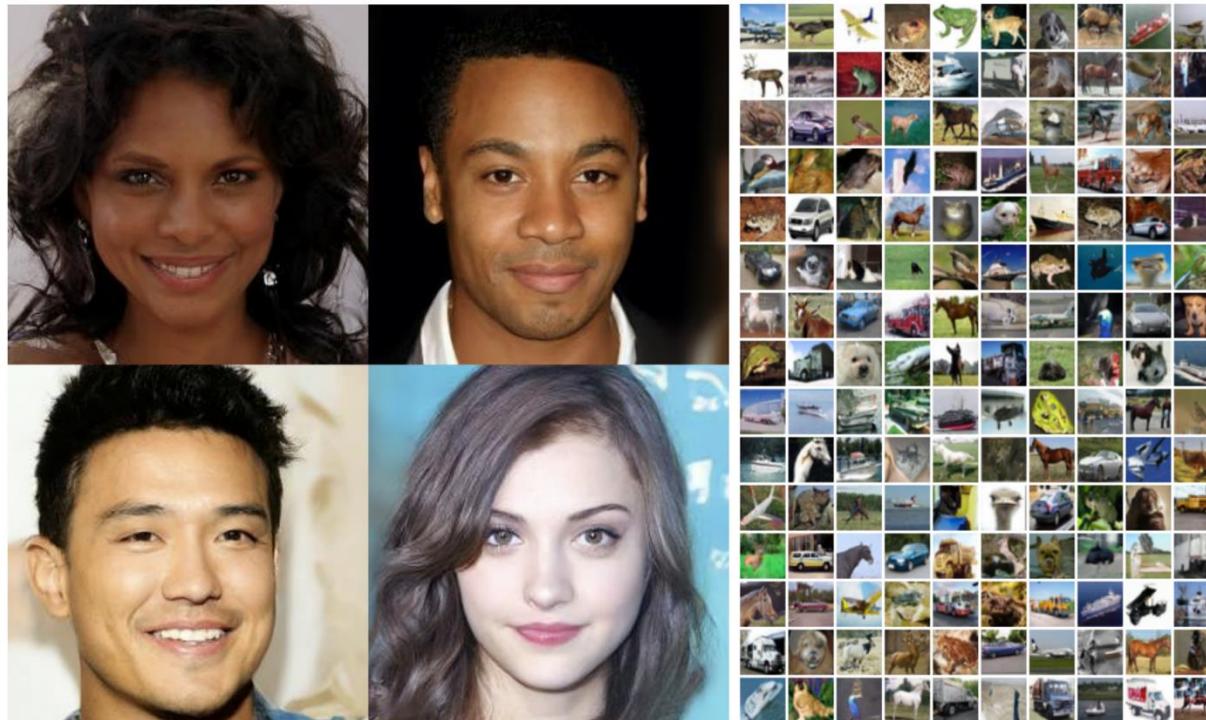
$$\mathbb{E}_{\mathcal{E}(x), y, \epsilon \sim \mathcal{N}(0,1), t} \left[ \|\epsilon - \epsilon_\theta(z_t, t, \tau_\theta(y))\|_2^2 \right]$$

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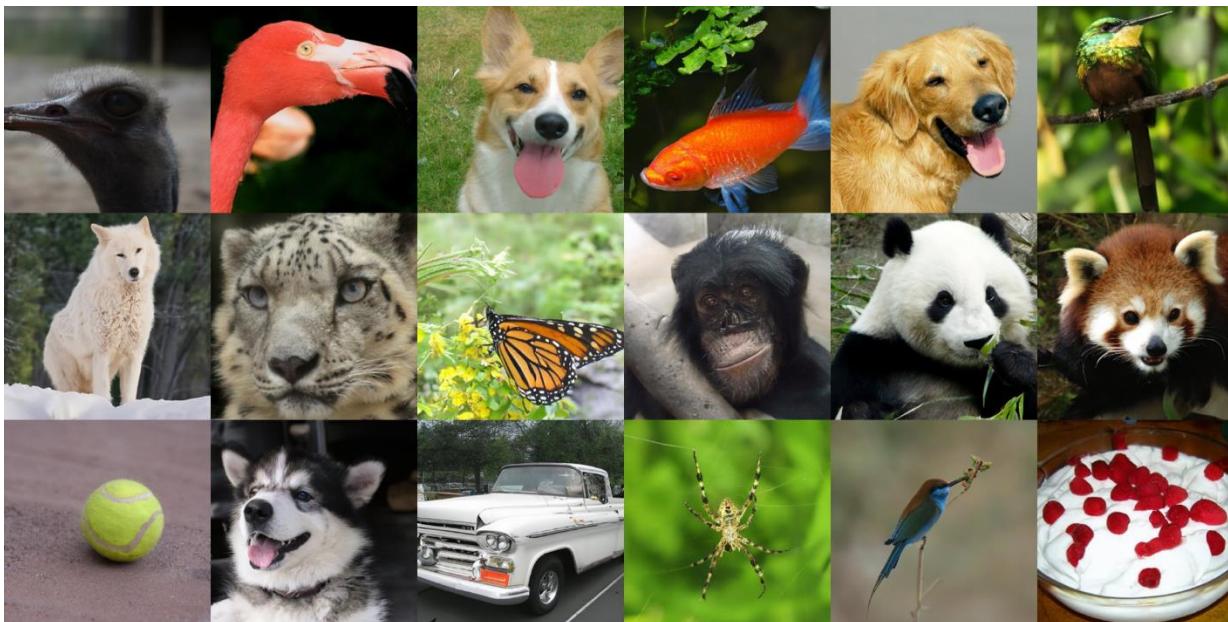
# DDPM

- Training diffusion models on raw images with a U-Net model



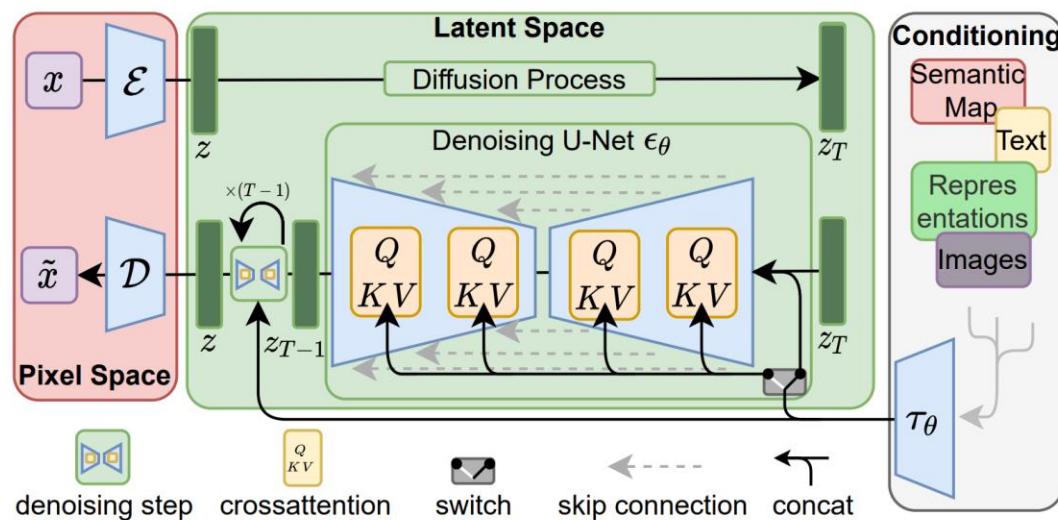
# Diffusion Models Beat GANs

- Larger denoising model with sophisticated design
  - Adaptive group normalization
  - Attention layers in U-Net



# Latent Diffusion Models (LDMs)

- Learn diffusion on VAE's latent
  - Yet another VAE! Except pre-trained.

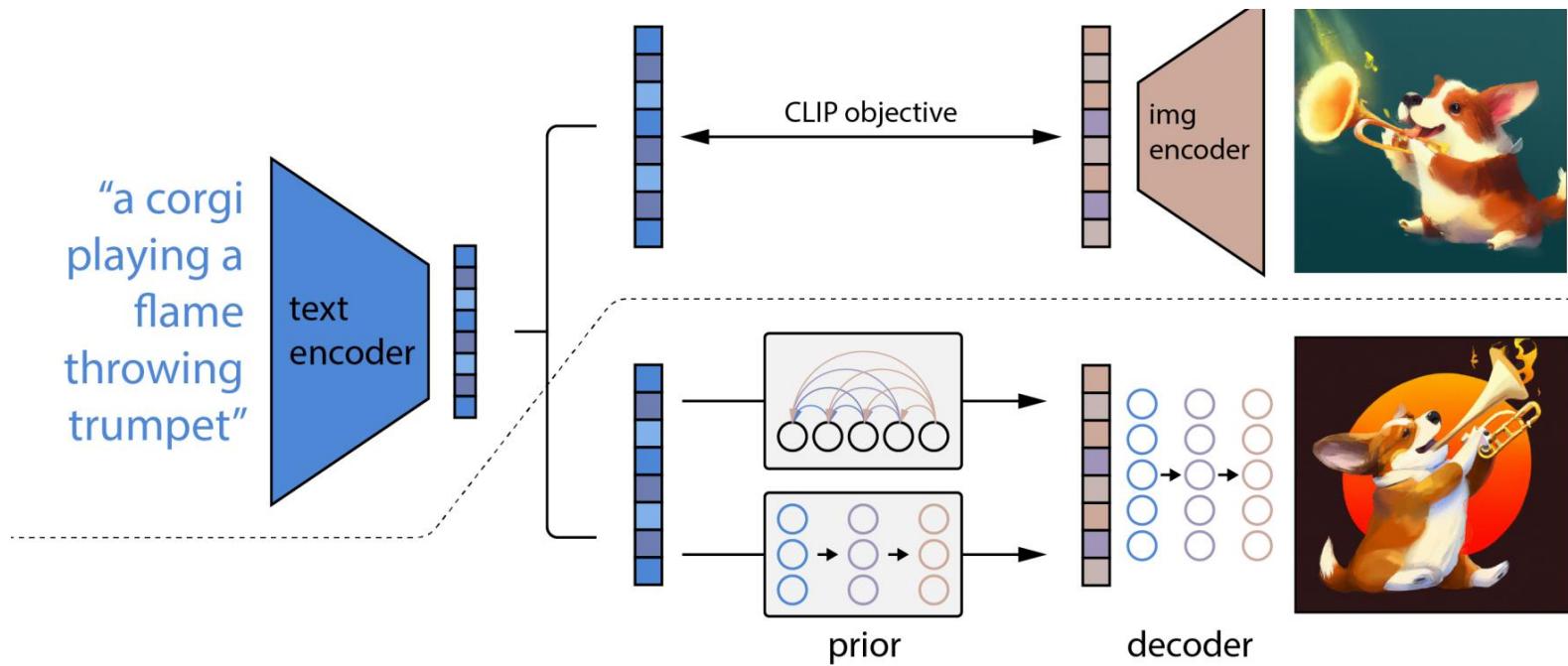


# Stable Diffusion

- Large-scale text-conditional LDMs
  - With VAEs trained also on larger datasets

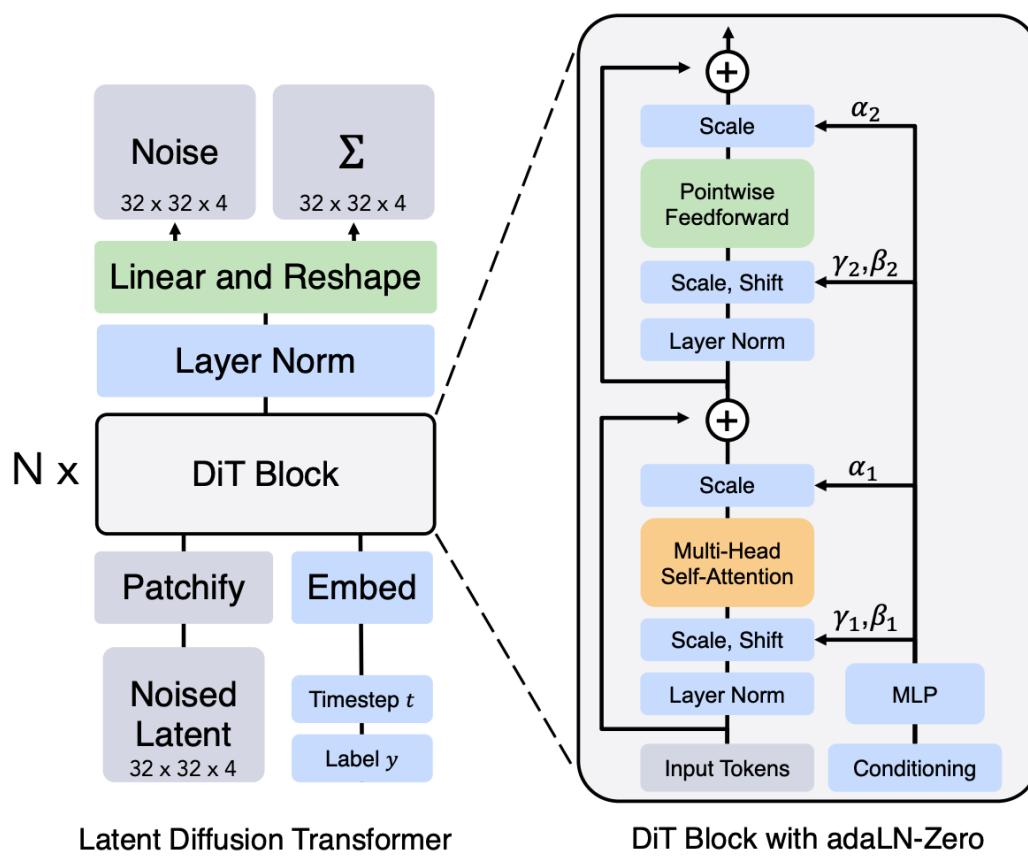


# DALLE



# DiT

- A transformer architecture for diffusion models



# MAR

- An autoregressive model with diffusion loss

