

# Deep Generative Models

## Lecture 9

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## Recap of Previous Lecture

Let us perturb the original data with Gaussian noise

$$q(\mathbf{x}_\sigma | \mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma^2 \cdot \mathbf{I}).$$

$$q(\mathbf{x}_\sigma) = \int q(\mathbf{x}_\sigma | \mathbf{x}) p_{\text{data}}(\mathbf{x}) d\mathbf{x}.$$

Then the solution of

$$\frac{1}{2} \mathbb{E}_{q(\mathbf{x}_\sigma)} \| \mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma) \|_2^2 \rightarrow \min_{\theta}$$

satisfies  $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) \approx \mathbf{s}_{\theta, 0}(\mathbf{x}_0) = \mathbf{s}_{\theta}(\mathbf{x})$  if  $\sigma$  is sufficiently small.

## Theorem (Denoising Score Matching)

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} \| \mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma) \|_2^2 &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma | \mathbf{x})} \| \mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma | \mathbf{x}) \|_2^2 + \text{const}(\theta) \end{aligned}$$

Here,  $\nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma | \mathbf{x}) = -\frac{\mathbf{x}_\sigma - \mathbf{x}}{\sigma^2} = -\frac{\epsilon}{\sigma}$ .

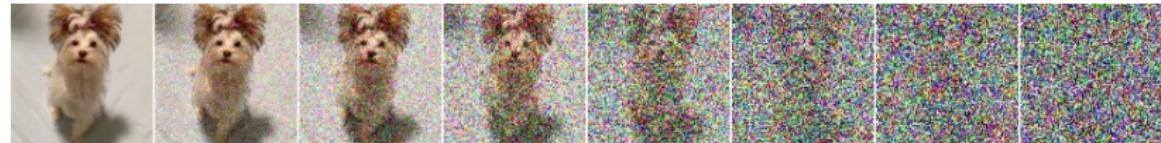
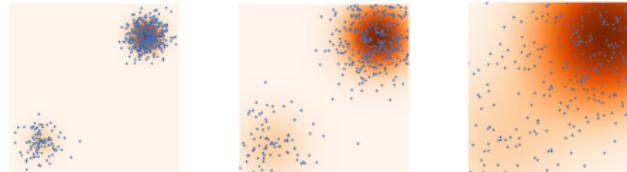
- ▶ We don't need to compute  $\nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)$  on the RHS.
- ▶  $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma)$  attempts to denoise a corrupted sample.

# Recap of Previous Lecture

## Noise-Conditioned Score Network

- ▶ Define a sequence of noise levels:  $\sigma_1 < \sigma_2 < \dots < \sigma_T$ .
- ▶ Train a denoised score function  $s_{\theta, \sigma_t}(\mathbf{x}_t)$  for each noise level:  
$$\sum_{t=1}^T \sigma_t^2 \cdot \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x})} \| s_{\theta, \sigma_t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}) \|_2^2 \rightarrow \min_{\theta}$$
- ▶ Sample using **annealed** Langevin dynamics (for  $t = 1, \dots, T$ ).

$$\sigma_1 < \sigma_2 < \sigma_3$$



# Recap of Previous Lecture

## NCSN Training

1. Obtain a sample  $\mathbf{x}_0 \sim p_{\text{data}}(\mathbf{x})$ .
2. Sample noise level  $t \sim U\{1, T\}$  and noise  $\epsilon \sim \mathcal{N}(0, \mathbf{I})$ .
3. Construct noisy image  $\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \epsilon$ .
4. Compute the loss  $\mathcal{L} = \sigma_t^2 \cdot \|\mathbf{s}_{\theta, \sigma_t}(\mathbf{x}_t) + \frac{\epsilon}{\sigma_t}\|^2$ .

## NCSN Sampling (Annealed Langevin Dynamics)

- ▶ Sample  $\mathbf{x}_0 \sim \mathcal{N}(0, \sigma_T^2 \cdot \mathbf{I}) \approx q(\mathbf{x}_T)$ .
- ▶ Apply  $L$  steps of Langevin dynamics:

$$\mathbf{x}_l = \mathbf{x}_{l-1} + \frac{\eta_t}{2} \cdot \mathbf{s}_{\theta, \sigma_t}(\mathbf{x}_{l-1}) + \sqrt{\eta_t} \cdot \epsilon_l.$$

- ▶ Update  $\mathbf{x}_0 := \mathbf{x}_L$  and proceed to the next  $\sigma_t$ .

# Recap of Previous Lecture

## Forward Gaussian Diffusion Process

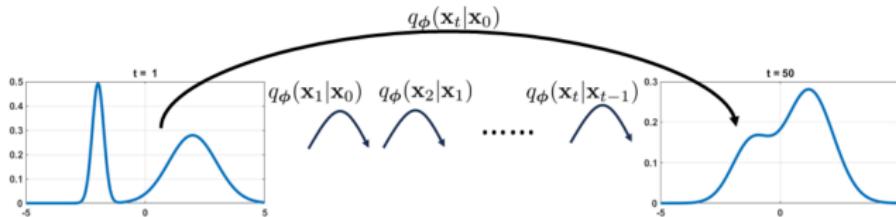
Let  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$ ,  $\beta_t \ll 1$ ,  $\alpha_t = 1 - \beta_t$  and  $\bar{\alpha}_t = \prod_{s=1}^t \alpha_s$ .

$$\mathbf{x}_t = \sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \boldsymbol{\epsilon}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I});$$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

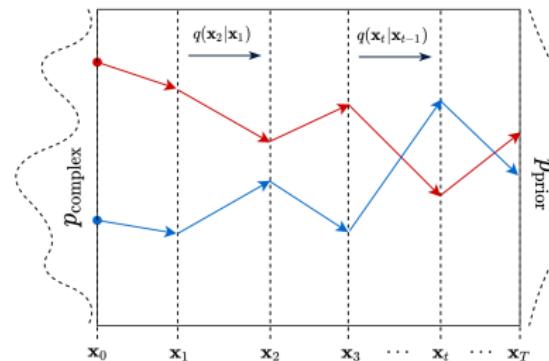
$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1}, \beta_t \cdot \mathbf{I});$$

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



# Recap of Previous Lecture

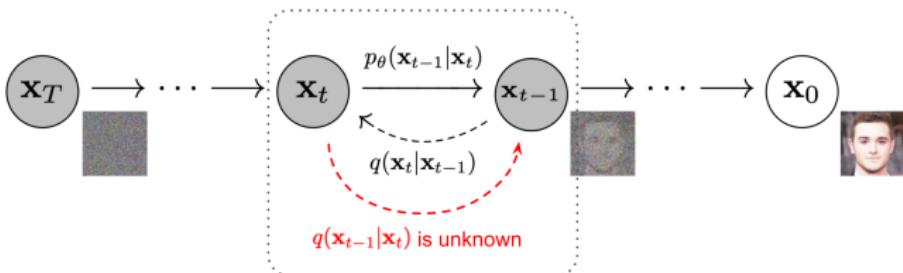
**Diffusion** describes the process where particles migrate from regions of high density to regions of low density.



1.  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x});$
2.  $\mathbf{x}_t = \sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \boldsymbol{\epsilon}, \text{ with } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}), t \geq 1;$
3.  $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I}), \text{ for } T \gg 1.$

If we can invert this process, we would have a way to sample  $\mathbf{x} \sim p_{\text{data}}(\mathbf{x})$  using noise samples, i.e.  $p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$ . Hence, our objective becomes to reverse this process.

# Recap of Previous Lecture



## Reverse Process (Ancestral Sampling)

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t) = \frac{q(\mathbf{x}_t | \mathbf{x}_{t-1}) q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)} \approx p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t) = \mathcal{N}(\mu_{\theta,t}(\mathbf{x}_t), \sigma_{\theta,t}^2(\mathbf{x}_t))$$

The Feller theorem guarantees this approximation is valid.

## Forward Process

1.  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x});$
2.  $\mathbf{x}_t = \sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \boldsymbol{\epsilon};$
3.  $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I}).$

## Reverse Process

1.  $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I});$
2.  $\mathbf{x}_{t-1} = \boldsymbol{\sigma}_{\theta,t}(\mathbf{x}_t) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t);$
3.  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x});$

# Outline

## 1. Denoising Diffusion Probabilistic Model (DDPM)

Gaussian Diffusion Model as VAE

ELBO Derivation

Reparametrization

Overview

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# Conditioned Reverse Distribution

Reverse Kernel (**Intractable**)

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t) = \frac{q(\mathbf{x}_t | \mathbf{x}_{t-1}) q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)}$$

# Conditioned Reverse Distribution

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Conditioned Reverse Kernel (**Tractable**)

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) = \frac{q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0) q(\mathbf{x}_{t-1} | \mathbf{x}_0)}{q(\mathbf{x}_t | \mathbf{x}_0)}$$

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Reverse Kernel (**Intractable**)

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Conditioned Reverse Kernel (**Tractable**)

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# Conditioned Reverse Distribution

## Reverse Kernel (**Intractable**)

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Here,

$$\begin{aligned} \tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) &= \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \cdot \mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t)}{1 - \bar{\alpha}_t} \cdot \mathbf{x}_0; \\ \tilde{\boldsymbol{\beta}}_t &= \frac{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} = \text{const.} \end{aligned}$$

## Distribution Summary

**Forward process** maps any distribution  $p_{\text{data}}(\mathbf{x})$  to  $\mathcal{N}(0, \mathbf{I})$  by injection of noise:

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

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**Reverse process** refers to an intractable distribution that can be approximated by a normal distribution (with unknown parameters) for small  $\beta_t$ :

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t) = \frac{q(\mathbf{x}_t | \mathbf{x}_{t-1}) q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)} \approx \mathcal{N}(\boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \boldsymbol{\sigma}_{\theta,t}^2(\mathbf{x}_t))$$

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**Conditioned reverse process** is a normal distribution with known parameters, describing how to denoise a noisy image  $\mathbf{x}_t$  when we know the clean image  $\mathbf{x}_0$ .

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

# Outline

## 1. Denoising Diffusion Probabilistic Model (DDPM)

Gaussian Diffusion Model as VAE

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# Gaussian Diffusion Model as VAE

Let's treat  $\mathbf{z} = (\mathbf{x}_1, \dots, \mathbf{x}_T)$  as a latent variable (**note:** each  $\mathbf{x}_t$  has the same dimension), and  $\mathbf{x} = \mathbf{x}_0$  as the observed variable.

## Latent Variable Model

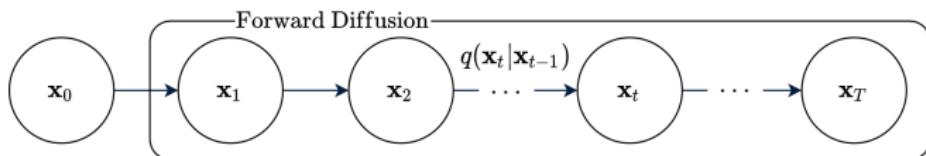
$$p_{\theta}(\mathbf{x}, \mathbf{z}) = p_{\theta}(\mathbf{x}|\mathbf{z})p_{\theta}(\mathbf{z})$$

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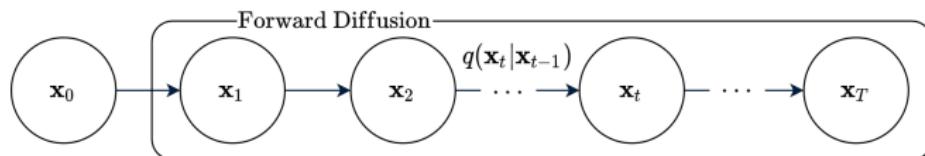


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## Latent Variable Model

$$p_{\theta}(\mathbf{x}, \mathbf{z}) = p_{\theta}(\mathbf{x}|\mathbf{z})p_{\theta}(\mathbf{z})$$



## Forward Diffusion

- ▶ Variational posterior distribution (encoder)

$$q(\mathbf{z}|\mathbf{x}) = q(\mathbf{x}_1, \dots, \mathbf{x}_T | \mathbf{x}_0) = \prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1}).$$

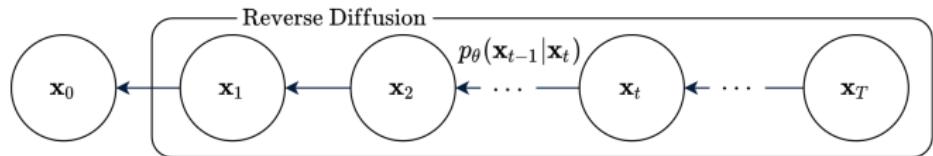
- ▶ **Note:** there are no learnable parameters.

# Gaussian Diffusion Model as VAE

$$p_{\theta}(\mathbf{x}, \mathbf{z}) = p_{\theta}(\mathbf{x}|\mathbf{z})p_{\theta}(\mathbf{z})$$

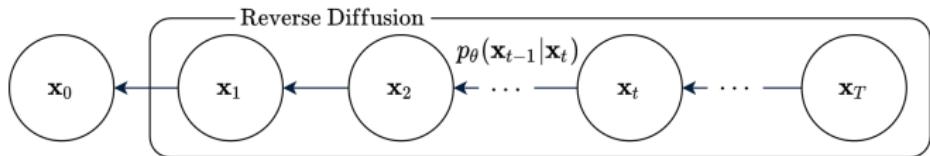
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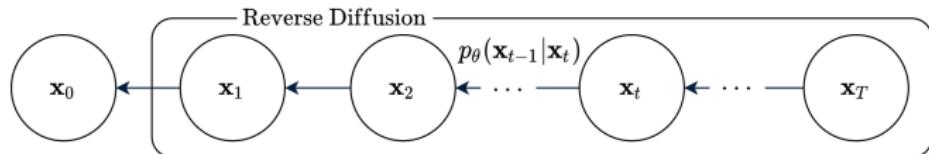
## Reverse Diffusion

- ▶ Generative distribution (decoder)

$$p_{\theta}(\mathbf{x}|\mathbf{z}) = p_{\theta}(\mathbf{x}_0|\mathbf{x}_1).$$

# Gaussian Diffusion Model as VAE

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## Reverse Diffusion

- ▶ Generative distribution (decoder)

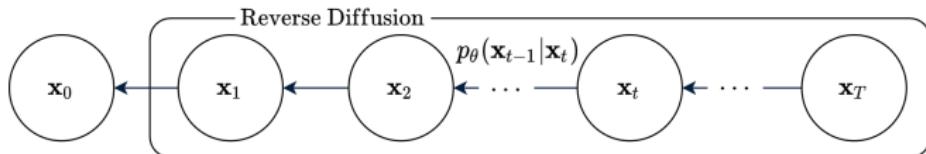
$$p_{\theta}(\mathbf{x}|\mathbf{z}) = p_{\theta}(\mathbf{x}_0|\mathbf{x}_1).$$

- ▶ Prior distribution

$$p_{\theta}(\mathbf{z}) = p_{\theta}(\mathbf{x}_1, \dots, \mathbf{x}_T) = \prod_{t=2}^T p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) \cdot p(\mathbf{x}_T).$$

# Gaussian Diffusion Model as VAE

$$p_{\theta}(\mathbf{x}, \mathbf{z}) = p_{\theta}(\mathbf{x}|\mathbf{z})p_{\theta}(\mathbf{z})$$



## Reverse Diffusion

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- ▶ Prior distribution

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**Note:** This differs from the vanilla VAE due to the complex decoder  $p_{\theta}(\mathbf{x}|\mathbf{z})$  and the standard normal prior  $p(\mathbf{z})$ .

# Outline

## 1. Denoising Diffusion Probabilistic Model (DDPM)

Gaussian Diffusion Model as VAE

**ELBO Derivation**

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# ELBO for Gaussian Diffusion Model

## Standard ELBO

$$\log p_{\theta}(\mathbf{x}) \geq \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\mathbf{x})} = \mathcal{L}_{\phi, \theta}(\mathbf{x}) \rightarrow \max_{q, \theta}$$

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## Derivation

$$\mathcal{L}_{\phi, \theta}(\mathbf{x}) = \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \log \frac{p_{\theta}(\mathbf{x}_0, \mathbf{x}_{1:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}$$

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## Derivation

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- ▶ Let's try to decompose the ELBO into individual KL divergence terms.
- ▶ We need to replace  $q(\mathbf{x}_t|\mathbf{x}_{t-1})$  with  $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$  in the denominator.
- ▶ Let's condition on  $\mathbf{x}_0$  to make the reverse  $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$  tractable.

## ELBO for Gaussian Diffusion Model

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0) = \frac{q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) q(\mathbf{x}_t | \mathbf{x}_0)}{q(\mathbf{x}_{t-1} | \mathbf{x}_0)}$$

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Derivation (continued)

$$\mathcal{L}_{\phi, \theta}(\mathbf{x}) = \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) \prod_{t=1}^T p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t)}{\prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1})}$$

## ELBO for Gaussian Diffusion Model

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Derivation (continued)

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# ELBO for Gaussian Diffusion Model

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0) = \frac{q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) q(\mathbf{x}_t | \mathbf{x}_0)}{q(\mathbf{x}_{t-1} | \mathbf{x}_0)}$$

Derivation (continued)

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) \prod_{t=1}^T p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t)}{\prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1})} \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) \prod_{t=1}^T p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t)}{\prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0)} \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) p_{\theta}(\mathbf{x}_0 | \mathbf{x}_1) \prod_{t=2}^T p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t)}{q(\mathbf{x}_1 | \mathbf{x}_0) \prod_{t=2}^T q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0)}\end{aligned}$$

# ELBO for Gaussian Diffusion Model

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0) = \frac{q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) q(\mathbf{x}_t | \mathbf{x}_0)}{q(\mathbf{x}_{t-1} | \mathbf{x}_0)}$$

Derivation (continued)

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)}{\prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1})} \\&= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)}{\prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0)} \\&= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) p_\theta(\mathbf{x}_0 | \mathbf{x}_1) \prod_{t=2}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)}{q(\mathbf{x}_1 | \mathbf{x}_0) \prod_{t=2}^T q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0)} \\&= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) p_\theta(\mathbf{x}_0 | \mathbf{x}_1) \prod_{t=2}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)}{q(\mathbf{x}_1 | \mathbf{x}_0) \prod_{t=2}^T \frac{q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) q(\mathbf{x}_t | \mathbf{x}_0)}{q(\mathbf{x}_{t-1} | \mathbf{x}_0)}}\end{aligned}$$

# ELBO for Gaussian Diffusion Model

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0) = \frac{q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) q(\mathbf{x}_t | \mathbf{x}_0)}{q(\mathbf{x}_{t-1} | \mathbf{x}_0)}$$

Derivation (continued)

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)}{\prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1})} \\&= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)}{\prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0)} \\&= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) p_\theta(\mathbf{x}_0 | \mathbf{x}_1) \prod_{t=2}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)}{q(\mathbf{x}_1 | \mathbf{x}_0) \prod_{t=2}^T q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0)} \\&= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) p_\theta(\mathbf{x}_0 | \mathbf{x}_1) \prod_{t=2}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)}{q(\mathbf{x}_1 | \mathbf{x}_0) \prod_{t=2}^T \frac{q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) q(\mathbf{x}_t | \mathbf{x}_0)}{q(\mathbf{x}_{t-1} | \mathbf{x}_0)}} \\&= \mathbb{E}_{q(\mathbf{x}_{1:T} | \mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) p_\theta(\mathbf{x}_0 | \mathbf{x}_1) \prod_{t=2}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)}{q(\mathbf{x}_T | \mathbf{x}_0) \prod_{t=2}^T q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0)}\end{aligned}$$

# ELBO for Gaussian Diffusion Model

## Derivation (continued)

$$\mathcal{L}_{\phi, \theta}(\mathbf{x}) = \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) \prod_{t=2}^T p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_T|\mathbf{x}_0) \prod_{t=2}^T q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)}$$

# ELBO for Gaussian Diffusion Model

## Derivation (continued)

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) \prod_{t=2}^T p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_T|\mathbf{x}_0) \prod_{t=2}^T q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} = \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[ \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) + \log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_0)} + \sum_{t=2}^T \log \left( \frac{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} \right) \right]\end{aligned}$$

# ELBO for Gaussian Diffusion Model

## Derivation (continued)

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) \prod_{t=2}^T p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_T|\mathbf{x}_0) \prod_{t=2}^T q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} = \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[ \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) + \log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_0)} + \sum_{t=2}^T \log \left( \frac{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} \right) \right] = \\ &= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) + \mathbb{E}_{q(\mathbf{x}_T|\mathbf{x}_0)} \log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_0)} + \\ &\quad + \sum_{t=2}^T \mathbb{E}_{q(\mathbf{x}_{t-1}, \mathbf{x}_t|\mathbf{x}_0)} \log \left( \frac{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} \right)\end{aligned}$$

# ELBO for Gaussian Diffusion Model

## Derivation (continued)

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \log \frac{p(\mathbf{x}_T) p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) \prod_{t=2}^T p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_T|\mathbf{x}_0) \prod_{t=2}^T q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} = \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[ \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) + \log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_0)} + \sum_{t=2}^T \log \left( \frac{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} \right) \right] = \\ &= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) + \mathbb{E}_{q(\mathbf{x}_T|\mathbf{x}_0)} \log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_0)} + \\ &\quad + \sum_{t=2}^T \mathbb{E}_{q(\mathbf{x}_{t-1}, \mathbf{x}_t|\mathbf{x}_0)} \log \left( \frac{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} \right) = \\ &= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0) \| p(\mathbf{x}_T)) - \\ &\quad - \sum_{t=2}^T \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \| p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{\mathcal{L}_t}\end{aligned}$$

# ELBO for Gaussian Diffusion Model

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) = & \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)) - \\ & - \sum_{t=2}^T \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{\mathcal{L}_t}\end{aligned}$$

# ELBO for Gaussian Diffusion Model

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) = & \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)) - \\ & - \sum_{t=2}^T \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{\mathcal{L}_t}\end{aligned}$$

- ▶ First term is the decoder distribution

$$\log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) = \log \mathcal{N}(\mathbf{x}_0|\mu_{\theta,t}(\mathbf{x}_1), \sigma_{\theta,t}^2(\mathbf{x}_1)),$$

with  $\mathbf{x}_1 \sim q(\mathbf{x}_1|\mathbf{x}_0)$ .

# ELBO for Gaussian Diffusion Model

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) = & \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)) - \\ & - \sum_{t=2}^T \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{\mathcal{L}_t}\end{aligned}$$

- ▶ First term is the decoder distribution

$$\log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) = \log \mathcal{N}(\mathbf{x}_0|\boldsymbol{\mu}_{\theta,t}(\mathbf{x}_1), \boldsymbol{\sigma}_{\theta,t}^2(\mathbf{x}_1)),$$

with  $\mathbf{x}_1 \sim q(\mathbf{x}_1|\mathbf{x}_0)$ .

- ▶ Second term is constant:

- ▶  $p(\mathbf{x}_T) = \mathcal{N}(0, \mathbf{I})$ ;
- ▶  $q(\mathbf{x}_T|\mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_T} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_T) \cdot \mathbf{I})$ .

# ELBO for Gaussian Diffusion Model

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) = & \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)) - \\ & - \sum_{t=2}^T \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{\mathcal{L}_t}\end{aligned}$$

- ▶ First term is the decoder distribution

$$\log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) = \log \mathcal{N}(\mathbf{x}_0|\boldsymbol{\mu}_{\theta,t}(\mathbf{x}_1), \boldsymbol{\sigma}_{\theta,t}^2(\mathbf{x}_1)),$$

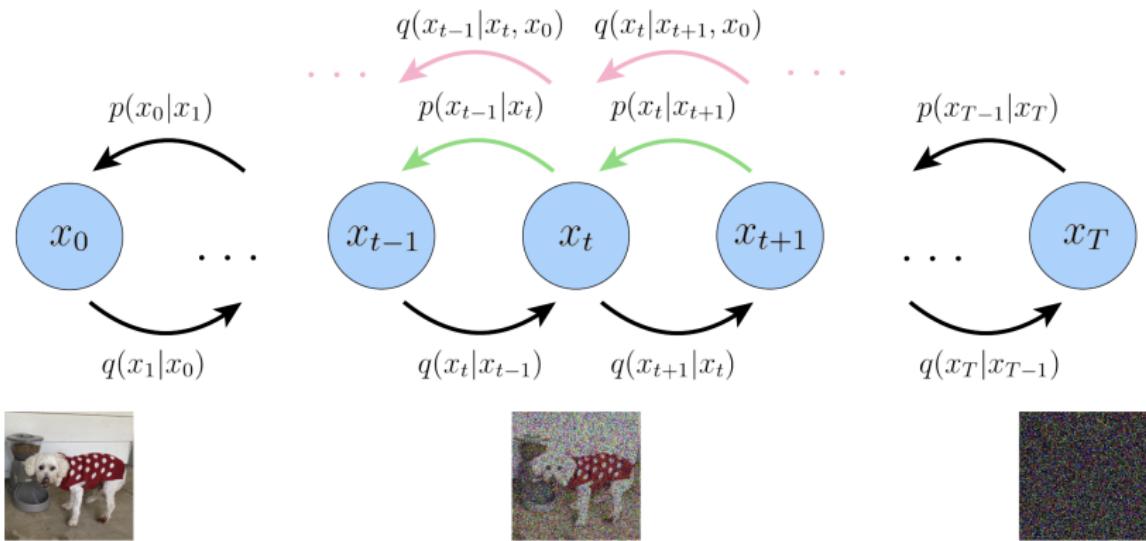
with  $\mathbf{x}_1 \sim q(\mathbf{x}_1|\mathbf{x}_0)$ .

- ▶ Second term is constant:

- ▶  $p(\mathbf{x}_T) = \mathcal{N}(0, \mathbf{I})$ ;
- ▶  $q(\mathbf{x}_T|\mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_T} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_T) \cdot \mathbf{I})$ .

- ▶ Third term is the main contributor to the ELBO.

# ELBO for Gaussian Diffusion Model



$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \| p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))$$

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

$$p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1} | \boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \boldsymbol{\sigma}_{\theta,t}^2(\mathbf{x}_t))$$

## ELBO for Gaussian Diffusion Model

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \| p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))$$

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

$$p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1} | \boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \boldsymbol{\sigma}_{\theta,t}^2(\mathbf{x}_t))$$

## ELBO for Gaussian Diffusion Model

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \| p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))$$

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

$$p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1} | \boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \boldsymbol{\sigma}_{\theta,t}^2(\mathbf{x}_t))$$

Let's assume that

$$\boldsymbol{\sigma}_{\theta,t}^2(\mathbf{x}_t) = \tilde{\beta}_t \mathbf{I} \quad \Rightarrow \quad p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1} | \boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \tilde{\beta}_t \mathbf{I}).$$

## ELBO for Gaussian Diffusion Model

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \| p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))$$

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

$$p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1} | \boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \boldsymbol{\sigma}_{\theta,t}^2(\mathbf{x}_t))$$

Let's assume that

$$\boldsymbol{\sigma}_{\theta,t}^2(\mathbf{x}_t) = \tilde{\beta}_t \mathbf{I} \quad \Rightarrow \quad p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1} | \boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \tilde{\beta}_t \mathbf{I}).$$

Theoretically, the optimal  $\boldsymbol{\sigma}_{\theta,t}^2(\mathbf{x}_t)$  lies in  $[\tilde{\beta}_t, \beta_t]$ :

- ▶  $\beta_t$  is optimal for  $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$ ;
- ▶  $\tilde{\beta}_t$  is optimal for  $\mathbf{x}_0 \sim \delta(\mathbf{x}_0 - \mathbf{x}^*)$ .

## ELBO for Gaussian Diffusion Model

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}\left(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \| p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)\right)$$

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

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

Let's assume that

$$\sigma_{\theta,t}^2(\mathbf{x}_t) = \tilde{\beta}_t \mathbf{I} \quad \Rightarrow \quad p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1} | \mu_{\theta,t}(\mathbf{x}_t), \tilde{\beta}_t \mathbf{I}).$$

Theoretically, the optimal  $\sigma_{\theta,t}^2(\mathbf{x}_t)$  lies in  $[\tilde{\beta}_t, \beta_t]$ :

- ▶  $\beta_t$  is optimal for  $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$ ;
- ▶  $\tilde{\beta}_t$  is optimal for  $\mathbf{x}_0 \sim \delta(\mathbf{x}_0 - \mathbf{x}^*)$ .

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}\left(\mathcal{N}(\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}) \| \mathcal{N}(\mu_{\theta,t}(\mathbf{x}_t), \tilde{\beta}_t \mathbf{I})\right)$$

## ELBO for Gaussian Diffusion Model

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \| p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))$$

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

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

Let's assume that

$$\sigma_{\theta,t}^2(\mathbf{x}_t) = \tilde{\beta}_t \mathbf{I} \quad \Rightarrow \quad p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1} | \mu_{\theta,t}(\mathbf{x}_t), \tilde{\beta}_t \mathbf{I}).$$

Theoretically, the optimal  $\sigma_{\theta,t}^2(\mathbf{x}_t)$  lies in  $[\tilde{\beta}_t, \beta_t]$ :

- ▶  $\beta_t$  is optimal for  $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$ ;
- ▶  $\tilde{\beta}_t$  is optimal for  $\mathbf{x}_0 \sim \delta(\mathbf{x}_0 - \mathbf{x}^*)$ .

$$\begin{aligned}\mathcal{L}_t &= \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}\left(\mathcal{N}(\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}) \| \mathcal{N}(\mu_{\theta,t}(\mathbf{x}_t), \tilde{\beta}_t \mathbf{I})\right) \\ &= \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t)\|^2 \right]\end{aligned}$$

# ELBO for Gaussian Diffusion Model

## Training

1. Obtain a sample  $\mathbf{x}_0 \sim p_{\text{data}}(\mathbf{x})$ .
2. Generate a noisy image  $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$ , with  $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$ .
3. Compute the ELBO

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)) - \\ &\quad - \underbrace{\sum_{t=2}^T \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta, t}(\mathbf{x}_t)\|^2 \right]}_{\mathcal{L}_t}\end{aligned}$$

# ELBO for Gaussian Diffusion Model

## Training

1. Obtain a sample  $\mathbf{x}_0 \sim p_{\text{data}}(\mathbf{x})$ .
2. Generate a noisy image  $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$ , with  $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$ .
3. Compute the ELBO

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_1 | \mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0 | \mathbf{x}_1) - \text{KL}(q(\mathbf{x}_T | \mathbf{x}_0) \| p(\mathbf{x}_T)) - \\ &\quad - \underbrace{\sum_{t=2}^T \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta, t}(\mathbf{x}_t)\|^2 \right]}_{\mathcal{L}_t}\end{aligned}$$

## Sampling

1. Sample  $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$ .
2. Denoise:  $\mathbf{x}_{t-1} = \mu_{\theta, t}(\mathbf{x}_t) + \sqrt{\tilde{\beta}_t} \cdot \boldsymbol{\epsilon}$ ,  $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$ .

# Outline

## 1. Denoising Diffusion Probabilistic Model (DDPM)

Gaussian Diffusion Model as VAE

ELBO Derivation

Reparametrization

Overview

# Reparametrization of DDPM

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \cdot \mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t)}{1 - \bar{\alpha}_t} \cdot \mathbf{x}_0$$

# Reparametrization of DDPM

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \cdot \mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t)}{1 - \bar{\alpha}_t} \cdot \mathbf{x}_0$$

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

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- ▶ There is a linear relationship between  $\boldsymbol{\epsilon}$ ,  $\mathbf{x}_t$ , and  $\mathbf{x}_0$ .
- ▶ Let's try to rewrite this mean using only  $\mathbf{x}_t$  and  $\boldsymbol{\epsilon}$ .

# Reparametrization of DDPM

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \cdot \mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t)}{1 - \bar{\alpha}_t} \cdot \mathbf{x}_0$$

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$$\tilde{\mu}_t(\mathbf{x}_t, \boldsymbol{\epsilon}) = \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \cdot \mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t)}{1 - \bar{\alpha}_t} \cdot \left( \frac{\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}}{\sqrt{\bar{\alpha}_t}} \right)$$

# Reparametrization of DDPM

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

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- ▶ There is a linear relationship between  $\epsilon$ ,  $\mathbf{x}_t$ , and  $\mathbf{x}_0$ .
- ▶ Let's try to rewrite this mean using only  $\mathbf{x}_t$  and  $\epsilon$ .

$$\begin{aligned}\tilde{\mu}_t(\mathbf{x}_t, \epsilon) &= \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \cdot \mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t)}{1 - \bar{\alpha}_t} \cdot \left( \frac{\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t} \cdot \epsilon}{\sqrt{\bar{\alpha}_t}} \right) \\ &= \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \epsilon\end{aligned}$$

# Reparametrization of DDPM

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

## Reparametrization

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \boldsymbol{\epsilon}$$

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$$\mu_{\theta,t}(\mathbf{x}_t) = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \boldsymbol{\epsilon}_{\theta,t}(\mathbf{x}_t)$$

# Reparametrization of DDPM

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

## Reparametrization

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

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$$\mathcal{L}_t = \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[ \frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \|\epsilon - \epsilon_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

# Reparametrization of DDPM

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \left\| \tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t) \right\|^2 \right]$$

## Reparametrization

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \boldsymbol{\epsilon}$$

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$$= \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})} \left[ \frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \left\| \boldsymbol{\epsilon} - \epsilon_{\theta,t}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}) \right\|^2 \right]$$

# Reparametrization of DDPM

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[ \frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

## Reparametrization

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

$$\mu_{\theta,t}(\mathbf{x}_t) = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \epsilon_{\theta,t}(\mathbf{x}_t)$$

$$\mathcal{L}_t = \mathbb{E}_{\epsilon \sim \mathcal{N}(0, I)} \left[ \frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \|\epsilon - \epsilon_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

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

At every step of the reverse process, we attempt to predict the noise  $\epsilon$  that was used in the forward diffusion process!

# Reparametrization of DDPM

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) = & \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)) - \\ & - \sum_{t=2}^T \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{\mathcal{L}_t}\end{aligned}$$

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$$\mathcal{L}_t = \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[ \frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \left\| \epsilon - \epsilon_{\theta, t}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon) \right\|^2 \right]$$

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$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)) - \\ &\quad - \sum_{t=2}^T \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{\mathcal{L}_t} \\ \mathcal{L}_t &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[ \frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \left\| \epsilon - \epsilon_{\theta, t}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon) \right\|^2 \right]\end{aligned}$$

Let's drop the scaling coefficient.

## Simplified Objective

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

# Outline

## 1. Denoising Diffusion Probabilistic Model (DDPM)

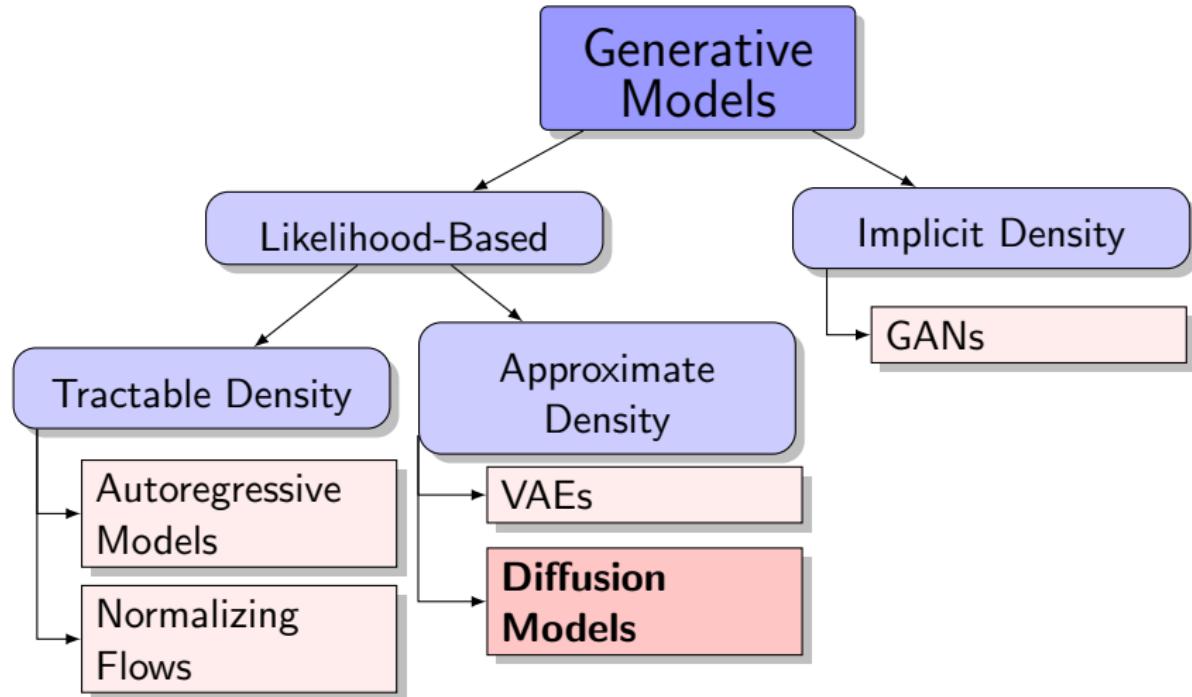
Gaussian Diffusion Model as VAE

ELBO Derivation

Reparametrization

Overview

# Generative Models Zoo



# Denoising Diffusion Probabilistic Model (DDPM)

## DDPM is a VAE Model

- ▶ The encoder is a fixed Gaussian Markov chain  $q(\mathbf{x}_1, \dots, \mathbf{x}_T | \mathbf{x}_0)$ .
- ▶ The latent variable is hierarchical (at each step, its dimension equals the input's).
- ▶ The decoder is a simple Gaussian model  $p_\theta(\mathbf{x}_0 | \mathbf{x}_1)$ .
- ▶ The prior distribution is given by a parametric Gaussian Markov chain  $p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)$ .

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## Forward Process

1.  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$ ;
2.  $\mathbf{x}_t = \sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \boldsymbol{\epsilon}$ ;
3.  $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$ .

# Denoising Diffusion Probabilistic Model (DDPM)

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### Reverse Process

1.  $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$ ;
2.  $\mathbf{x}_{t-1} = \sigma_{\theta, t}(\mathbf{x}_t) \cdot \boldsymbol{\epsilon} + \mu_{\theta, t}(\mathbf{x}_t)$ ;
3.  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$ ;

# Denoising Diffusion Probabilistic Model (DDPM)

## Training

1. Obtain a sample  $\mathbf{x}_0 \sim p_{\text{data}}(\mathbf{x})$ .
2. Sample time index  $t \sim U\{1, T\}$  and noise  $\epsilon \sim \mathcal{N}(0, \mathbf{I})$ .
3. Generate noisy image  $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \epsilon$ .
4. Compute the loss  $\mathcal{L}_{\text{simple}} = \|\epsilon - \epsilon_{\theta, t}(\mathbf{x}_t)\|^2$ .

# Denoising Diffusion Probabilistic Model (DDPM)

## Training

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## Sampling (Ancestral Sampling)

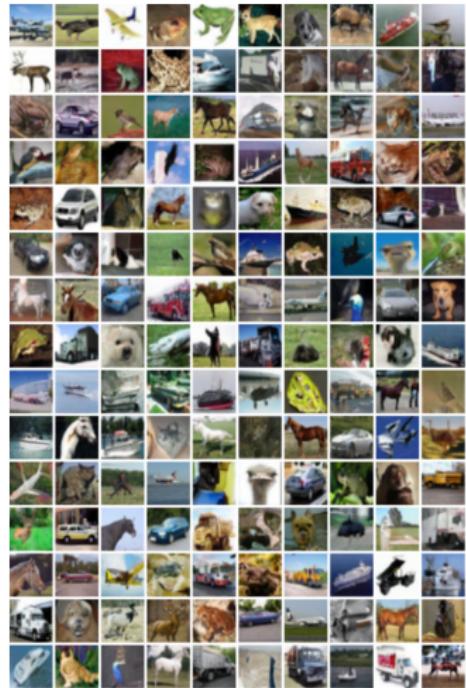
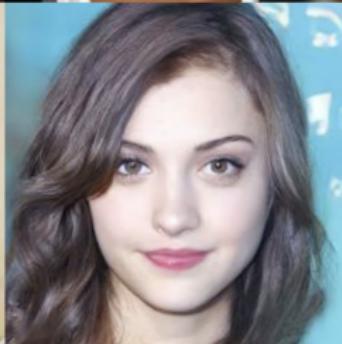
1. Sample  $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$ .
2. Compute the mean of  $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t) = \mathcal{N}(\boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \tilde{\beta}_t \cdot \mathbf{I})$ :

$$\boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t) = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \epsilon_{\theta,t}(\mathbf{x}_t)$$

3. Denoise:  $\mathbf{x}_{t-1} = \boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t) + \sqrt{\tilde{\beta}_t} \cdot \epsilon, \epsilon \sim \mathcal{N}(0, \mathbf{I})$ .

# Denoising Diffusion Probabilistic Model (DDPM)

## Samples



## Summary

- ▶ DDPM approximates the reverse process using normality assumptions.
- ▶ DDPM can be interpreted as a VAE with a hierarchy of latent variables.
- ▶ The ELBO for DDPM may be formulated as a sum over many KL divergence terms.
- ▶ At each step, DDPM predicts the noise that was injected in the forward process.
- ▶ DDPM is a VAE model that tries to invert the forward diffusion process via variational inference.
- ▶ DDPMs are quite slow, since the model must be applied  $T$  times for sampling.