

Deep Generative Models

Lecture 9

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Recap of Previous Lecture

Let us perturb the original data with Gaussian noise

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

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

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 σ is sufficiently small.

Theorem (Denoising Score Matching)

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

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

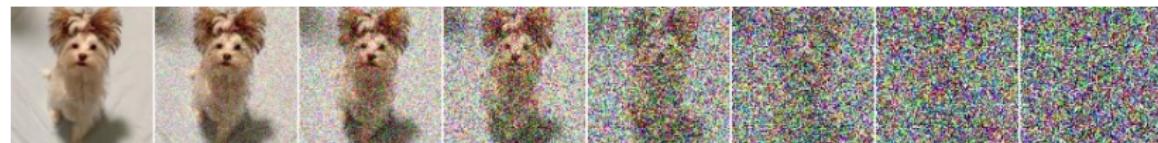
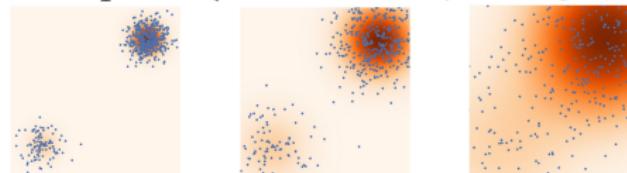
Noise-Conditioned Score Network

- ▶ 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:

$$\sum_{t=1}^T \sigma_t^2 \cdot \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x})} \| s_{\theta, \sigma_t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}) \|_2^2 \rightarrow \min_{\theta}$$

- ▶ 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 $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
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 σ_t .

Recap of Previous Lecture

Forward Gaussian Diffusion Process

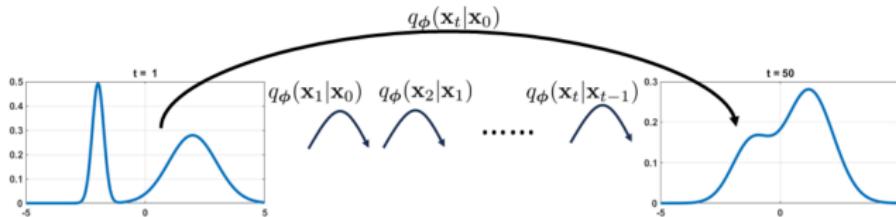
Let $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$, $\beta_t \ll 1$, $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{s=1}^t \alpha_s$.

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

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

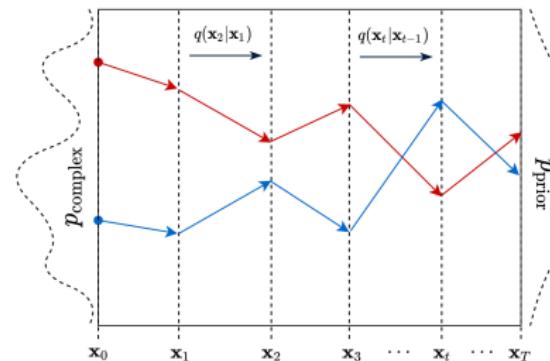
$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1}, \beta_t \cdot \mathbf{I});$$

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



Recap of Previous Lecture

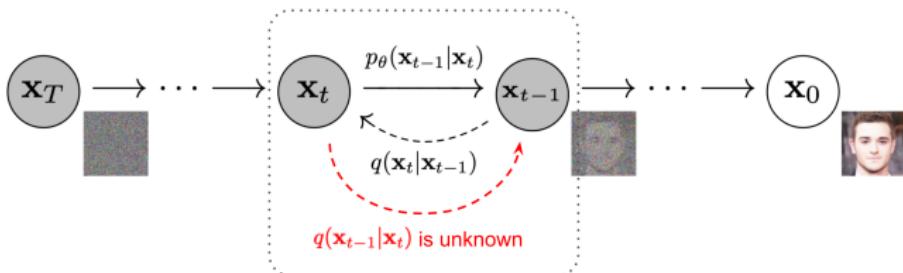
Diffusion describes the process where particles migrate from regions of high density to regions of low density.



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

If we can invert this process, we would have a way to sample $\mathbf{x} \sim \pi(\mathbf{x})$ 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)

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

The Feller theorem guarantees this approximation is valid.

Forward Process

1. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$
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. $\mathbf{x}_{t-1} = \boldsymbol{\sigma}_{\boldsymbol{\theta},t}(\mathbf{x}_t) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t);$
3. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$

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

Reverse Kernel (**Intractable**)

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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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Conditioned Reverse Kernel (**Tractable**)

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Conditioned Reverse Distribution

Reverse Kernel (**Intractable**)

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Conditioned Reverse Kernel (**Tractable**)

$$\begin{aligned} q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) &= \frac{q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{x}_0) q(\mathbf{x}_{t-1} | \mathbf{x}_0)}{q(\mathbf{x}_t | \mathbf{x}_0)} \\ &= \frac{\mathcal{N}(\sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1}, \beta_t \mathbf{I}) \cdot \mathcal{N}(\sqrt{\bar{\alpha}_{t-1}} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_{t-1}) \cdot \mathbf{I})}{\mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_t) \cdot \mathbf{I})} \\ &= \mathcal{N}(\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\boldsymbol{\beta}}_t \cdot \mathbf{I}) \end{aligned}$$

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 $\pi(\mathbf{x})$ 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 β_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

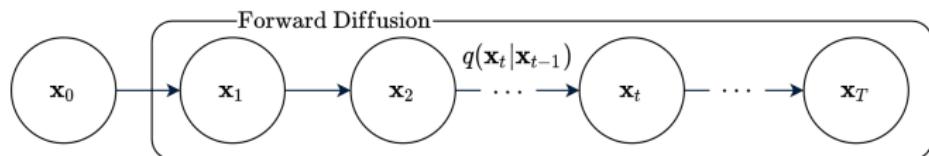
$$p(\mathbf{x}, \mathbf{z} | \theta) = p(\mathbf{x} | \mathbf{z}, \theta)p(\mathbf{z} | \theta)$$

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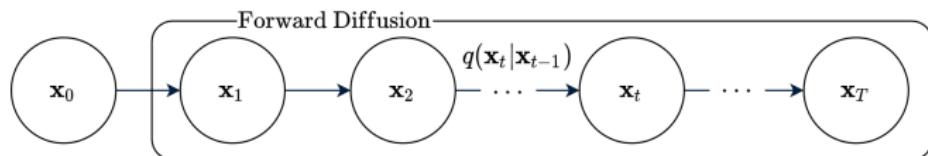


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Latent Variable Model

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



Forward Diffusion

- ▶ Variational posterior distribution (encoder)

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

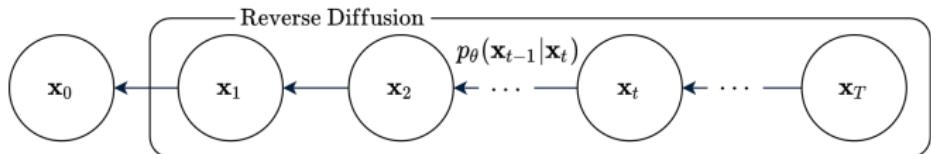
- ▶ **Note:** there are no learnable parameters.

Gaussian Diffusion Model as VAE

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

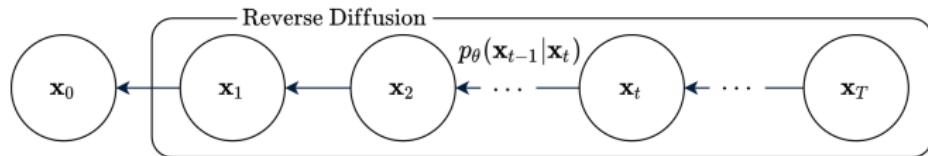
Gaussian Diffusion Model as VAE

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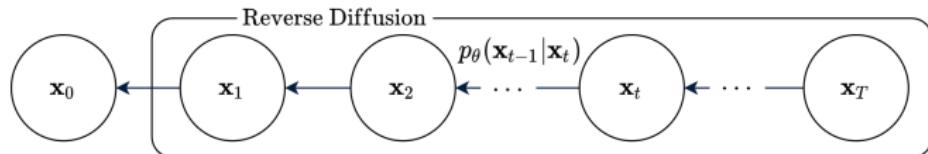
Reverse Diffusion

- ▶ Generative distribution (decoder)

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

Gaussian Diffusion Model as VAE

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



Reverse Diffusion

- ▶ Generative distribution (decoder)

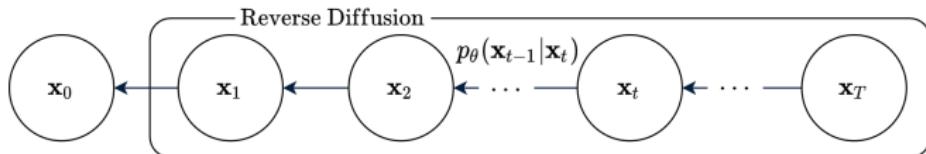
$$p(\mathbf{x} | \mathbf{z}, \theta) = p(\mathbf{x}_0 | \mathbf{x}_1, \theta).$$

- ▶ Prior distribution

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

Gaussian Diffusion Model as VAE

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



Reverse Diffusion

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- ▶ Prior distribution

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

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

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ELBO for Gaussian Diffusion Model

Standard ELBO

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

ELBO for Gaussian Diffusion Model

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Derivation

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

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ELBO for Gaussian Diffusion Model

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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)

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

ELBO for Gaussian Diffusion Model

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Derivation (continued)

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

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)

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

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)

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

ELBO for Gaussian Diffusion Model

Derivation (continued)

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

ELBO for Gaussian Diffusion Model

Derivation (continued)

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

ELBO for Gaussian Diffusion Model

Derivation (continued)

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

ELBO for Gaussian Diffusion Model

Derivation (continued)

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

ELBO for Gaussian Diffusion Model

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

ELBO for Gaussian Diffusion Model

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

- ▶ First term is the decoder distribution

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

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

ELBO for Gaussian Diffusion Model

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

- ▶ First term is the decoder distribution

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

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

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

- ▶ First term is the decoder distribution

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

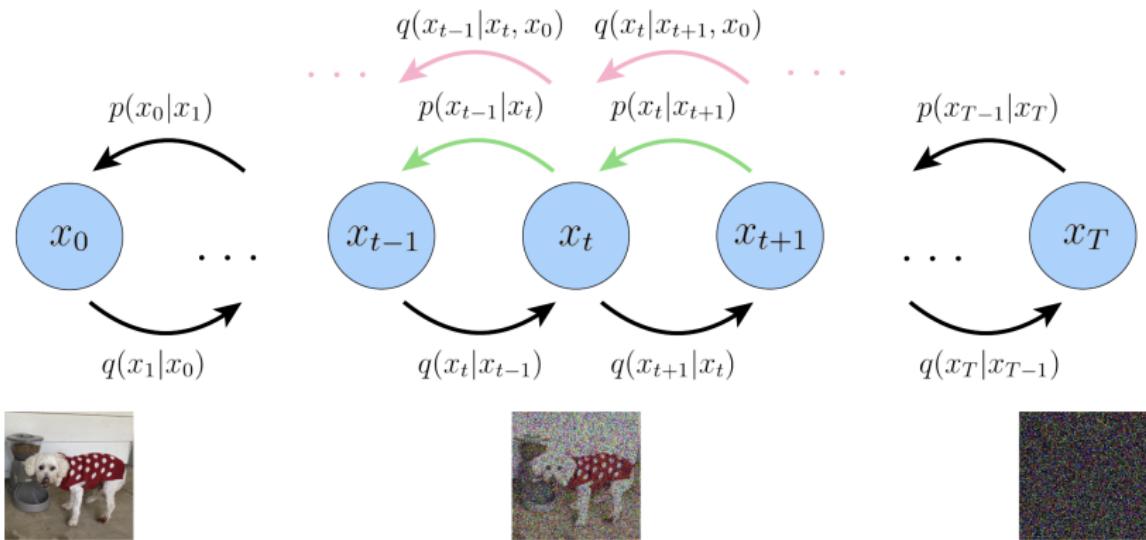
with $\mathbf{x}_1 \sim q(\mathbf{x}_1|\mathbf{x}_0)$.

- ▶ 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



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

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

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

ELBO for Gaussian Diffusion Model

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

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

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

ELBO for Gaussian Diffusion Model

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

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

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

Let's assume that

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

ELBO for Gaussian Diffusion Model

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

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

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

Let's assume that

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

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

- ▶ β_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

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

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

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

Let's assume that

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

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

- ▶ β_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

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

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

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

Let's assume that

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

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

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

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

ELBO for Gaussian Diffusion Model

Training

1. Obtain a sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
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

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

ELBO for Gaussian Diffusion Model

Training

1. Obtain a sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
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 $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
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$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p(\mathbf{x}_0|\mathbf{x}_1, \theta) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)) - \\ &\quad - \underbrace{\sum_{t=2}^T \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[\frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta, t}(\mathbf{x}_t)\|^2 \right]}_{\mathcal{L}_t}\end{aligned}$$

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

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

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

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

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

Reparametrization of DDPM

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

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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

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

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- ▶ Let's try to rewrite this mean using only \mathbf{x}_t and $\boldsymbol{\epsilon}$.

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

Reparametrization of DDPM

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

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

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

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

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

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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Reparametrization

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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

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Reparametrization

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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

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Reparametrization

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

Reparametrization of DDPM

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

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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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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)

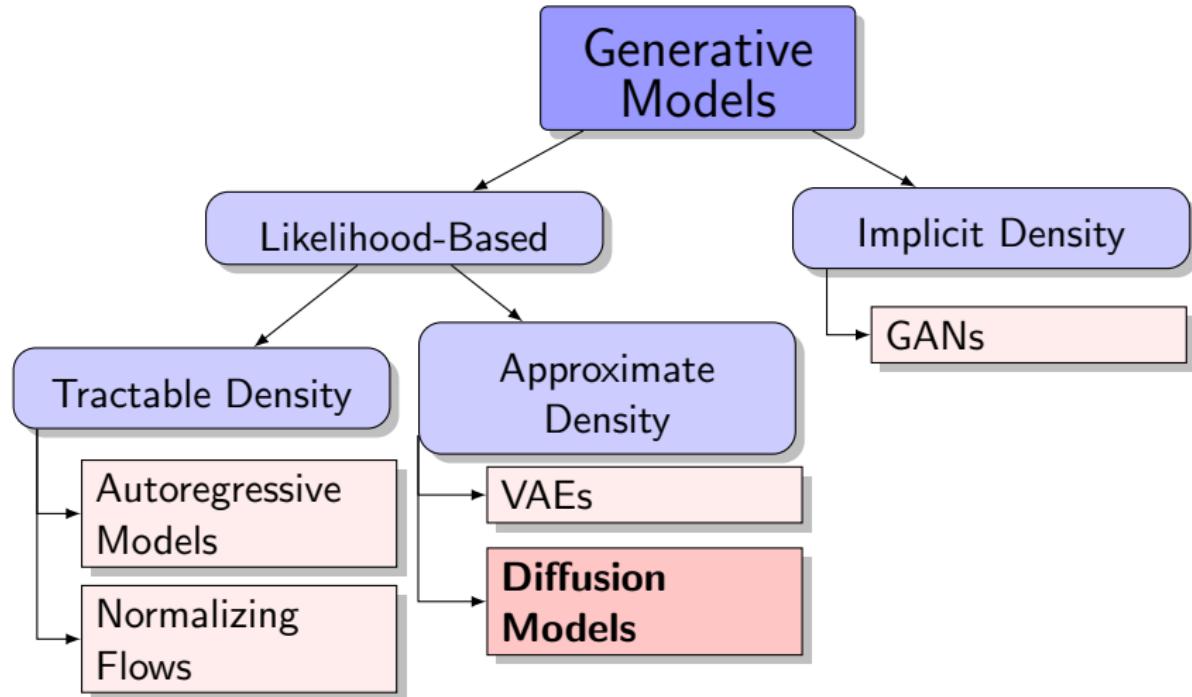
Gaussian Diffusion Model as VAE

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 $p(\mathbf{x}_0 | \mathbf{x}_1, \theta)$.
- ▶ The prior distribution is given by a parametric Gaussian Markov chain $p(\mathbf{x}_{t-1} | \mathbf{x}_t, \theta)$.

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Forward Process

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

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Reverse Process

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

Denoising Diffusion Probabilistic Model (DDPM)

Training

1. Obtain a sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
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)

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Sampling (Ancestral Sampling)

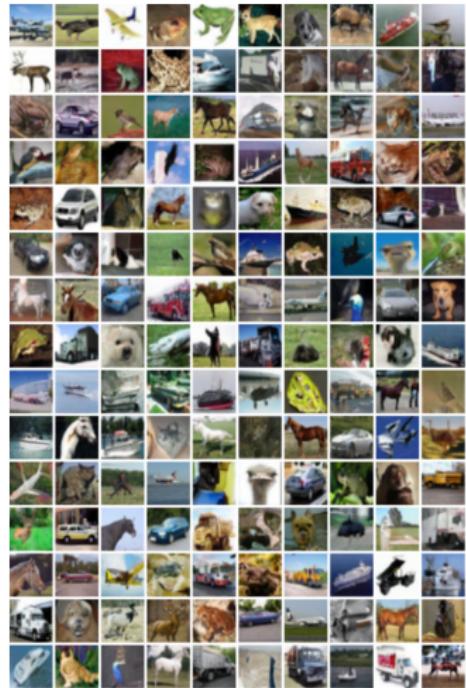
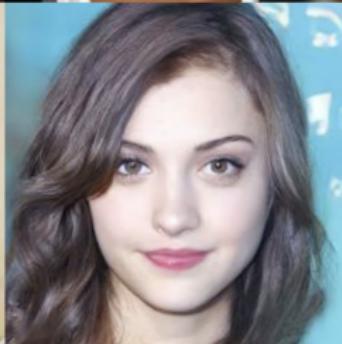
1. Sample $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$.
2. Compute the mean of $p(\mathbf{x}_{t-1} | \mathbf{x}_t, \theta) = \mathcal{N}(\mu_{\theta, t}(\mathbf{x}_t), \tilde{\beta}_t \cdot \mathbf{I})$:

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

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

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.