Deep Generative Models

Lecture 8

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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

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

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

Theorem (Denoising Score Matching)

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

Here, $\nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma | \mathbf{x}) = -\frac{\mathbf{x}_\sigma - \mathbf{x}}{\sigma^2} = -\frac{\boldsymbol{\epsilon}}{\sigma}$. $\mathbf{s}_{\boldsymbol{\theta},\sigma}(\mathbf{x}_\sigma)$ attempts to **denoise** a corrupted sample.

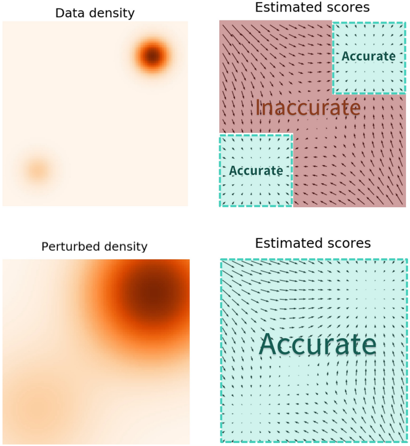
Vincent P. A Connection Between Score Matching and Denoising Autoencoders, 2010

Recap of Previous Lecture

$$\mathbb{E}_{p_{\text{data}}(\mathbf{x})}\mathbb{E}_{\mathcal{N}(0,\mathbf{I})}\left\|\mathbf{s}_{\boldsymbol{\theta},\sigma}(\mathbf{x}+\sigma\boldsymbol{\epsilon})+\frac{\boldsymbol{\epsilon}}{\sigma}\right\|_2^2 \to \min_{\boldsymbol{\theta}}$$

$$\mathbf{x}_{l+1} = \mathbf{x}_l + \frac{\eta}{2}\cdot\mathbf{s}_{\boldsymbol{\theta},\sigma}(\mathbf{x}_l) + \sqrt{\eta}\cdot\boldsymbol{\epsilon}_l$$

- For **small** σ, $\mathbf{s}_{\boldsymbol{\theta},\sigma}(\mathbf{x})$ becomes inaccurate and Langevin dynamics fails to traverse modes
- For **large** σ, robustness in low-density regions is achieved, but the model learns a distribution that is overly corrupted



Song Y. Generative Modeling by Estimating Gradients of the Data Distribution, blog post, 2021

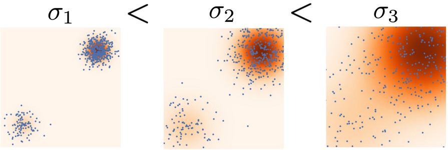
Recap of Previous Lecture

Noise-Conditioned Score Network

- Define a sequence of noise levels: $\sigma_1 < \sigma_2 < \dots < \sigma_T$.
- Train a denoised score function $\mathbf{s}_{\boldsymbol{\theta}, \sigma_t}(\mathbf{x}_t)$ for each noise level:

$$\sum_{t=1}^{T} \sigma_t^2 \cdot \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x})} \left\| \mathbf{s}_{\boldsymbol{\theta}, \sigma_t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}) \right\|_2^2 \to \min_{\boldsymbol{\theta}}$$

- Sample using **annealed** Langevin dynamics (for $t = 1, \dots, T$).



Song Y. et al. Generative Modeling by Estimating Gradients of the Data Distribution, 2019

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 $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
3. Construct noisy image $\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}$.
4. Compute the loss $\mathcal{L} = \sigma_t^2 \cdot \|\mathbf{s}_{\boldsymbol{\theta},\sigma_t}(\mathbf{x}_t) + \frac{\boldsymbol{\epsilon}}{\sigma_t}\|^2$.

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:

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

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

Song Y. et al. Improved Techniques for Training Score-Based Generative Models, 2020

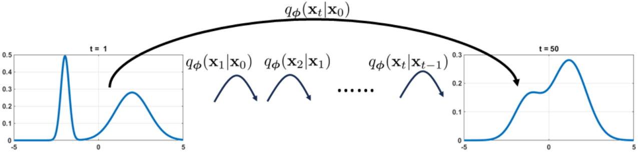
Recap of Previous Lecture

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 $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$.

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

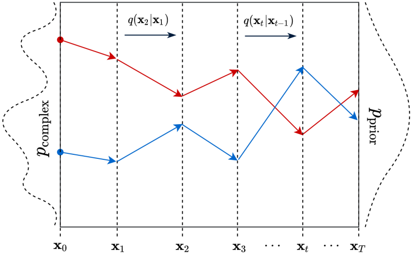
$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t} \cdot \mathbf{x}_{t-1}, \beta_t \cdot \mathbf{I});$$
$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1-\bar{\alpha}_t) \cdot \mathbf{I}).$$



Chan S. Tutorial on Diffusion Models for Imaging and Vision, 2024

Recap of Previous Lecture

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

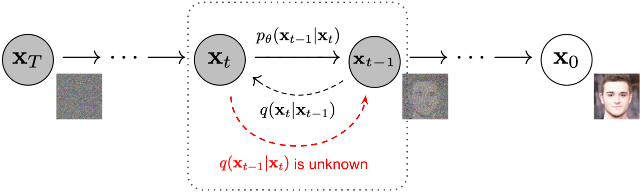


1. $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$;
2. $\mathbf{x}_t = \sqrt{1-\beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \boldsymbol{\epsilon}$, with $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$, $t \geq 1$;
3. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0,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

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

Das A. An Introduction to Diffusion Probabilistic Models, blog post, 2021

Recap of Previous Lecture



Reverse Process (Ancestral Sampling)

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

The Feller theorem guarantees this approximation is valid.

Forward Process

1. $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$;
2. $\mathbf{x}_t = \sqrt{1-\beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \epsilon$;
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. $\mathbf{x}_{t-1} = \boldsymbol{\sigma}_{\boldsymbol{\theta},t}(\mathbf{x}_t) \cdot \epsilon + \boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t)$;
3. $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$;

Weng L. What are Diffusion Models?, blog post, 2021

Outline

1. Conditioned Reverse Distribution

2. Gaussian Diffusion Model as VAE

3. ELBO Derivation

4. Reparametrization

5. Denoising Diffusion Probabilistic Model (DDPM)

Outline

1. Conditioned Reverse Distribution
2. Gaussian Diffusion Model as VAE
3. ELBO Derivation
4. Reparametrization
5. Denoising Diffusion Probabilistic Model (DDPM)

Conditioned Reverse Distribution

Reverse Kernel (**Intractable**)

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

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 Kernel (**Tractable**)

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

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 Kernel (**Tractable**)

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

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 Kernel (**Tractable**)

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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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&= \mathcal{N}(\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \cdot \mathbf{I})
\end{aligned}$$

Here,

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

$$\tilde{\beta}_t = \frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t} = \text{const.}$$

Ho J. Denoising Diffusion Probabilistic Models, 2020

Distribution Summary

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

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

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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:

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

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\end{aligned}
$$

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

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

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 $\mathbf{x}_0$.

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Outline

Gaussian Diffusion Model as VAE

Let's treat $\mathbf{z} = (\mathbf{x}_1, \ldots, \mathbf{x}_T)$ 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

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

Das A. An Introduction to Diffusion Probabilistic Models, blog post, 2021

Gaussian Diffusion Model as VAE

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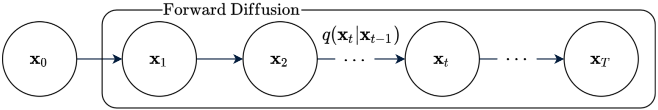

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Gaussian Diffusion Model as VAE

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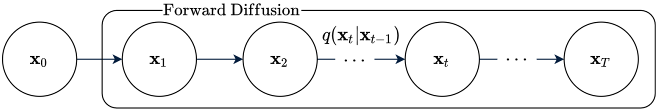
Latent Variable Model

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



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.

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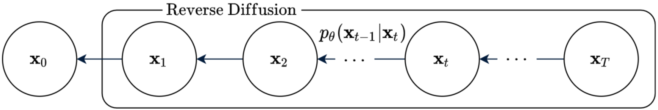
Gaussian Diffusion Model as VAE

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

Das A. An Introduction to Diffusion Probabilistic Models, blog post, 2021

Gaussian Diffusion Model as VAE

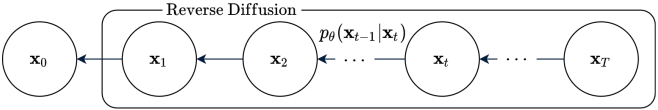
$$p_\theta(\mathbf{x}, \mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})$$



Das A. An Introduction to Diffusion Probabilistic Models, blog post, 2021

Gaussian Diffusion Model as VAE

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



Reverse Diffusion

- Generative distribution (decoder)

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

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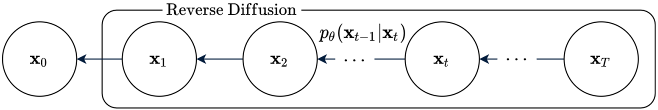
Gaussian Diffusion Model as VAE

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



Reverse Diffusion

- Generative distribution (decoder)

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

- Prior distribution

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

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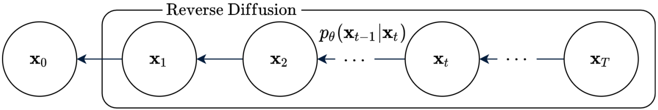
Gaussian Diffusion Model as VAE

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



Reverse Diffusion

- Generative distribution (decoder)

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

- Prior distribution

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

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

Das A. An Introduction to Diffusion Probabilistic Models, blog post, 2021

Outline

ELBO for Gaussian Diffusion Model

Standard ELBO

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian Diffusion Model

Standard ELBO

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

Derivation

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian Diffusion Model

Standard ELBO

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

Derivation

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian Diffusion Model

Standard ELBO

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

Derivation

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

- 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.

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian Diffusion Model

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

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)

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

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)

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

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)

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

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)

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

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)

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

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ELBO for Gaussian Diffusion Model

Derivation (continued)

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian Diffusion Model

Derivation (continued)

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

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

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ELBO for Gaussian Diffusion Model

Derivation (continued)

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

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

$$= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) + \mathbb{E}_{q(\mathbf{x}_T|\mathbf{x}_0)} \log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_0)} +$$

$$+ \sum_{t=2}^{T} \mathbb{E}_{q(\mathbf{x}_{t-1}, \mathbf{x}_t|\mathbf{x}_0)} \log \left(\frac{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} \right) \Bigg]$$

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ELBO for Gaussian Diffusion Model

Derivation (continued)

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

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ELBO for Gaussian Diffusion Model

$$\mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\boldsymbol{\theta}}(\mathbf{x}_0|\mathbf{x}_1) - \mathrm{KL}\big(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)\big) -$$

$$- \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \mathrm{KL}\big(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}|\mathbf{x}_t)\big)}_{\mathcal{L}_t}$$

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian Diffusion Model

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

- First term is the decoder distribution

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

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian Diffusion Model

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

- First term is the decoder distribution

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

  with $\mathbf{x}_1 \sim q(\mathbf{x}_1|\mathbf{x}_0)$.
- Second term is constant:
  - $p(\mathbf{x}_T) = \mathcal{N}(0, \mathbf{I})$;
  - $q(\mathbf{x}_T|\mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_T} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_T) \cdot \mathbf{I})$.

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian Diffusion Model

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

- First term is the decoder distribution

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

  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.

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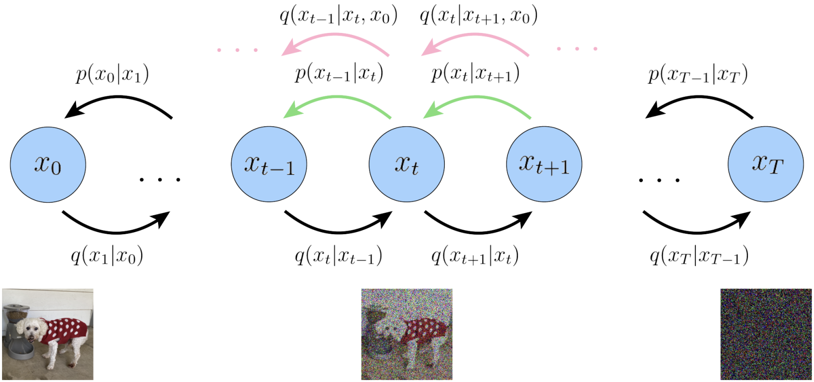
ELBO for Gaussian Diffusion Model



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

$$\begin{aligned} q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) &= \mathcal{N}(\mathbf{x}_{t-1}|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}), \\ p_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}|\mathbf{x}_t) &= \mathcal{N}\big(\mathbf{x}_{t-1}|\boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t), \boldsymbol{\sigma}^2_{\boldsymbol{\theta},t}(\mathbf{x}_t)\big) \end{aligned}$$

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ELBO for Gaussian Diffusion Model

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

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

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian Diffusion Model

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

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}),$$
$$p_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}\big(\mathbf{x}_{t-1}|\boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t), \boldsymbol{\sigma}^2_{\boldsymbol{\theta},t}(\mathbf{x}_t)\big)$$

Let's assume that

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian Diffusion Model

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

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}),$$
$$p_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}\big(\mathbf{x}_{t-1}|\boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t), \boldsymbol{\sigma}^2_{\boldsymbol{\theta},t}(\mathbf{x}_t)\big)$$

Let's assume that

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

Theoretically, the optimal $\boldsymbol{\sigma}^2_{\boldsymbol{\theta},t}(\mathbf{x}_t)$ 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 $\mathbf{x}_0 \sim \delta(\mathbf{x}_0 - \mathbf{x}^*)$.

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ELBO for Gaussian Diffusion Model

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

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}),$$
$$p_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}\big(\mathbf{x}_{t-1}|\boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t), \boldsymbol{\sigma}^2_{\boldsymbol{\theta},t}(\mathbf{x}_t)\big)$$

Let's assume that

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

Theoretically, the optimal $\boldsymbol{\sigma}^2_{\boldsymbol{\theta},t}(\mathbf{x}_t)$ 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 $\mathbf{x}_0 \sim \delta(\mathbf{x}_0 - \mathbf{x}^*)$.

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} KL\Big(\mathcal{N}\big(\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}\big) \| \mathcal{N}\big(\boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t), \tilde{\beta}_t \mathbf{I}\big)\Big)$$

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ELBO for Gaussian Diffusion Model

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

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}),$$
$$p_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}\big(\mathbf{x}_{t-1}|\boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t), \boldsymbol{\sigma}^2_{\boldsymbol{\theta},t}(\mathbf{x}_t)\big)$$

Let's assume that

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

Theoretically, the optimal $\boldsymbol{\sigma}^2_{\boldsymbol{\theta},t}(\mathbf{x}_t)$ 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 $\mathbf{x}_0 \sim \delta(\mathbf{x}_0 - \mathbf{x}^*)$.

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

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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

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

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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 $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
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$$\mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\boldsymbol{\theta}}(\mathbf{x}_0|\mathbf{x}_1) - \mathrm{KL}\big(q(\mathbf{x}_T|\mathbf{x}_0) \| p(\mathbf{x}_T)\big) - \\ - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[\frac{1}{2\tilde{\beta}_t} \left\| \tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t) \right\|^2 \right]}_{\mathcal{L}_t}$$

Sampling

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

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Outline

Reparametrization of DDPM

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

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

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Reparametrization of DDPM

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

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

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

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Reparametrization of DDPM

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

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

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

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Reparametrization of DDPM

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

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

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

- 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 $\boldsymbol{\epsilon}$.

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Reparametrization of DDPM

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

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

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

- 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 $\boldsymbol{\epsilon}$.

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

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Reparametrization of DDPM

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

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

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

- 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 $\boldsymbol{\epsilon}$.

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

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Reparametrization of DDPM

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

Reparametrization

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

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Reparametrization of DDPM

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

Reparametrization

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

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

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Reparametrization of DDPM

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

Reparametrization

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

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

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

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Reparametrization of DDPM

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

Reparametrization

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

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

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

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Reparametrization of DDPM

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

Reparametrization

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

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

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

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

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

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Reparametrization of DDPM

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

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Reparametrization of DDPM

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

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

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Reparametrization of DDPM

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

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

Let's drop the scaling coefficient.

Simplified Objective

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

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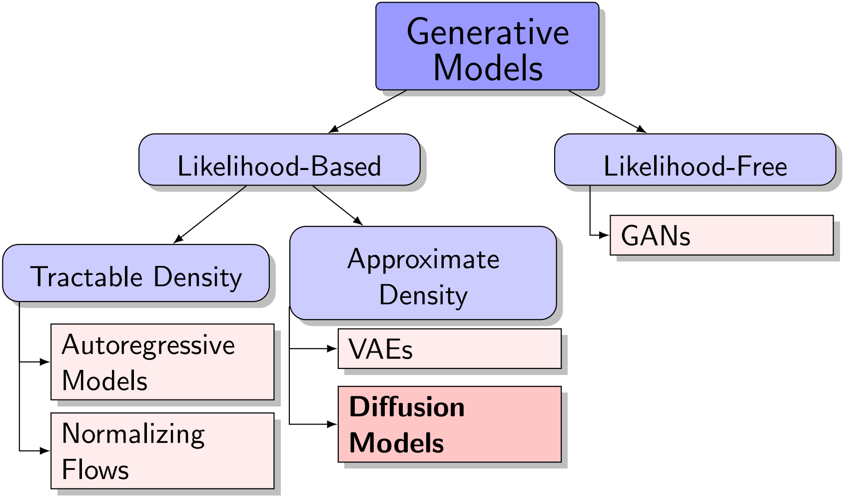
Outline

1. Conditioned Reverse Distribution
2. Gaussian Diffusion Model as VAE
3. ELBO Derivation
4. Reparametrization
5. Denoising Diffusion Probabilistic Model (DDPM)

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

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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. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$.

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Denoising Diffusion Probabilistic Model (DDPM)

DDPM is a VAE Model

- The encoder is a fixed Gaussian Markov chain $q(\mathbf{x}_1, \dots, \mathbf{x}_T | \mathbf{x}_0)$.
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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. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$.

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. $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$;

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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 $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
3. Generate noisy image $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$.
4. Compute the loss $\mathcal{L}_{\text{simple}} = \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t)\|^2$.

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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 $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
3. Generate noisy image $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$.
4. Compute the loss $\mathcal{L}_{\text{simple}} = \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t)\|^2$.

Sampling (Ancestral Sampling)

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

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

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

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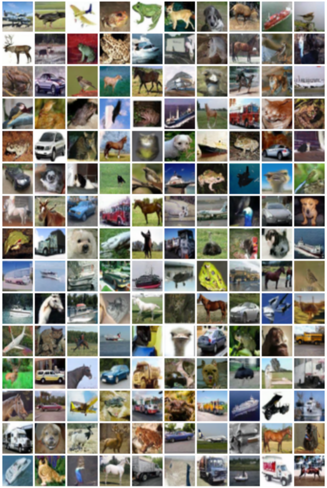
Denoising Diffusion Probabilistic Model (DDPM)

Samples



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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.