Deep Generative Models

Lecture 9

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AI Masters

2025, Spring

Recap of previous lecture

Let perturb original data by normal 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

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

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 small enough.

Theorem (denoising score matching)

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

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

- We do not need to compute $\nabla_{\mathbf{x}_\sigma}\log q(\mathbf{x}_\sigma)$ at the RHS.
- $\mathbf{s}_{\boldsymbol{\theta},\sigma}(\mathbf{x}_\sigma)$ tries to **denoise** a corrupted sample.

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

Recap of previous lecture

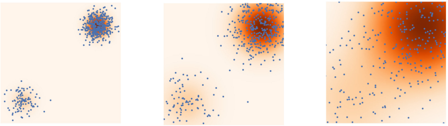
Noise conditioned score network

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

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

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

$\sigma_1 < \sigma_2 < \sigma_3$



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

Recap of previous lecture

NCSN training

1. Get the sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Sample noise level $t \sim U\{1, T\}$ and the noise $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}$.
4. Compute 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 dynamic

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

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

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

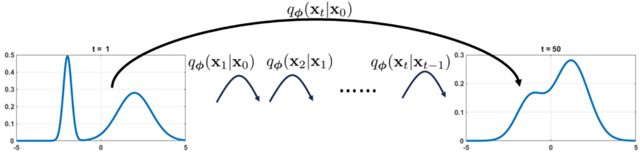
Recap of previous lecture

Forward Gaussian diffusion process

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

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

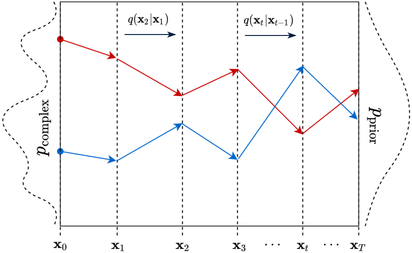
$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t} \cdot \mathbf{x}_{t-1}, \beta_t \cdot \mathbf{I});$$
$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1-\bar{\alpha}_t) \cdot \mathbf{I}).$$



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

Recap of previous lecture

Diffusion refers to the flow of particles from high-density regions towards low-density regions.



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

If we are able to invert this process, we will get the way to sample $\mathbf{x} \sim \pi(\mathbf{x})$ using noise samples $p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$.
Now our goal is to revert this process.

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

Outline

1. Denoising Diffusion Probabilistic Model (DDPM)
   - Gaussian diffusion model as VAE
   - ELBO derivation

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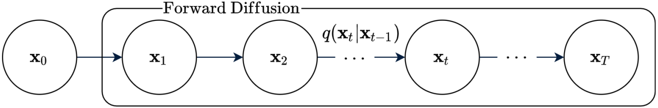
Outline

Gaussian diffusion model as VAE

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

Latent Variable Model

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



Forward diffusion

- Variational posterior distribution (encoder)

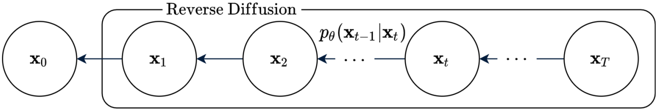
$$q(\mathbf{z}|\mathbf{x}) = q(\mathbf{x}_1, \dots, \mathbf{x}_T|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}).$$

- **Note:** there is no learnable parameters.

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

Gaussian diffusion model as VAE

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



Reverse diffusion

- Generative distribution (decoder)

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

- Prior distribution

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

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

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

Outline

1. Denoising Diffusion Probabilistic Model (DDPM)
   Gaussian diffusion model as VAE
   ELBO derivation

ELBO for Gaussian diffusion model

Standard ELBO

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

Derivation

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

- Let try to decompose the ELBO to separate KL divergences.
- We have to swap the distribution $q(\mathbf{x}_t|\mathbf{x}_{t-1})$ to $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ in the denominator.
- Let add conditioning on $\mathbf{x}_0$ to make reverse distribution $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ tractable.

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian diffusion model

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

Derivation (continued)

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian diffusion model

Derivation (continued)

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

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

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

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

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

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian diffusion model

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

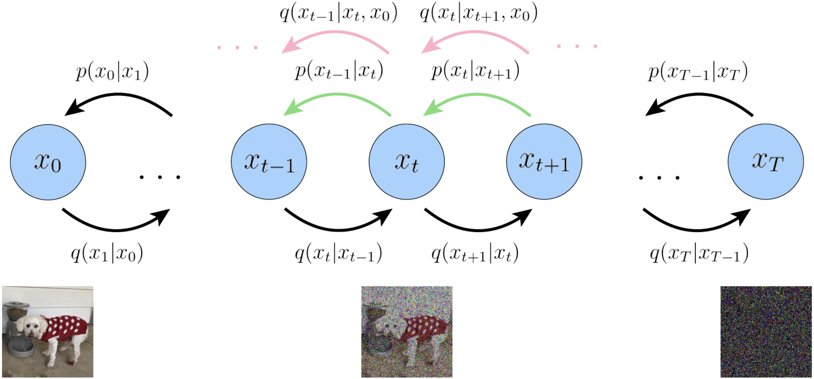
- First term is a decoder distribution

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

  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 makes the main contribution to the ELBO.

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian diffusion model



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

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

Luo C. Understanding Diffusion Models: A Unified Perspective, 2022

ELBO for Gaussian diffusion model

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

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

Let assume

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

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

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

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for Gaussian diffusion model

Training

1. Get the sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Get noisy image $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
3. Compute ELBO

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

Sampling

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Summary

- DDPM approximates the reverse process using Normal assumption.
- One could treat DDPM as VAE model with hierarchical latent variables.
- ELBO of DDPM could be represented as a sum of large number of the KL terms.