Deep Generative Models

Lecture 12

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AI Masters

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Recap of previous lecture

Let perturb original data by normal noise $q(\mathbf{x}'|\mathbf{x}, \sigma) = \mathcal{N}(\mathbf{x}, \sigma^2\mathbf{I})$

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

Then the solution of

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

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

Theorem (denoising score matching)

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

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

- The RHS does not need to compute $\nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma)$ and even more $\nabla_{\mathbf{x}'} \log \pi(\mathbf{x}')$.
- $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma)$ tries to **denoise** a corrupted sample.
- Score function $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma)$ parametrized by σ.

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

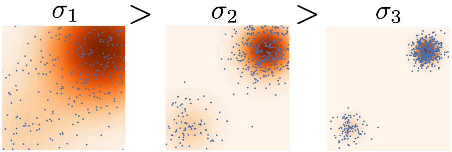
Recap of previous lecture

Noise conditioned score network

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

$$\sum_{t=1}^{T} \sigma_t^2 \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}'|\mathbf{x}, \sigma_t)} \left\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma_t) - \nabla'_{\mathbf{x}} \log q(\mathbf{x}'|\mathbf{x}, \sigma_t) \right\|_2^2 \to \min_{\boldsymbol{\theta}}$$

- Sample from **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. 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 $\mathbf{x}' = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}$.
4. Compute loss $\mathcal{L} = \|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma_t) + \frac{\boldsymbol{\epsilon}}{\sigma_t}\|^2$.

NCSN sampling (annealed Langevin dynamics)

- Sample $\mathbf{x}_0 \sim \mathcal{N}(0, \sigma_1 \mathbf{I}) \approx \pi(\mathbf{x}|\sigma_1)$.
- Apply T steps of Langevin dynamic

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

- 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

Outline

1. Gaussian diffusion process
   - Forward gaussian diffusion process
   - Denoising score matching
   - Reverse gaussian diffusion process
2. Gaussian diffusion model as VAE

Outline

1. Gaussian diffusion process
   Forward gaussian diffusion process
   Denoising score matching
   Reverse gaussian diffusion process

2. Gaussian diffusion model as VAE

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2. Gaussian diffusion model as VAE

Forward gaussian diffusion process

Let $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$, $\beta_t \in (0, 1)$. Define the Markov chain

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

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

Statement 1

Let denote $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$. Then

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

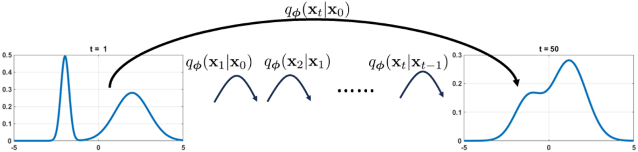
We are able to sample from any timestamp using only $\mathbf{x}_0$!

$$\begin{aligned}
\mathbf{x}_t &= \sqrt{\alpha_t} \cdot \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \cdot \boldsymbol{\epsilon}_t = \\
&= \sqrt{\alpha_t}(\cdot \sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \cdot \boldsymbol{\epsilon}_{t-1}) + \sqrt{1 - \alpha_t} \cdot \boldsymbol{\epsilon}_t = \\
&= \sqrt{\alpha_t \alpha_{t-1}} \cdot \mathbf{x}_{t-2} + (\sqrt{\alpha_t (1 - \alpha_{t-1})} \cdot \boldsymbol{\epsilon}_{t-1} + \sqrt{1 - \alpha_t} \cdot \boldsymbol{\epsilon}_t) = \\
&= \sqrt{\alpha_t \alpha_{t-1}} \cdot \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1} \alpha_t} \cdot \boldsymbol{\epsilon}'_t = \\
&= \cdots = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).
\end{aligned}$$

Sohl-Dickstein J. Deep Unsupervised Learning using Nonequilibrium Thermodynamics, 2015

Forward gaussian diffusion process

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



Statement 2

Applying the Markov chain to samples from any $\pi(\mathbf{x})$ we will get $\mathbf{x}_\infty \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$. Here $p_\infty(\mathbf{x})$ is a **stationary** and **limiting** distribution:

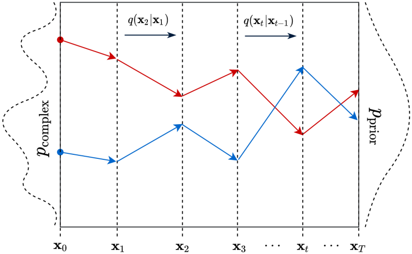
$$p_\infty(\mathbf{x}) = \int q(\mathbf{x}|\mathbf{x}')p_\infty(\mathbf{x}')d\mathbf{x}'.$$

$$p_\infty(\mathbf{x}) = \int q(\mathbf{x}_\infty|\mathbf{x}_0)\pi(\mathbf{x}_0)d\mathbf{x}_0 \approx \mathcal{N}(0, \mathbf{I}) \int \pi(\mathbf{x}_0)d\mathbf{x}_0 = \mathcal{N}(0, \mathbf{I})$$

Chan S. Tutorial on Diffusion Models for Imaging and Vision, 2024
Sohl-Dickstein J. Deep Unsupervised Learning using Nonequilibrium Thermodynamics, 2015

Forward gaussian diffusion process

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 $T >> 1$.

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

Denoising score matching

NCSN

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}, \sigma_t^2 \mathbf{I})$$

$$\pi(\mathbf{x}'|\sigma_1) \approx \mathcal{N}(0, \sigma_1^2 \mathbf{I}), \quad \pi(\mathbf{x}'|\sigma_T) \approx \pi(\mathbf{x}).$$

Gaussian diffusion

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

$$q(\mathbf{x}_1) \approx \pi(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \mathbf{I}).$$

Theorem

$$\mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \big\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma) - \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \big\|_2^2 =$$

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

Gradient of the noise kernel

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

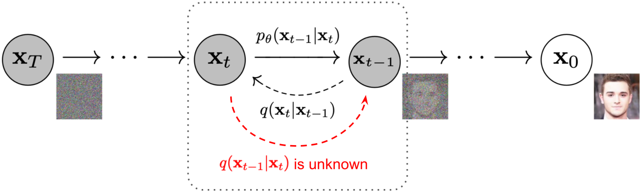
$$\nabla_{\mathbf{x}'} \log q(\mathbf{x}'|\mathbf{x}, \sigma) = \nabla_{\mathbf{x}'} \log \mathcal{N}(\mathbf{x}, \sigma^2 \mathbf{I}) = \mathbf{x}' - \mathbf{x}$$

Outline

1. Gaussian diffusion process
   - Forward gaussian diffusion process
   - Denoising score matching
   - Reverse gaussian diffusion process

2. Gaussian diffusion model as VAE

Reverse gaussian diffusion process



Forward process

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

Reverse process

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)} \approx p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta})$$

- $q(\mathbf{x}_{t-1})$, $q(\mathbf{x}_t)$ are intractable.
- If β_t is small enough, $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ will be Gaussian (Feller, 1949).

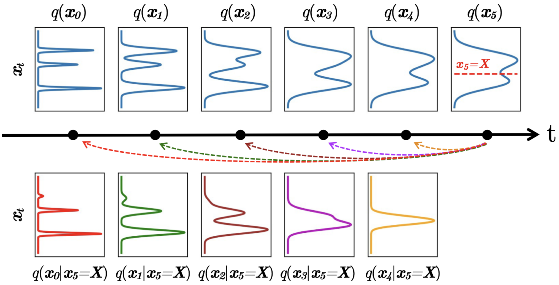
Feller W. On the theory of stochastic processes, with particular reference to applications, 1949

Reverse gaussian diffusion process

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

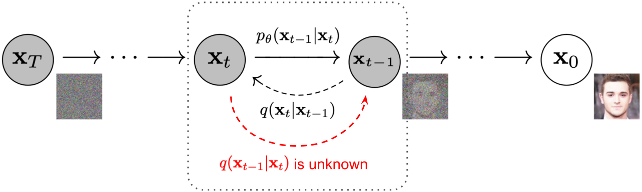
$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} = \mathcal{N}(\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I})$$

- $q(\mathbf{x}_{t-1})$, $q(\mathbf{x}_t)$ are intractable.
- If β_t is small enough, $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ will be Gaussian (Feller, 1949).



Xiao Z., Kreis K., Vahdat A. Tackling the generative learning trilemma with denoising diffusion GANs, 2021

Reverse gaussian diffusion process



Let define the reverse process

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

Forward process

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

Reverse process

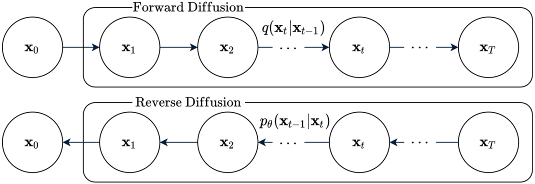
1. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$;
2. $\mathbf{x}_{t-1} = \boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_t, t)$;
3. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$;

Note: The forward process does not have any learnable parameters!

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

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).
- Variational posterior distribution (**note:** there is no learnable parameters)

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

- Probabilistic model

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

- Generative distribution and prior

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = p(\mathbf{x}_0|\mathbf{x}_1, \boldsymbol{\theta}); \quad p(\mathbf{z}|\boldsymbol{\theta}) = \prod_{t=2}^{T} p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) \cdot p(\mathbf{x}_T)$$

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

ELBO for gaussian diffusion model

Standard ELBO

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

Derivation

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

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for gaussian diffusion model

Derivation (continued)

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

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

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

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

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

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for gaussian diffusion model

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

- First term is a decoder distribution

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

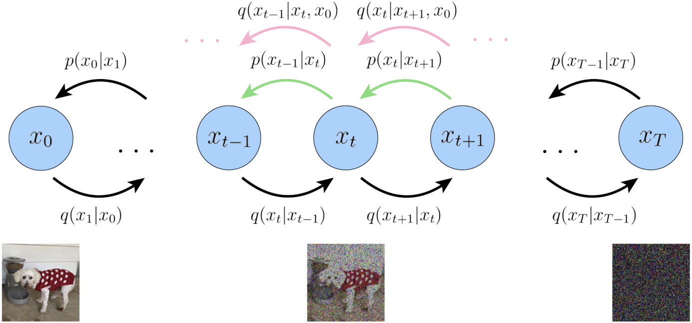
- Second term is constant ($p(\mathbf{x}_T)$ is a standard Normal, $q(\mathbf{x}_T|\mathbf{x}_0)$ is a non-parametrical Normal).

Ho J. Denoising Diffusion Probabilistic Models, 2020

ELBO for gaussian diffusion model

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

$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ defines how to denoise a noisy image $\mathbf{x}_t$ with access to what the final, completely denoised image $\mathbf{x}_0$ should be.



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

Summary

- Gaussian diffusion process is a Markov chain that injects special form of Gaussian noise to the samples.
- Reverse process allows to sample from the real distribution $\pi(\mathbf{x})$ using samples from noise.
- Diffusion model is a VAE model which reverts gaussian diffusion process using variational inference.
- ELBO of DDPM could be represented as a sum of KL terms.