

Deep Generative Models

Lecture 11

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AI Masters

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Recap of previous lecture

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

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

Then the solution of

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

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

Theorem (denoising score matching)

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

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

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

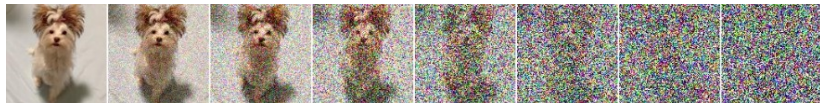
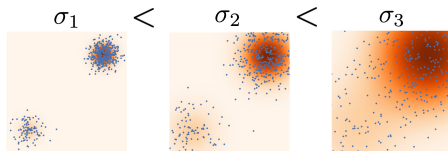
Recap of previous lecture

Noise conditioned score network

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

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

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

NCSN sampling (annealed Langevin dynamics)

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

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

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

Recap of previous lecture

Forward gaussian diffusion process

Let $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$, $\beta_t \in (0, 1)$, $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{s=1}^t \alpha_s$.

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

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

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

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

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

Outline

1. Diffusion denoising score matching
2. Reverse gaussian diffusion process
3. Gaussian diffusion model as VAE
4. Reparametrization of gaussian diffusion model

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Denoising score matching

NCSN

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_0, \sigma_t^2 \cdot \mathbf{I}), \quad q(\mathbf{x}_1) \approx \pi(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \sigma_T^2 \cdot \mathbf{I}).$$

$$\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}) = -\frac{\mathbf{x}_t - \mathbf{x}}{\sigma_t^2}$$

Gaussian diffusion

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_t) \cdot \mathbf{I}), \quad q(\mathbf{x}_1) \approx \pi(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \mathbf{I})$$

$$\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}_0) = -\frac{\mathbf{x}_t - \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0}{1 - \bar{\alpha}_t}$$

Theorem (denoising score matching)

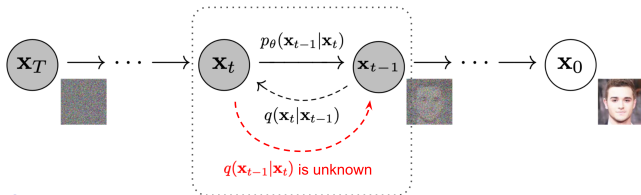
$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_t)} \left\| \mathbf{s}_{\theta,t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t) \right\|_2^2 &= \\ &= \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x})} \left\| \mathbf{s}_{\theta,t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x})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

Note: We are able to apply NCSN approach with annealed Langevin dynamics to get diffusion denoising model.

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1. Diffusion denoising score matching
2. Reverse gaussian diffusion process
3. Gaussian diffusion model as VAE
4. Reparametrization of gaussian diffusion model

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

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

$q(\mathbf{x}_{t-1})$, $q(\mathbf{x}_t)$ are intractable:

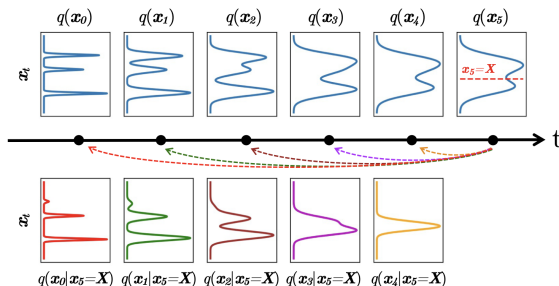
$$q(\mathbf{x}_t) = \int q(\mathbf{x}_t|\mathbf{x}_0)\pi(\mathbf{x}_0)d\mathbf{x}_0$$

Reverse gaussian diffusion process

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

Theorem (Feller, 1949)

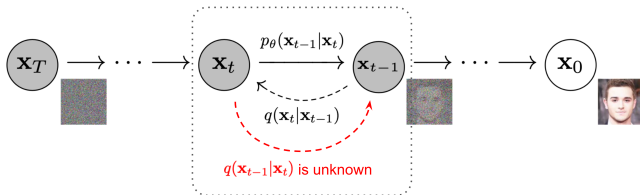
If β_t is small enough, $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ will be Gaussian (that is why diffusion needs $T \approx 1000$ steps to converge).



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

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

Feller theorem shows that it is a reasonable assumption.

Forward process

1. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$;
2. $\mathbf{x}_t = \sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \epsilon$;
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. $\mathbf{x}_{t-1} = \sigma_{\theta,t}(\mathbf{x}_t) \cdot \epsilon + \mu_{\theta,t}(\mathbf{x}_t)$;
3. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$;

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

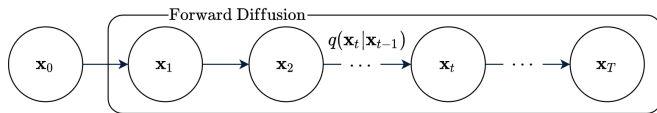
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4. Reparametrization of gaussian diffusion model

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). Probabilistic model is

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



Forward diffusion

- Variational posterior distribution (encoder)

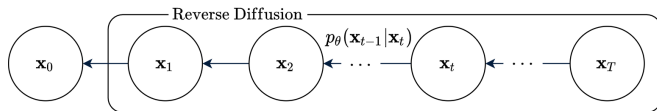
$$q(\mathbf{z} | \mathbf{x}) = q(\mathbf{x}_1, \dots, \mathbf{x}_T | \mathbf{x}_0) = \prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1}).$$

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

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). Probabilistic model is

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



Reverse diffusion

- Generative distribution (decoder)

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

- Prior distribution

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

Conditioned reverse distribution

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

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

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

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

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

ELBO for gaussian diffusion model

Standard ELBO

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

Derivation

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

We add conditioning on \mathbf{x}_0 to make reverse distribution $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ tractable and to get KL divergences.

ELBO for gaussian diffusion model

Derivation (continued)

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

ELBO for gaussian diffusion model

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

- **First term** is a decoder distribution

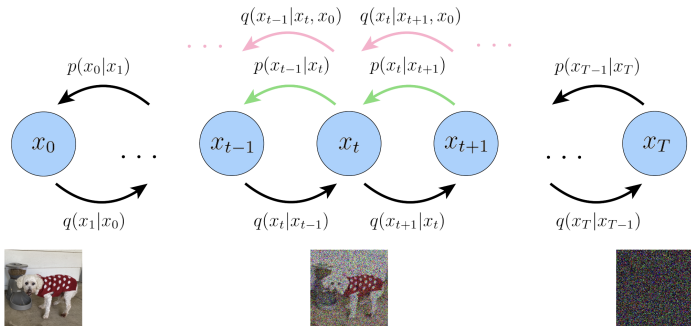
$$\log p(\mathbf{x}_0|\mathbf{x}_1, \theta) = \log \mathcal{N}(\mathbf{x}_0 | \mu_{\theta, t}(\mathbf{x}_1), \sigma_{\theta, t}^2(\mathbf{x}_1)).$$

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

ELBO for gaussian diffusion model

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

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



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Reparametrization of DDPM

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

\mathcal{L}_t is the mean of KL between two normal distributions:

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

Here $\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0)$, $\tilde{\beta}_t = \frac{\beta_t(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}$ have analytical expressions. Let assume

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

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

Reparametrization of DDPM

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

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

Use the formula for KL between two normal distributions:

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

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

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

Reparametrization of DDPM

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

Reparametrization

$$\begin{aligned}\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) &= \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \epsilon \\ \mu_{\theta,t}(\mathbf{x}_t) &= \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \epsilon_{\theta,t}(\mathbf{x}_t)\end{aligned}$$

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

At each step of reverse diffusion process we try to predict the noise ϵ that we used in the forward diffusion process!

Reparametrization of DDPM

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

Simplified objective

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

Summary

- ▶ Denoising score matching is applicable to gaussian diffusion process.
- ▶ Reverse process allows to sample from the real distribution $\pi(\mathbf{x})$ using samples from noise, but it is intractable.
- ▶ We will use approximation to get the reverse process.
- ▶ 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.
- ▶ DDPM is a VAE model with hierarchical latent variables.
- ▶ At each step DDPM predicts the noise that was used in the forward diffusion process.