

Deep Generative Models

Lecture 11

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Recap of previous lecture

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

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

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

- ▶ 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.
- ▶ Score function $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma)$ parametrized by σ .

Recap of previous lecture

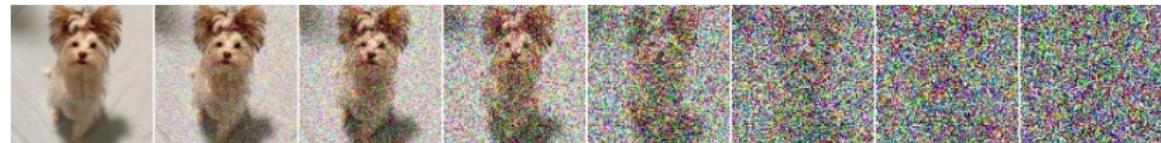
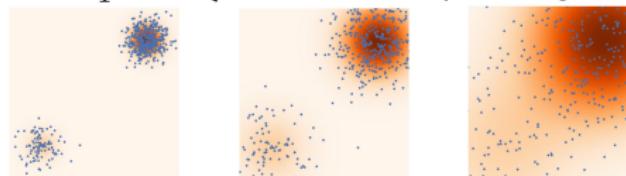
Noise conditioned score network

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

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

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

$$\sigma_1 < \sigma_2 < \sigma_3$$



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 $\mathcal{L} = \|\mathbf{s}_{\theta, \sigma_t}(\mathbf{x}_t) + \frac{\epsilon}{\sigma_t}\|^2$.

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 .

Outline

1. Gaussian diffusion model as VAE
2. Reparametrization of gaussian diffusion model
3. Denoising Diffusion Probabilistic Model (DDPM)

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

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

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

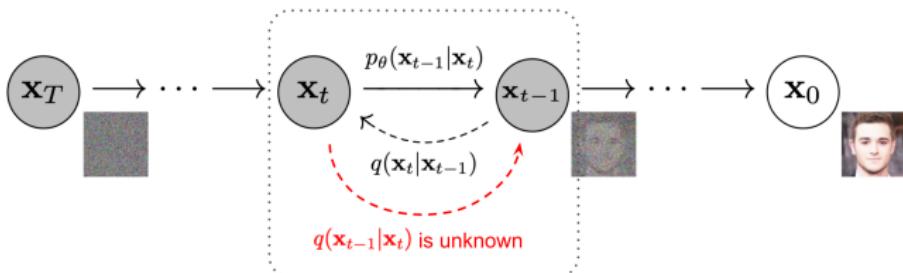
$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t | \sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1}, \beta_t \cdot \mathbf{I});$$

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

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

Recap of previous lecture



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.
- ▶ 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

Recap of previous lecture

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

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

Let define the reverse process

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

Forward process

$$1. \quad \mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$$

$$2. \quad \mathbf{x}_t = \sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \boldsymbol{\epsilon}, \quad 2. \quad \mathbf{x}_{t-1} =$$

where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$, $t \geq 1$; $2. \quad \sigma_\theta(\mathbf{x}_t, t) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}_\theta(\mathbf{x}_t, t);$

$$3. \quad \mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I}). \quad 3. \quad \mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$$

Reverse process

$$1. \quad \mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I});$$

$$2. \quad \mathbf{x}_{t-1} =$$

$\sigma_\theta(\mathbf{x}_t, t) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}_\theta(\mathbf{x}_t, t);$

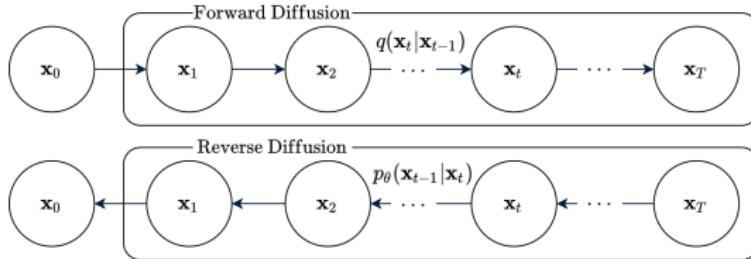
$$3. \quad \mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$$

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

Outline

1. Gaussian diffusion model as VAE
2. Reparametrization of gaussian diffusion model
3. Denoising Diffusion Probabilistic Model (DDPM)

Gaussian diffusion model as VAE



- ▶ Let treat $\mathbf{z} = (x_1, \dots, x_T)$ as a latent variable (**note**: each x_t has the same size).
- ▶ Variational posterior distribution (**note**: there is no learnable parameters)

$$q(\mathbf{z}|\mathbf{x}) = q(x_1, \dots, x_T | x_0) = \prod_{t=1}^T q(x_t | x_{t-1}).$$

- ▶ 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

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = p(x_0|x_1, \boldsymbol{\theta}); \quad p(\mathbf{z}|\boldsymbol{\theta}) = \prod_{t=2}^T p(x_{t-1}|x_t, \boldsymbol{\theta}) \cdot p(x_T)$$

ELBO for gaussian diffusion model

Standard ELBO

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

Derivation

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

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

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

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

- ▶ First term is a decoder distribution

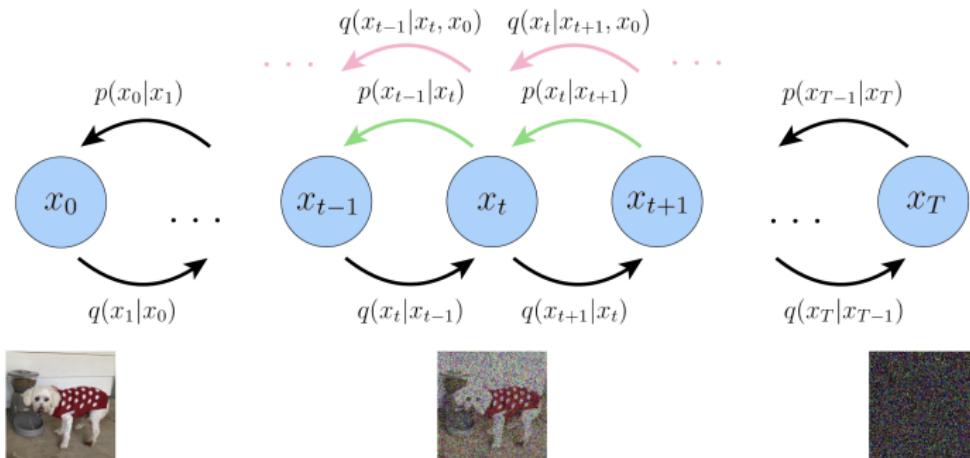
$$\log p(\mathbf{x}_0|\mathbf{x}_1, \theta) = \log \mathcal{N}(\mathbf{x}_0|\mu_\theta(\mathbf{x}_1, t), \sigma_\theta^2(\mathbf{x}_1, t)).$$

- ▶ 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

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

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



Outline

1. Gaussian diffusion model as VAE
2. Reparametrization of gaussian diffusion model
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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:

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

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

Here

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

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

Let assume

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

Reparametrization of DDPM

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

Use the formula for KL between two normal distributions:

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

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

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

Reparametrization of DDPM

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

Reparametrization

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

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

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

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

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

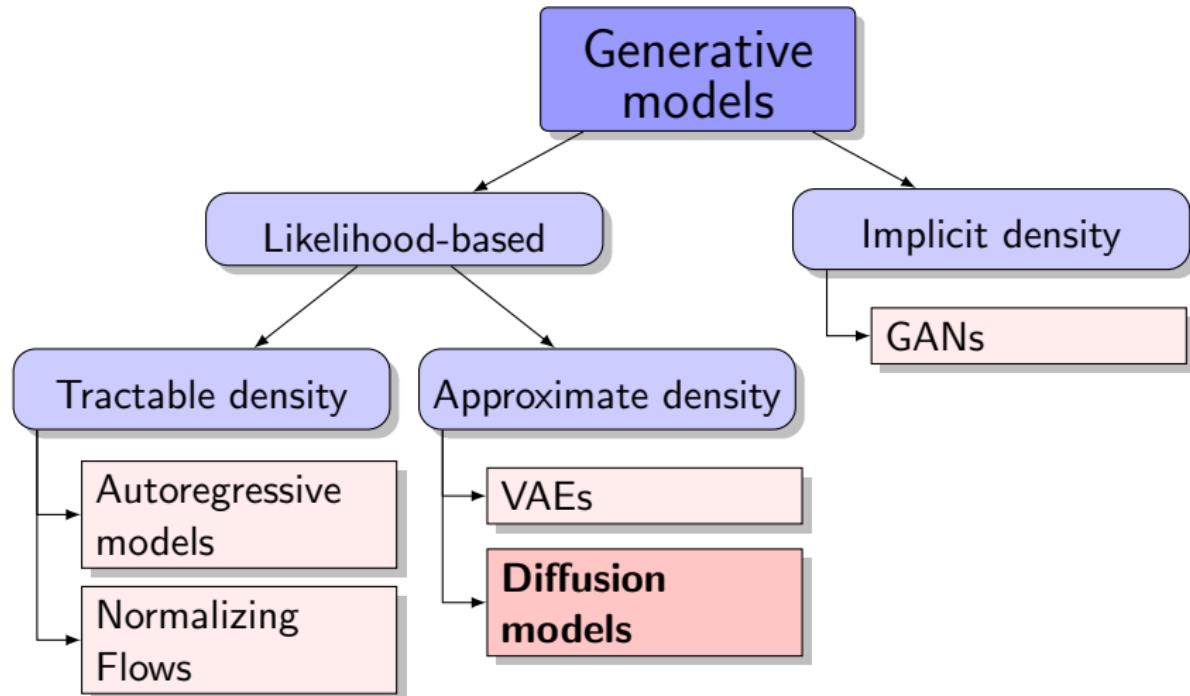
Simplified objective

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

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Generative models zoo



Denoising diffusion probabilistic model (DDPM)

DDPM is a VAE model

- ▶ Encoder is a fixed Gaussian Markov chain $q(\mathbf{x}_1, \dots, \mathbf{x}_T | \mathbf{x}_0)$.
- ▶ Latent variable is a hierarchical (in each step the dim. of the latent equals to the dim of the input).
- ▶ Decoder is a simple Gaussian model $p(\mathbf{x}_0 | \mathbf{x}_1, \theta)$.
- ▶ Prior distribution is given by parametric Gaussian Makov chain $p(\mathbf{x}_{t-1} | \mathbf{x}_t, \theta)$.

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

Denoising diffusion probabilistic model (DDPM)

Training

1. Get the sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Sample timestamp $t \sim U[1, T]$ and the noise $\epsilon \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon$.
4. Compute loss $\mathcal{L}_{\text{simple}} = \|\epsilon - \epsilon_{\theta}(\mathbf{x}_t, t)\|^2$.

Sampling

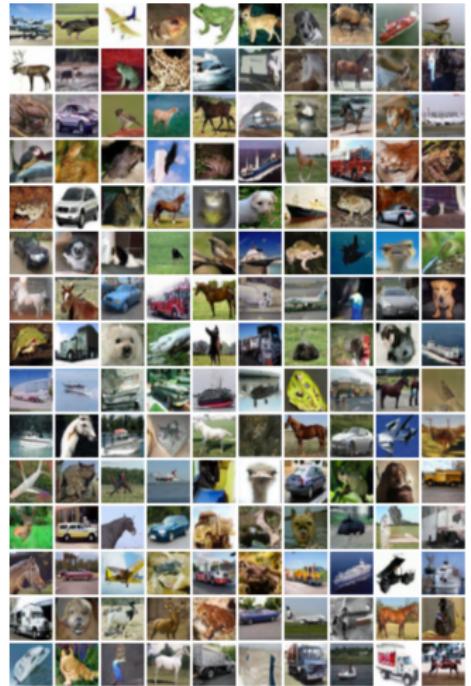
1. Sample $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$.
2. Compute mean of $p(\mathbf{x}_{t-1} | \mathbf{x}_t, \theta) = \mathcal{N}(\mu_{\theta}(\mathbf{x}_t, t), \tilde{\beta}_t \mathbf{I})$:

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

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

Denoising diffusion probabilistic model (DDPM)

Samples



Summary

- ▶ 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.
- ▶ DDPM is really slow, because we have to apply the model T times.