

Deep Generative Models

Lecture 11

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Recap of previous lecture

Consider Ordinary Differential Equation

$$\frac{d\mathbf{z}(t)}{dt} = f_{\theta}(\mathbf{z}(t), t); \quad \text{with initial condition } \mathbf{z}(t_0) = \mathbf{z}_0.$$

$$\mathbf{z}(t_1) = \int_{t_0}^{t_1} f_{\theta}(\mathbf{z}(t), t) dt + \mathbf{z}_0 = \text{ODESolve}(\mathbf{z}(t_0), f_{\theta}, t_0, t_1).$$

Euler update step

$$\frac{\mathbf{z}(t + \Delta t) - \mathbf{z}(t)}{\Delta t} = f_{\theta}(\mathbf{z}(t), t) \Rightarrow \mathbf{z}(t + \Delta t) = \mathbf{z}(t) + \Delta t \cdot f_{\theta}(\mathbf{z}(t), t)$$

Residual block

$$\mathbf{z}_{t+1} = \mathbf{z}_t + f_{\theta}(\mathbf{z}_t)$$

It is equivalent to Euler update step for solving ODE with $\Delta t = 1$!

In the limit of adding more layers and taking smaller steps we get:

$$\frac{d\mathbf{z}(t)}{dt} = f_{\theta}(\mathbf{z}(t), t); \quad \mathbf{z}(t_0) = \mathbf{x}; \quad \mathbf{z}(t_1) = \mathbf{y}.$$

Recap of previous lecture

Forward pass (loss function)

$$\begin{aligned} L(\mathbf{y}) &= L(\mathbf{z}(t_1)) = L\left(\mathbf{z}(t_0) + \int_{t_0}^{t_1} f_\theta(\mathbf{z}(t), t) dt\right) \\ &= L(\text{ODESolve}(\mathbf{z}(t_0), f_\theta, t_0, t_1)) \end{aligned}$$

Note: ODESolve could be any method (Euler step, Runge-Kutta methods).

Backward pass (gradients computation)

For fitting parameters we need gradients:

$$\mathbf{a}_z(t) = \frac{\partial L(\mathbf{y})}{\partial \mathbf{z}(t)}; \quad \mathbf{a}_\theta(t) = \frac{\partial L(\mathbf{y})}{\partial \theta(t)}.$$

In theory of optimal control these functions called **adjoint** functions. They show how the gradient of the loss depends on the hidden state $\mathbf{z}(t)$ and parameters θ .

Recap of previous lecture

$$\mathbf{a}_z(t) = \frac{\partial L(\mathbf{y})}{\partial \mathbf{z}(t)}; \quad \mathbf{a}_{\theta}(t) = \frac{\partial L(\mathbf{y})}{\partial \theta(t)} - \text{adjoint functions.}$$

Theorem (Pontryagin)

$$\frac{d\mathbf{a}_z(t)}{dt} = -\mathbf{a}_z(t)^T \cdot \frac{\partial f_{\theta}(\mathbf{z}(t), t)}{\partial \mathbf{z}}; \quad \frac{d\mathbf{a}_{\theta}(t)}{dt} = -\mathbf{a}_z(t)^T \cdot \frac{\partial f_{\theta}(\mathbf{z}(t), t)}{\partial \theta}.$$

Forward pass

$$\mathbf{z}(t_1) = \int_{t_0}^{t_1} f_{\theta}(\mathbf{z}(t), t) dt + \mathbf{z}_0 \quad \Rightarrow \quad \text{ODE Solver}$$

Backward pass

$$\left. \begin{aligned} \frac{\partial L}{\partial \theta(t_0)} &= \mathbf{a}_{\theta}(t_0) = - \int_{t_1}^{t_0} \mathbf{a}_z(t)^T \frac{\partial f_{\theta}(\mathbf{z}(t), t)}{\partial \theta(t)} dt + 0 \\ \frac{\partial L}{\partial \mathbf{z}(t_0)} &= \mathbf{a}_z(t_0) = - \int_{t_1}^{t_0} \mathbf{a}_z(t)^T \frac{\partial f_{\theta}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)} dt + \frac{\partial L}{\partial \mathbf{z}(t_1)} \\ \mathbf{z}(t_0) &= - \int_{t_1}^{t_0} f_{\theta}(\mathbf{z}(t), t) dt + \mathbf{z}_1. \end{aligned} \right\} \Rightarrow \text{ODE Solver}$$

Recap of previous lecture

Continuous-in-time normalizing flows

$$\frac{d\mathbf{z}(t)}{dt} = f_{\theta}(\mathbf{z}(t), t); \quad \frac{d \log p(\mathbf{z}(t), t)}{dt} = -\text{tr} \left(\frac{\partial f_{\theta}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)} \right).$$

Theorem (Picard)

If f is uniformly Lipschitz continuous in \mathbf{z} and continuous in t , then the ODE has a **unique** solution.

Forward transform + log-density

$$\begin{bmatrix} \mathbf{x} \\ \log p(\mathbf{x}|\boldsymbol{\theta}) \end{bmatrix} = \begin{bmatrix} \mathbf{z} \\ \log p(\mathbf{z}) \end{bmatrix} + \int_{t_0}^{t_1} \begin{bmatrix} f_{\theta}(\mathbf{z}(t), t) \\ -\text{tr} \left(\frac{\partial f_{\theta}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)} \right) \end{bmatrix} dt.$$

Hutchinson's trace estimator

$$\log p(\mathbf{z}(t_1)) = \log p(\mathbf{z}(t_0)) - \mathbb{E}_{p(\epsilon)} \int_{t_0}^{t_1} \left[\epsilon^T \frac{\partial f}{\partial \mathbf{z}} \epsilon \right] dt.$$

Outline

1. Gaussian diffusion process

Forward gaussian diffusion process

Reverse gaussian diffusion process

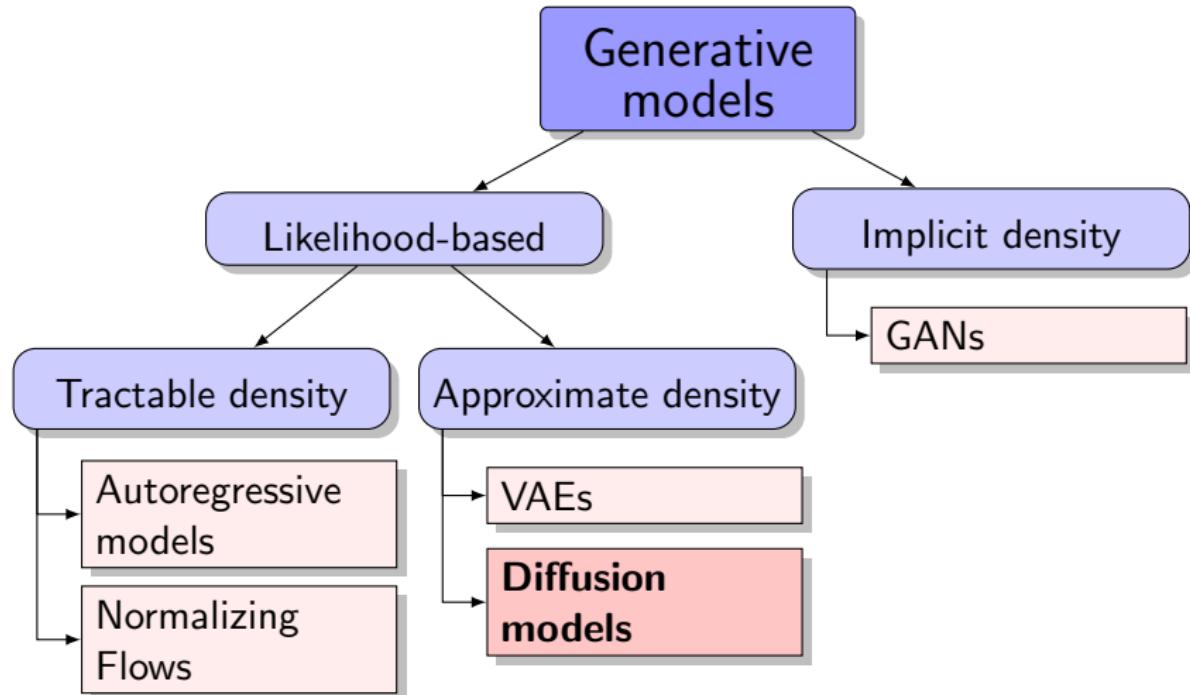
2. Denoising diffusion probabilistic model (DDPM)

Objective of DDPM

Reparametrization of DDPM

Overview of DDPM

Generative models zoo



Outline

1. Gaussian diffusion process

Forward gaussian diffusion process

Reverse gaussian diffusion process

2. Denoising diffusion probabilistic model (DDPM)

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Reparametrization of DDPM

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Forward gaussian diffusion process

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

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

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

Statement 1

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

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_t = \\ &= \sqrt{\alpha_t} (\sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \boldsymbol{\epsilon}_{t-1}) + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_t = \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + (\sqrt{\alpha_t(1 - \alpha_{t-1})} \boldsymbol{\epsilon}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_t) = \\ &= \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).\end{aligned}$$

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

We could sample from any timestamp using only \mathbf{x}_0 !

Forward gaussian diffusion process

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

At each step we

- ▶ scale magnitude of the signal at rate $\sqrt{1 - \beta_t}$;
- ▶ add noise with variance β_t .

Statement 2

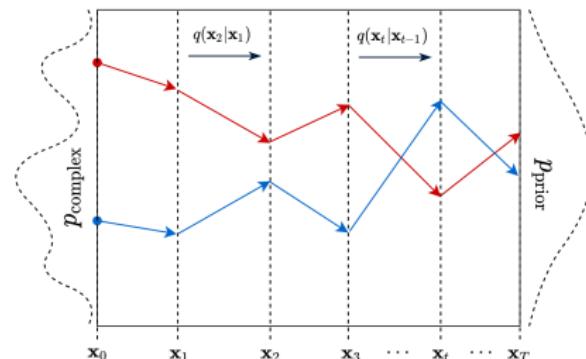
Applying the Markov chain to samples from any $\pi(\mathbf{x})$ we will get $\mathbf{x}_\infty \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$. Here $p_\infty(\mathbf{x})$ is a **stationary** and **limiting** distribution:

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

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

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

Now our goal is to revert this process.

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1. Gaussian diffusion process

Forward gaussian diffusion process

Reverse gaussian diffusion process

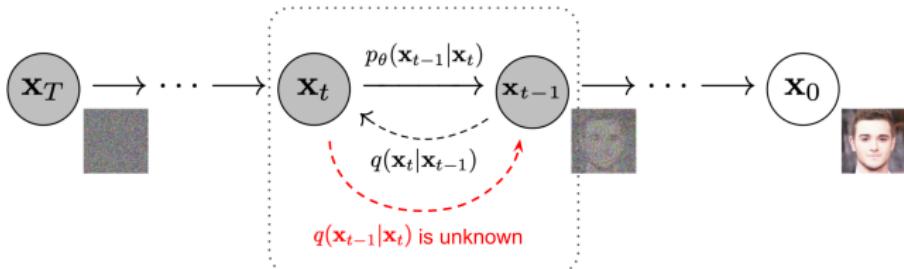
2. Denoising diffusion probabilistic model (DDPM)

Objective of DDPM

Reparametrization of DDPM

Overview of DDPM

Reverse gaussian diffusion process



Forward process

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

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).

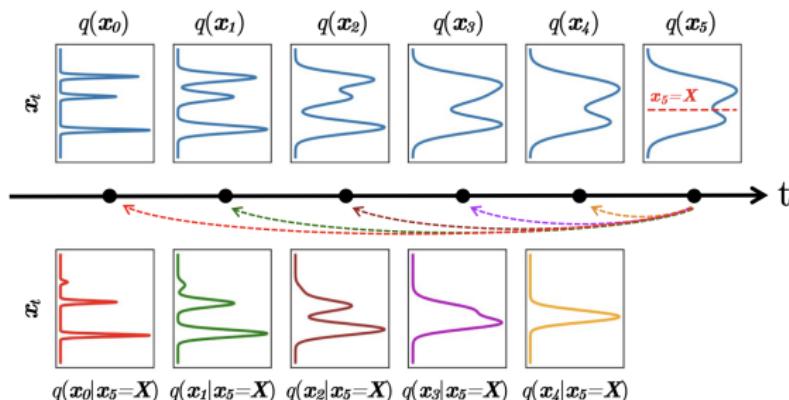
Feller W. On the theory of stochastic processes, with particular reference to applications, 1949

Reverse gaussian diffusion process

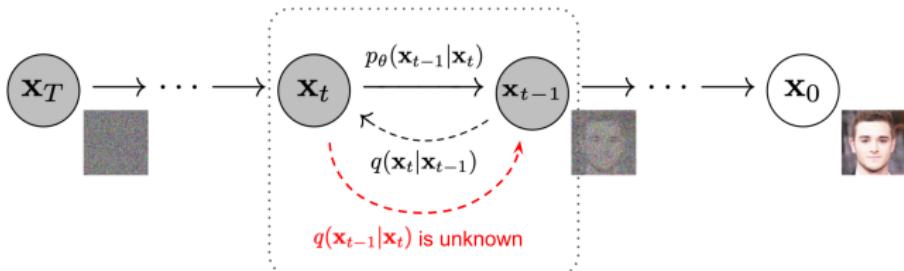
$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)}$$

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

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



Reverse gaussian diffusion process



Let define the reverse process

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

Forward process

1. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$
2. $\mathbf{x}_t = \sqrt{1 - \beta} \cdot \mathbf{x}_{t-1} + \sqrt{\beta} \cdot \boldsymbol{\epsilon},$ 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. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$

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

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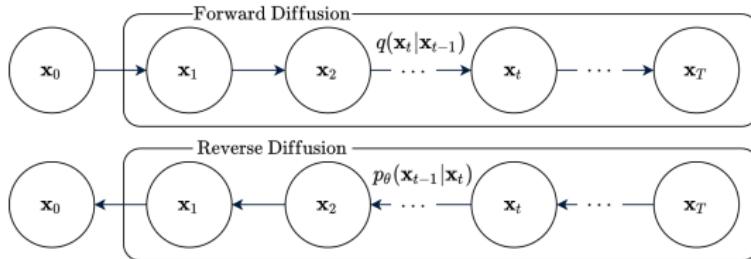
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Gaussian diffusion model as VAE



- ▶ 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

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

Objective of DDPM

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

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

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

Objective of DDPM

Derivation (continued)

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

Objective of DDPM

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

- ▶ First term is a decoder distribution

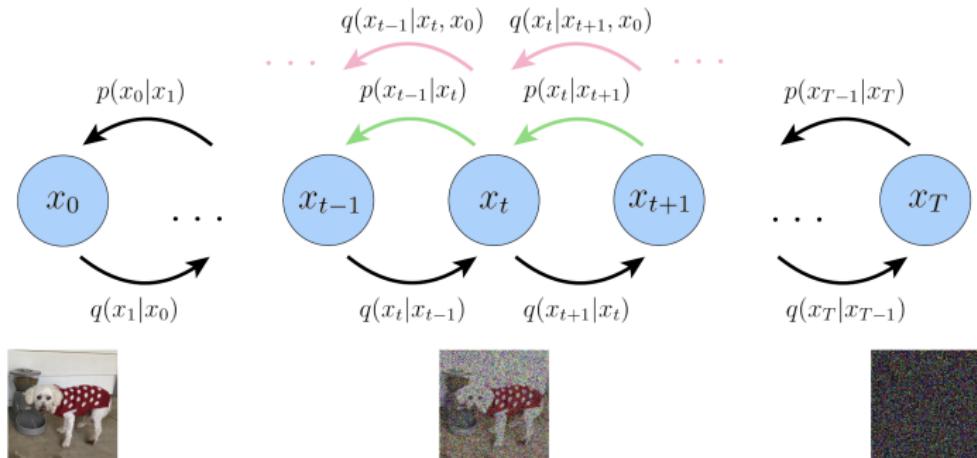
$$\log p(\mathbf{x}_0|\mathbf{x}_1, \theta) = \log \mathcal{N}(\mathbf{x}_0 | \mu_\theta(\mathbf{x}_1, t), \sigma_\theta^2(\mathbf{x}_1, t)).$$

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

Objective of DDPM

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

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



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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 a KL between two normal distributions:

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

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

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

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

Use KL formula between two normal distributions:

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

Here we used the analytic expression for $\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0)$.

Reparametrization

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

Reparametrization of DDPM

KL term

$$\begin{aligned}\mathcal{L}_t = \mathbb{E}_{\epsilon} \left[\frac{1}{2\tilde{\beta}_t} \left\| \frac{1}{\sqrt{1-\beta_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon \right) - \right. \right. \\ \left. \left. - \frac{1}{\sqrt{1-\beta_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon_{\theta}(\mathbf{x}_t, t) \right) \right\|^2 \right] = \\ \mathbb{E}_{\epsilon} \left[\frac{\beta_t^2}{2\tilde{\beta}_t(1-\beta_t)} \left\| \frac{\epsilon}{\sqrt{1-\bar{\alpha}_t}} - \frac{\epsilon_{\theta}(\textcolor{teal}{x}_t, t)}{\sqrt{1-\bar{\alpha}_t}} \right\|^2 \right]\end{aligned}$$

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

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

Outline

1. Gaussian diffusion process

Forward gaussian diffusion process

Reverse gaussian diffusion process

2. Denoising diffusion probabilistic model (DDPM)

Objective of DDPM

Reparametrization of DDPM

Overview of DDPM

Denoising diffusion probabilistic model (DDPM)

DDPM is a VAE model

- ▶ Encoder is a fixed Gaussian Markov chain.
- ▶ 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.
- ▶ Prior distribution is given by parametric Gaussian Makov chain.

Forward process

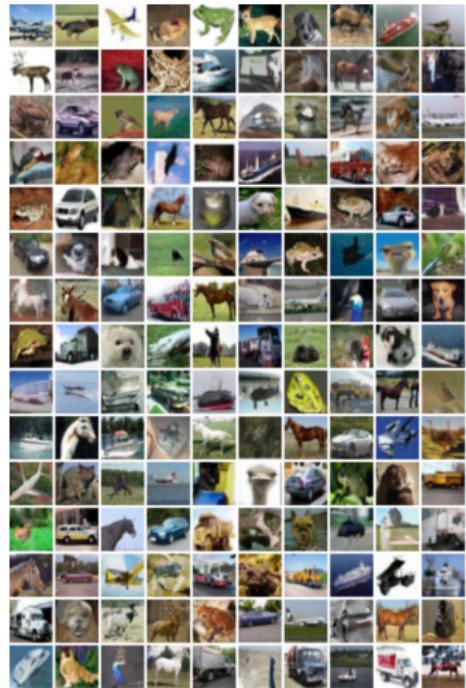
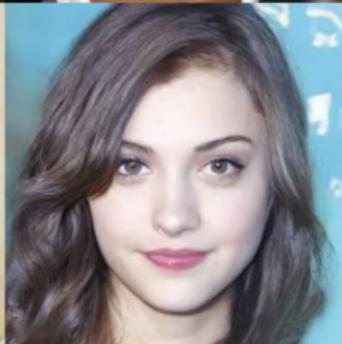
1. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$
2. $\mathbf{x}_t = \sqrt{1 - \beta} \cdot \mathbf{x}_{t-1} + \sqrt{\beta} \cdot \boldsymbol{\epsilon},$
where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, 1), t \geq 1;$
3. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, 1).$

Reverse process

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

Samples



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.
- ▶ At each step DDPM predicts the noise that was used in forward diffusion process.