

Deep Generative Models

Lecture 14

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Spring, 2022

Recap of previous lecture

Continuous dynamic

$$\frac{d\mathbf{z}(t)}{dt} = f(\mathbf{z}(t), \theta).$$

Forward pass

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

Backward pass

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

Recap of previous lecture

Continuous normalizing flows

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

Forward transform + log-density

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

Hutchinson's trace estimator

$$\begin{aligned} \log p(\mathbf{z}(t_1)) &= \log p(\mathbf{z}(t_0)) - \int_{t_0}^{t_1} \text{tr} \left(\frac{\partial f(\mathbf{z}(t), \boldsymbol{\theta})}{\partial \mathbf{z}(t)} \right) dt = \\ &= \log p(\mathbf{z}(t_0)) - \mathbb{E}_{p(\epsilon)} \int_{t_0}^{t_1} \left[\epsilon^T \frac{\partial f}{\partial \mathbf{z}} \epsilon \right] dt. \end{aligned}$$

Recap of previous lecture

SDE basics

Let define stochastic process $\mathbf{x}(t)$ with initial condition $\mathbf{x}(0) \sim p_0(\mathbf{x})$:

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w},$$

where $\mathbf{w}(t)$ is the standard Wiener process (Brownian motion)

$$\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, (t-s)\mathbf{I}), \quad d\mathbf{w} = \epsilon \cdot \sqrt{dt}, \text{ where } \epsilon \sim \mathcal{N}(0, \mathbf{I}).$$

Langevin dynamics

Let \mathbf{x}_0 be a random vector. Then under mild regularity conditions for small enough η samples from the following dynamics

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \eta \frac{1}{2} \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \theta) + \sqrt{\eta} \cdot \epsilon, \quad \epsilon \sim \mathcal{N}(0, \mathbf{I}).$$

will come from $p(\mathbf{x} | \theta)$.

The density $p(\mathbf{x} | \theta)$ is a **stationary** distribution for the Langevin SDE.

Outline

1. Score matching
2. Noise conditioned score network
3. Diffusion models

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Score matching

We could sample from the model if we have $\nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta)$.

Fisher divergence

$$D_F(\pi, p) = \frac{1}{2} \mathbb{E}_{\pi} \| \nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}) \|_2^2 \rightarrow \min_{\theta}$$

Score function

$$\mathbf{s}(\mathbf{x}, \theta) = \nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta)$$

Problem: we do not know $\nabla_{\mathbf{x}} \log \pi(\mathbf{x})$.

Theorem

Under some regularity conditions, it holds

$$\frac{1}{2} \mathbb{E}_{\pi} \| \mathbf{s}(\mathbf{x}, \theta) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}) \|_2^2 = \mathbb{E}_{\pi} \left[\frac{1}{2} \| \mathbf{s}(\mathbf{x}, \theta) \|_2^2 + \text{tr}(\nabla_{\mathbf{x}} \mathbf{s}(\mathbf{x}, \theta)) \right] + \text{const}$$

Here $\nabla_{\mathbf{x}} \mathbf{s}(\mathbf{x}, \theta) = \nabla_{\mathbf{x}}^2 \log p(\mathbf{x}|\theta)$ is a Hessian matrix.

Score matching

Theorem

$$\frac{1}{2} \mathbb{E}_\pi \| \mathbf{s}(\mathbf{x}, \boldsymbol{\theta}) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}) \|_2^2 = \mathbb{E}_\pi \left[\frac{1}{2} \| \mathbf{s}(\mathbf{x}, \boldsymbol{\theta}) \|_2^2 + \text{tr}(\nabla_{\mathbf{x}} \mathbf{s}(\mathbf{x}, \boldsymbol{\theta})) \right] + \text{const}$$

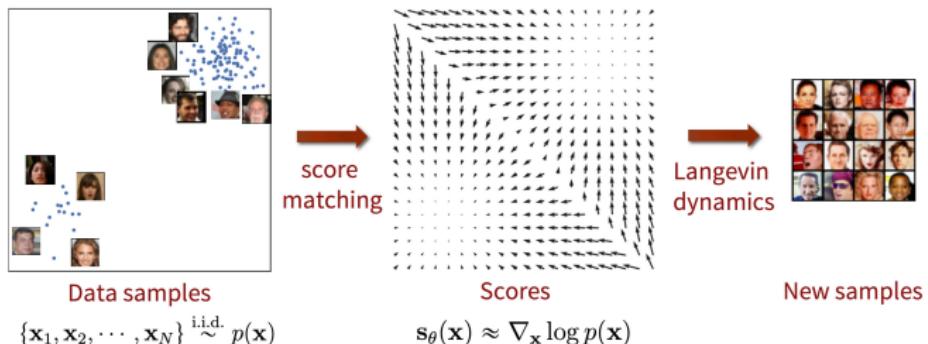
Proof (only for 1D)

$$\mathbb{E}_\pi \| s(x) - \nabla_x \log \pi(x) \|_2^2 = \mathbb{E}_\pi [s(x)^2 + (\nabla_x \log \pi(x))^2 - 2[s(x) \nabla_x \log \pi(x)]]$$

$$\begin{aligned}\mathbb{E}_\pi [s(x) \nabla_x \log \pi(x)] &= \int \pi(x) \nabla_x \log p(x) \nabla_x \log \pi(x) dx \\ &= \int \nabla_x \log p(x) \nabla_x \pi(x) dx = \pi(x) \nabla_x \log p(x) \Big|_{-\infty}^{+\infty} \\ &\quad - \int \nabla_x^2 \log p(x) \pi(x) dx = -\mathbb{E}_\pi \nabla_x^2 \log p(x)\end{aligned}$$

$$\frac{1}{2} \mathbb{E}_\pi \| s(x) - \nabla_x \log \pi(x) \|_2^2 = \frac{1}{2} \mathbb{E}_\pi [s(x)^2 + \nabla_x s(x)] + \text{const.}$$

Score matching



Theorem (implicit score matching)

$$\frac{1}{2}\mathbb{E}_\pi \|\mathbf{s}(\mathbf{x}, \theta) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x})\|_2^2 = \mathbb{E}_\pi \left[\frac{1}{2} \|\mathbf{s}(\mathbf{x}, \theta)\|_2^2 + \text{tr}(\nabla_{\mathbf{x}} \mathbf{s}(\mathbf{x}, \theta)) \right] + \text{const}$$

1. The left hand side is intractable due to unknown $\pi(\mathbf{x})$ – **denoising score matching**.
 2. The right hand side is complex due to Hessian matrix – **sliced score matching**.

Score matching

Sliced score matching (Hutchinson's trace estimation)

$$\text{tr}(\nabla_{\mathbf{x}} \mathbf{s}(\mathbf{x}, \theta)) = \mathbb{E}_{p(\epsilon)} \left[\epsilon^T \nabla_{\mathbf{x}} \mathbf{s}(\mathbf{x}, \theta) \epsilon \right],$$

where $\mathbb{E}[\epsilon] = 0$ and $\text{Cov}(\epsilon) = \mathbf{I}$.

Denoising score matching

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

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

Then the solution of

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

satisfies $\mathbf{s}(\mathbf{x}, \theta, \sigma) \approx \mathbf{s}(\mathbf{x}, \theta, 0) = \mathbf{s}(\mathbf{x}, \theta)$ using small enough noise scale σ .

Song Y. Sliced Score Matching: A Scalable Approach to Density and Score Estimation, 2019

Vincent P. A connection between score matching and denoising autoencoders. Neural computation, 2011

Denoising score matching

Theorem

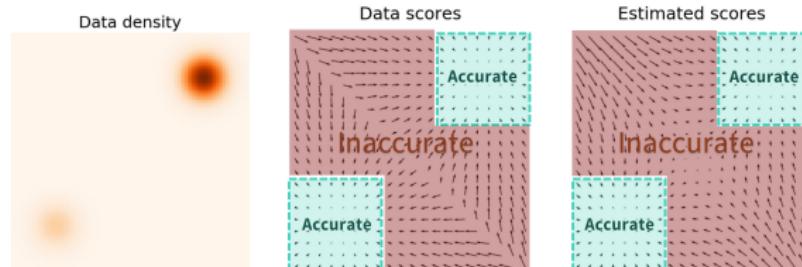
$$\begin{aligned}\mathbb{E}_{\pi(\mathbf{x}|\sigma)} \left\| \mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, \sigma) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}|\sigma) \right\|_2^2 &= \\ &= \mathbb{E}_{\pi(\mathbf{x}')} \mathbb{E}_{p(\mathbf{x}|\mathbf{x}', \sigma)} \left\| \mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, \sigma) - \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{x}', \sigma) \right\|_2^2\end{aligned}$$

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

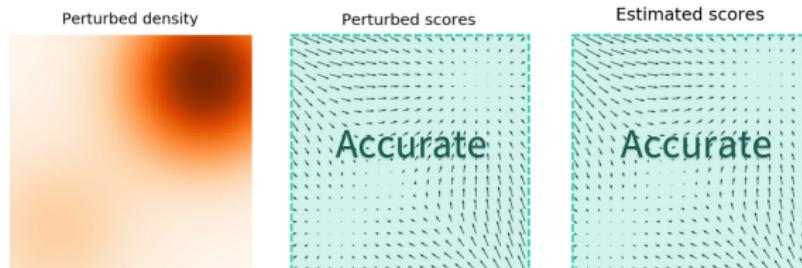
- ▶ The RHS does not need to compute $\nabla_{\mathbf{x}} \pi(\mathbf{x}|\sigma)$ and even more $\nabla_{\mathbf{x}} \pi(\mathbf{x})$.
- ▶ $\mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, \sigma)$ tries to **denoise** a corrupted sample.
- ▶ Score function $\mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, \sigma)$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

Denoising score matching

- If σ is **small**, the score function is not accurate and Langevin dynamics will probably fail to jump between modes.



- If σ is **large**, it is good for low-density regions and multimodal distributions, but we will learn too corrupted distribution.



Outline

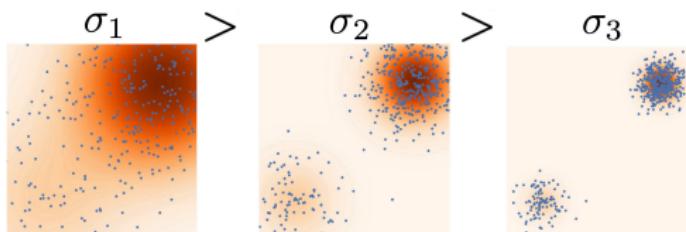
1. Score matching
2. Noise conditioned score network
3. Diffusion models

Noise conditioned score network

- ▶ Define the sequence of noise levels: $\sigma_1 > \sigma_2 > \dots > \sigma_L$.
- ▶ Perturb the original data with the different noise level to get $\pi(\mathbf{x}|\sigma_1), \dots, \pi(\mathbf{x}|\sigma_L)$.
- ▶ Train denoised score function $\mathbf{s}(\mathbf{x}, \theta, \sigma)$ for each noise level:

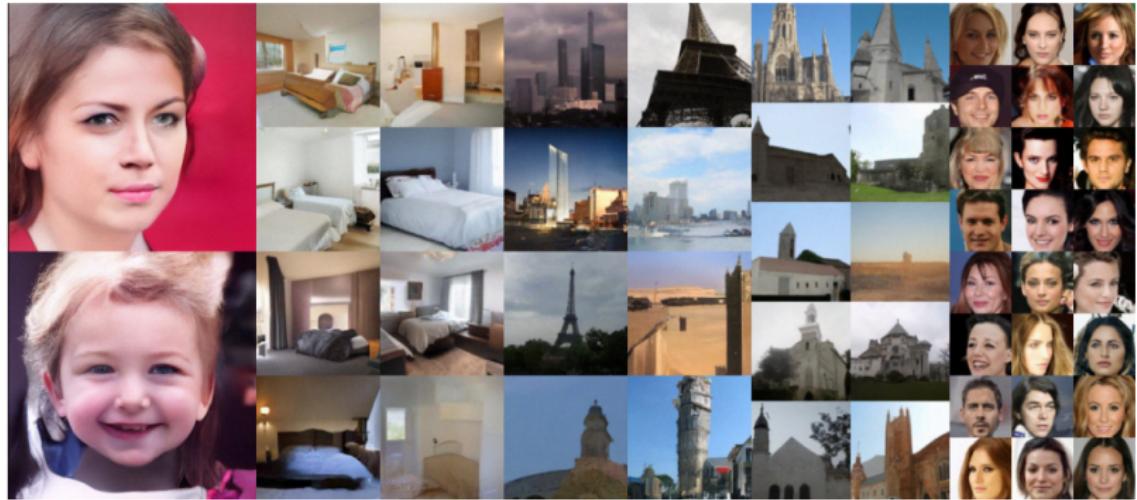
$$\sum_{l=1}^L \sigma_l^2 \mathbb{E}_{\pi(\mathbf{x}')} \mathbb{E}_{p(\mathbf{x}|\mathbf{x}', \sigma_l)} \| \mathbf{s}(\mathbf{x}, \theta, \sigma_l) - \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{x}', \sigma_l) \|_2^2 \rightarrow \min_{\theta}$$

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



Noise conditioned score network

Samples



Outline

1. Score matching
2. Noise conditioned score network
3. Diffusion models

Forward diffusion process

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

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

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

Statement

Applying the Markov chain to samples from any $\pi(\mathbf{x})$ we will get $\mathbf{x}_\infty \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, 1)$. Here $p_\infty(\mathbf{x})$ is a **stationary** distribution:

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

Statement

Denote $\alpha_t = 1 - \beta_t$, $\bar{\alpha}_t = \prod_{s=1}^t \alpha_s$. Then

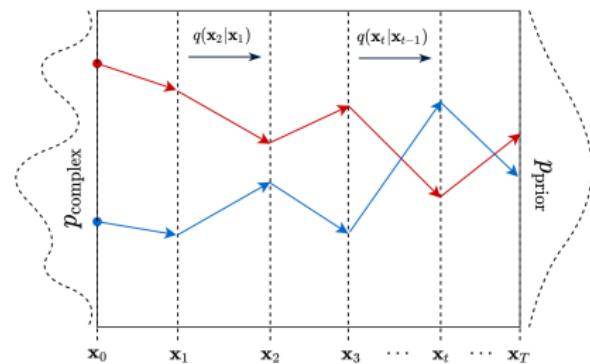
$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1)$$

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

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

Forward diffusion process

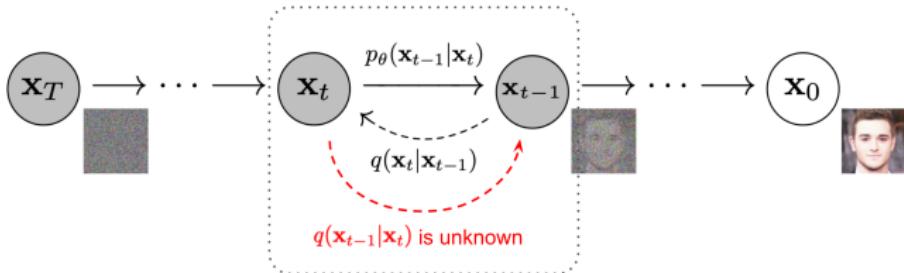
Diffusion refers to the flow of particles from high-density regions towards low-density regions.



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

Now our goal is to revert this process.

Reverse diffusion process



Let define the reverse process

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

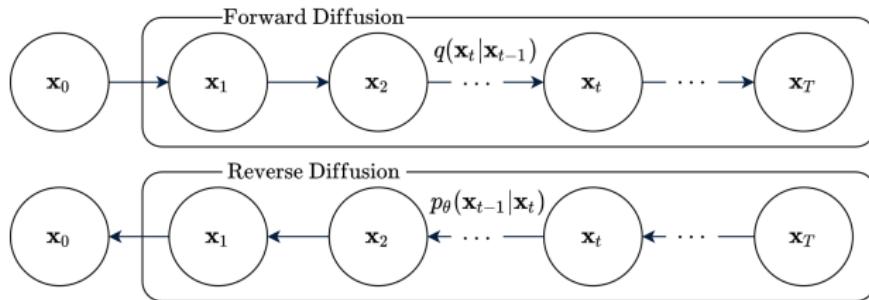
Forward process

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

Diffusion model



- ▶ Let treat $\mathbf{z} = (\mathbf{x}_1, \dots, \mathbf{x}_T)$ as a latent variable.
- ▶ Variational posterior distribution

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

- ▶ 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

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

Diffusion model

ELBO

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

Statement

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

- ▶ **First term** is constant (KL between two standard normals).
- ▶ **Third term** is a decoder distribution (could be AR model or discretized distribution (like mixture of logistics)).

Diffusion model

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

Here

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

$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0)$ and $\tilde{\beta}_t$ have analytical formulas (we omit it) and both dependent on β_t .

- ▶ Assume $\Sigma(\mathbf{x}_t, \theta, t) = \tilde{\beta}_t \mathbf{I}$ (reminder:
 $p(\mathbf{x}_{t-1}|\mathbf{x}_t, \theta) = \mathcal{N}(\mathbf{x}_{t-1}|\mu(\mathbf{x}_t, \theta, t), \Sigma(\mathbf{x}_t, \theta, t))$).
- ▶ Use KL formula for normal distributions.
- ▶ Use the fact $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}$

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

Diffusion model

Reparametrization

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

KL term

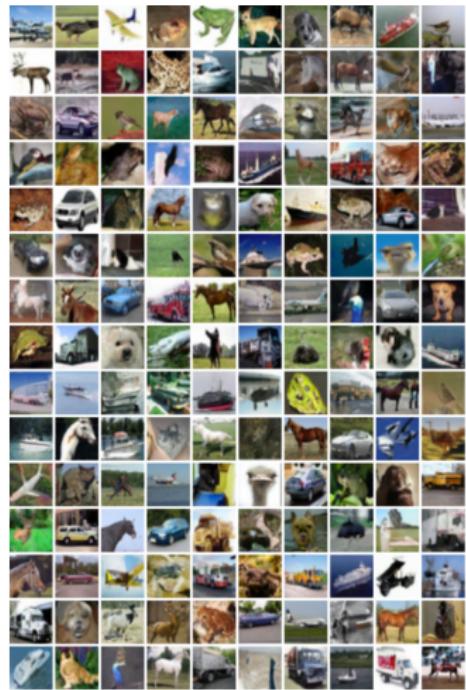
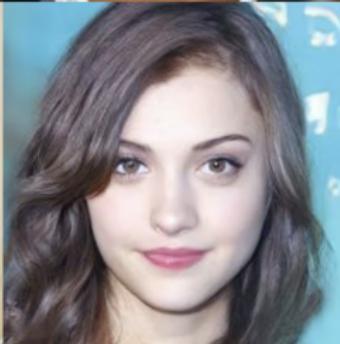
$$\begin{aligned} \mathcal{L}_t &= \mathbb{E}_{\epsilon} \left[\frac{1}{2\tilde{\beta}_t} \left\| \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1 - \bar{\alpha}_t}} \epsilon \right) - \mu(\mathbf{x}_t, \boldsymbol{\theta}, t) \right\|^2 \right] \\ &= \mathbb{E}_{\epsilon} \left[\frac{\beta_t^2}{2\tilde{\beta}_t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

Noise conditioned score network

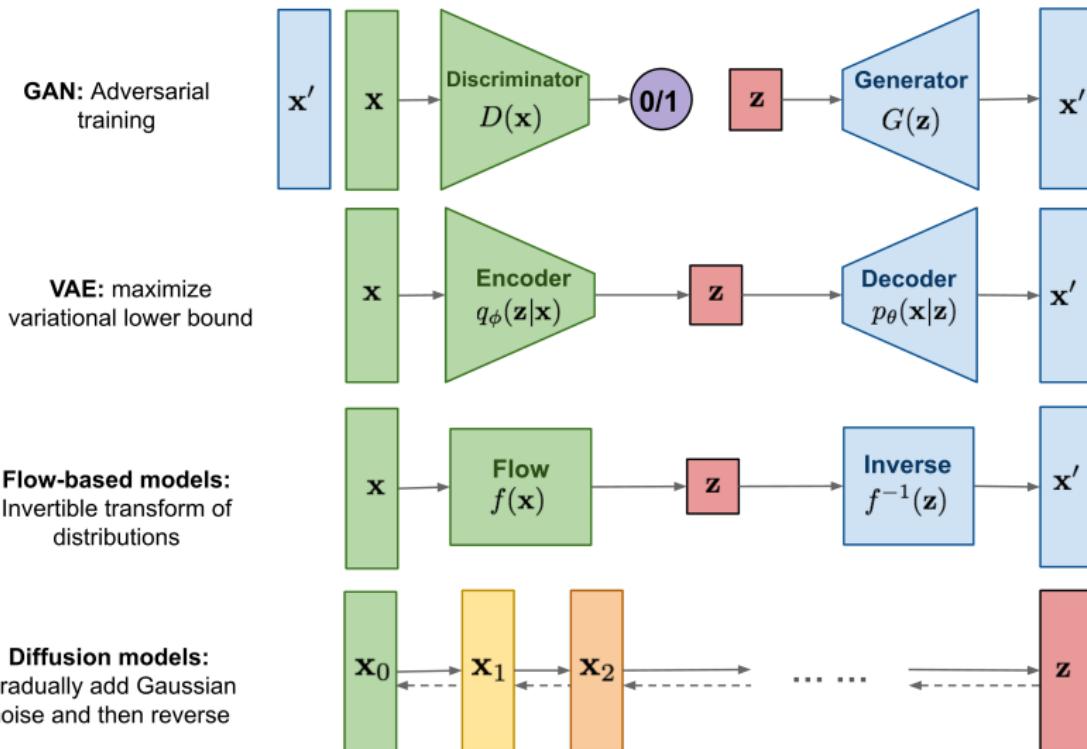
$$\mathbb{E}_{p(\mathbf{x}|\mathbf{x}', \sigma_I)} \|\mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, \sigma_I) - \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{x}', \sigma_I)\|_2^2 \rightarrow \min_{\boldsymbol{\theta}}$$

Denoising diffusion probabilistic model

Samples



The poorest course overview :)



Summary

- ▶ Score matching proposes to minimize Fisher divergence to get score function.
- ▶ Sliced score matching and denoising score matching are two techniques to get scalable algorithm for fitting Fisher divergence.
- ▶ Noise conditioned score nework uses multiple noise levels and annealed Langevin dynamics to fit score function.
- ▶ Gaussian diffusion process is a Markov chain that inject Gaussian noise.
- ▶ Diffusion model is a VAE model which revert gaussian diffusion process using variational inference.
- ▶ Objective of diffusion model is closely related to the noise conditioned score network.