Deep Generative Models

Lecture 13

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Recap of previous lecture

Continuous dynamic

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

Forward pass

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

Backward pass

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

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

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

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

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

Grathwohl W. et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models, 2018

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)

$$\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, t - s), \quad d\mathbf{w} = \boldsymbol{\epsilon} \cdot \sqrt{dt}, \text{ where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1).$$

Langevin dynamics

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

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

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

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

Welling M. Bayesian Learning via Stochastic Gradient Langevin Dynamics, 2011

Outline

1. Score matching

2. Diffusion models

Outline

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2. Diffusion models

Score matching

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

Fisher divergence

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

Score function

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

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

Theorem

Under some regularity conditions, it holds

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

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

Hyvarinen A. Estimation of non-normalized statistical models by score matching, 2005

Score matching

Theorem

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

Proof (only for 1D)

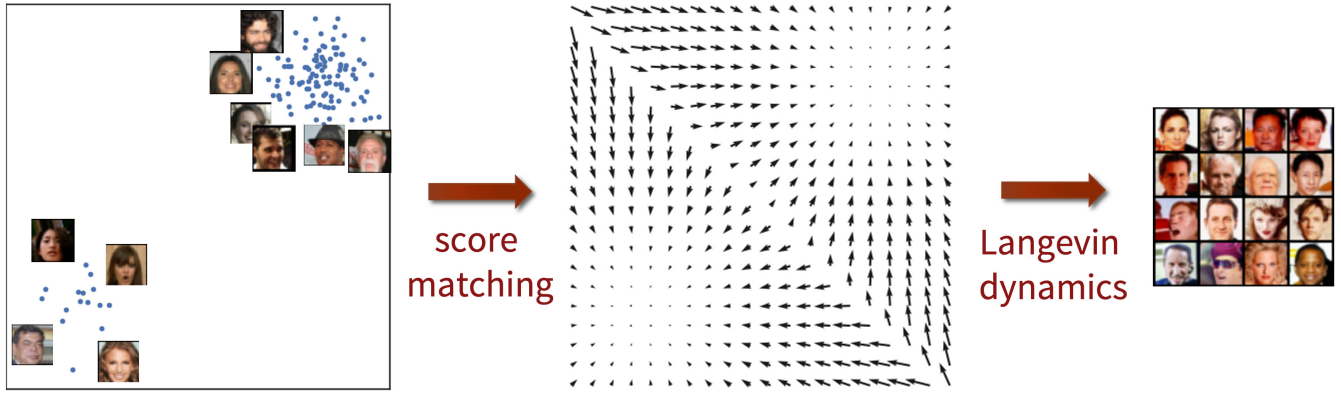
$$\mathbb{E}_\pi \left\| s(x) - \nabla_x \log \pi(x) \right\|_2^2 = \mathbb{E}_\pi \left[s(x)^2 + (\nabla_x \log \pi(x))^2 - 2[s(x) \nabla_x \log \pi(x)] \right]$$

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

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

Hyvarinen A. Estimation of non-normalized statistical models by score matching, 2005

Score matching



Data samples

$\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\} \overset{\text{i.i.d.}}{\sim} p(\mathbf{x})$

Scores

$\mathbf{s}_\theta(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p(\mathbf{x})$

New samples

Theorem (implicit score matching)

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

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**.

Song Y. Generative Modeling by Estimating Gradients of the Data Distribution, blog post, 2021

Score matching

Sliced score matching (Hutchinson's trace estimation)

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

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

Denoising score mathing

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

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

satisfies $\mathbf{s}(\mathbf{x},\boldsymbol{\theta},\sigma) \approx \mathbf{s}(\mathbf{x},\boldsymbol{\theta},0) = \mathbf{s}(\mathbf{x},\boldsymbol{\theta})$ 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

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

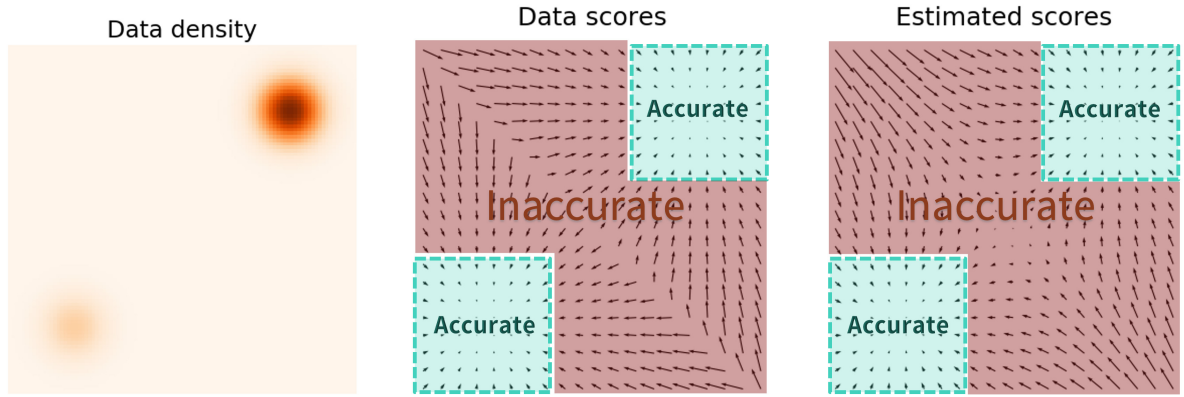
Here $\nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{x}',\sigma) = -\frac{\mathbf{x}-\mathbf{x}'}{\sigma^2}$.

- 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?

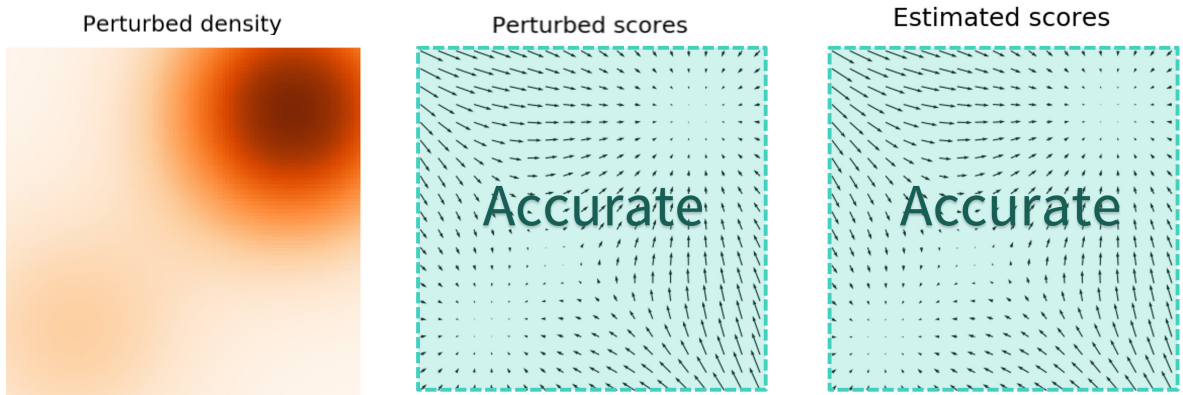
Vincent P. A Connection Between Score Matching and Denoising Autoencoders, 2010

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.



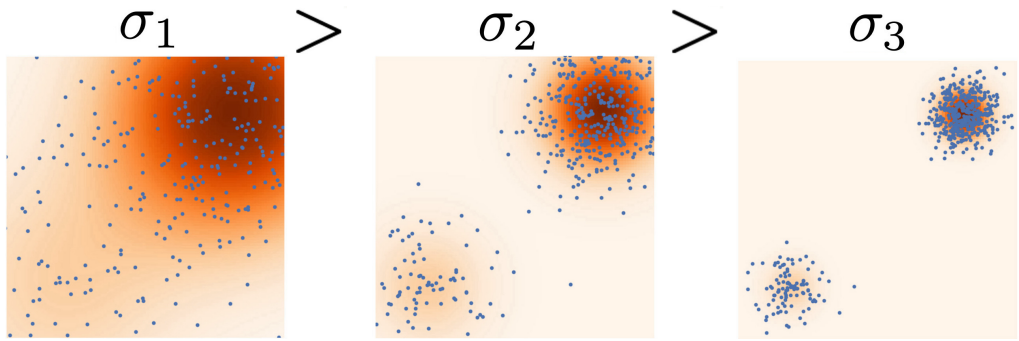
Song Y. Generative Modeling by Estimating Gradients of the Data Distribution, blog post, 2021

Noice conditioned score network

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

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

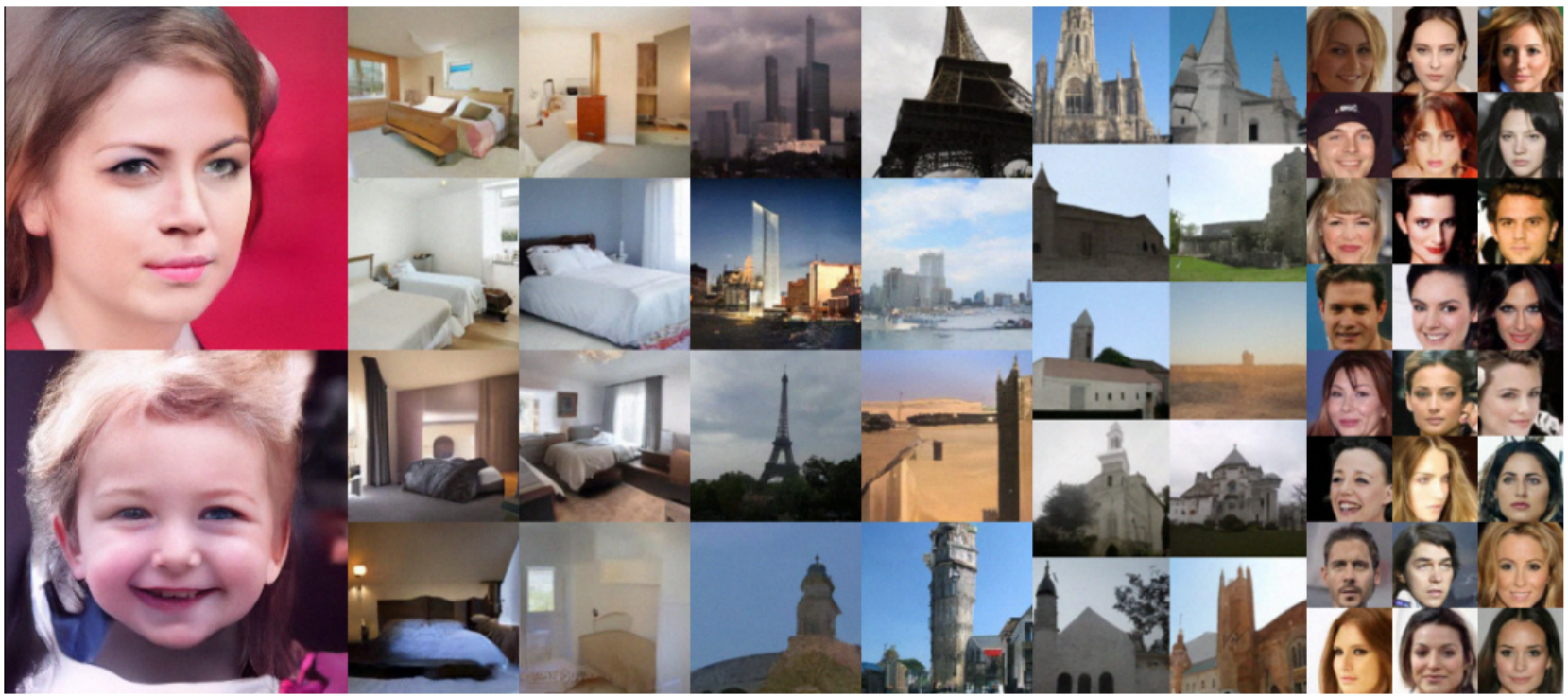
- Sample from **annealed** Langevin dynamics (for $l = 1, \ldots, L$).



Song Y. et al. Generative Modeling by Estimating Gradients of the Data Distribution, 2019

Noice conditioned score network

Samples



Song Y. et al. Improved Techniques for Training Score-Based Generative Models, 2020

Outline

1. Score matching
2. Diffusion models

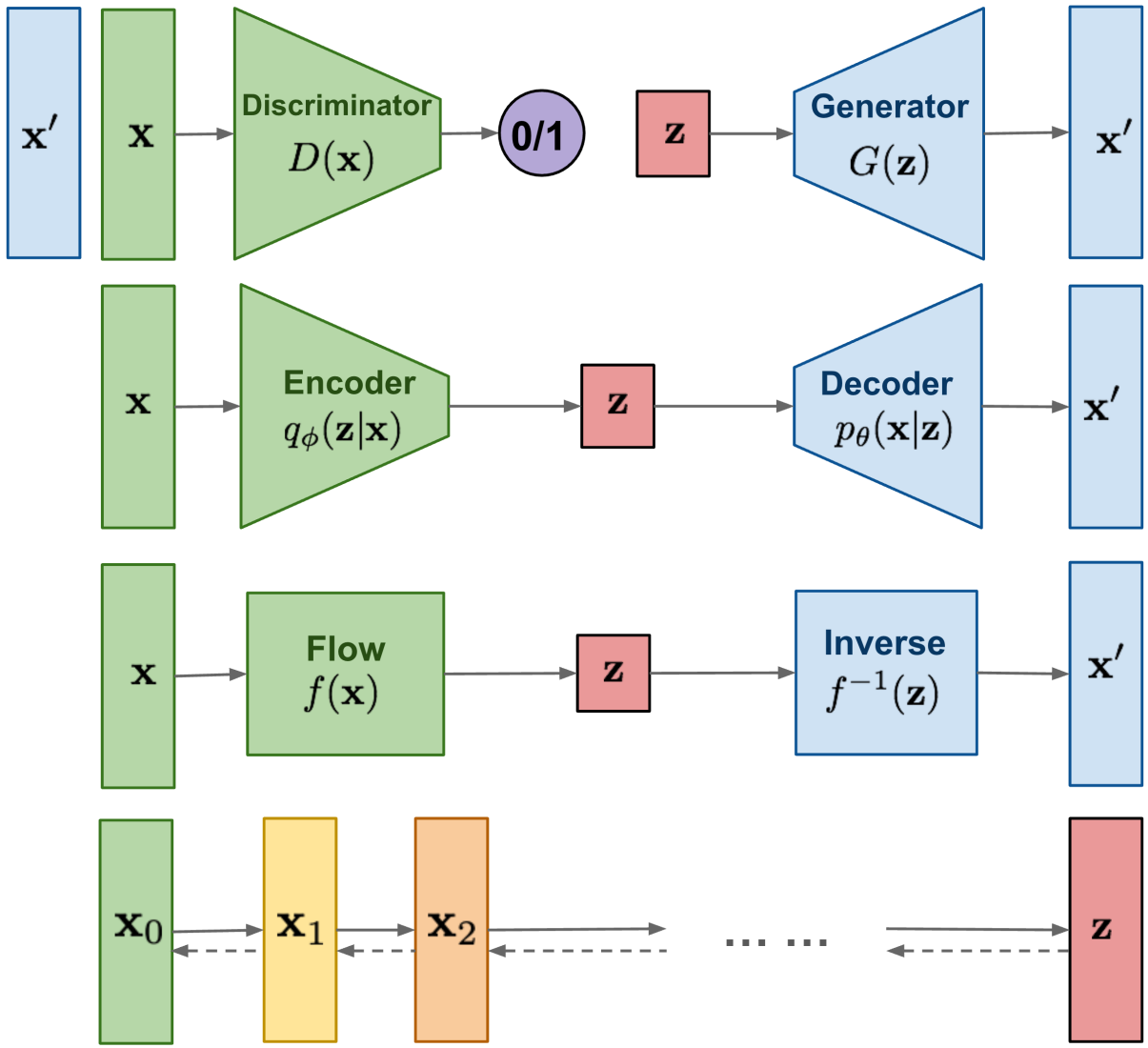
The poorest course overview :)

GAN: Adversarial training

VAE: maximize variational lower bound

Flow-based models: Invertible transform of distributions

Diffusion models: Gradually add Gaussian noise and then reverse



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

Summary

- Score matching proposes to minimize Fisher divergence to get score function.

- Sliced score matching and denoised score matching are two techniques to get scalable algorithm for fitting Fisher divergence.