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

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Score matching

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

Fisher divergence

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

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

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

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

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

Score matching

Theorem

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

Proof (only for 1D)

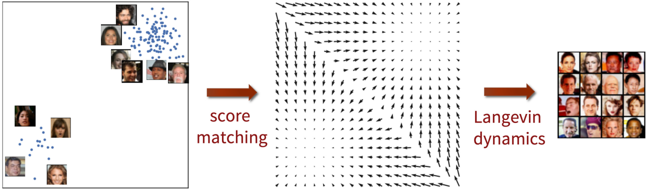
$$\mathbb{E}_{\pi}\left\|s(x)-\nabla_x\log\pi(x)\right\|_2^2=\mathbb{E}_{\pi}\left[s(x)^2+(\nabla_x\log\pi(x))^2-2[s(x)\nabla_x\log\pi(x)]\right]$$

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

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

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

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

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)

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

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

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

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.

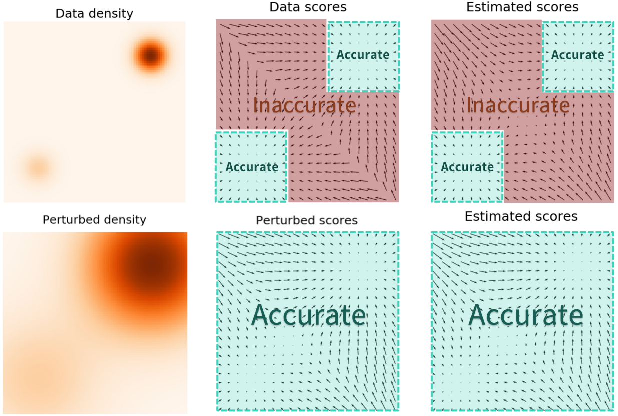
Song Y. Sliced Score Matching: A Scalable Approach to Density and Score Estimation, 2019

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

Denoising score matching

Theorem

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



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