Deep Generative Models

Lecture 13

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Outline

1. Score matching

Recap of previous lecture

Outline

1. Score matching

Score matching

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

Fisher divergence

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

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

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

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

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

Score matching

Theorem

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

Proof (only for 1D)

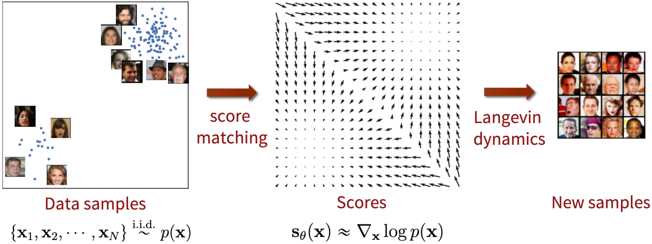
$$\mathbb{E}_\pi \left\| s(x) - \nabla_x \log \pi(x) \right\|_2^2 = \mathbb{E}_\pi \left[s(x)^2 + (\nabla_x \log \pi(x))^2 - 2[s(x) \nabla_x \log \pi(x)] \right]$$

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

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

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

Score matching



Theorem

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

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.

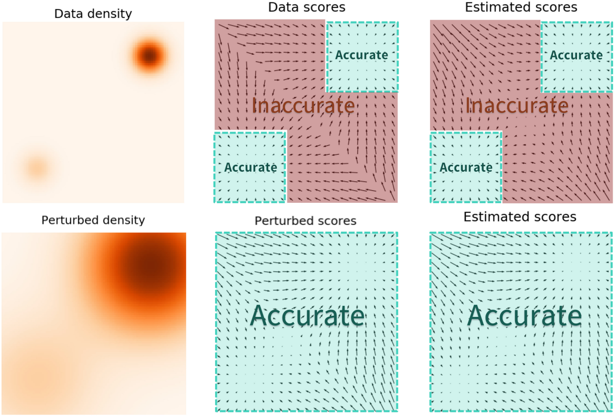
Song Y. Sliced Score Matching: A Scalable Approach to Density and Score Estimation, 2019

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.