

Deep Generative Models

Lecture 10

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Recap of previous lecture

How to evaluate likelihood-free models?

$p(y|x)$ – pretrained image classification model (e.g. ImageNet classifier).

What do we want from samples?

- ▶ Sharpness



$p(y|x)$ has low entropy (each image x should have distinctly recognizable object).

- ▶ Diversity



$p(y) = \int p(y|x)p(x)dx$ has high entropy (there should be as many classes generated as possible).

Recap of previous lecture

Let's take some pretrained image classification model to get the conditional label distribution $p(y|\mathbf{x})$ (e.g. ImageNet classifier).

Evaluation of likelihood-free models

- ▶ Sharpness \Rightarrow low $H(y|\mathbf{x}) = -\sum_y \int_{\mathbf{x}} p(y, \mathbf{x}) \log p(y|\mathbf{x}) d\mathbf{x}$.
- ▶ Diversity \Rightarrow high $H(y) = -\sum_y p(y) \log p(y)$.

Inception Score

$$IS = \exp(H(y) - H(y|\mathbf{x})) = \exp(\mathbb{E}_{\mathbf{x}} KL(p(y|\mathbf{x}) || p(y)))$$

Frechet Inception Distance

$$D^2(\pi, p) = \|\mathbf{m}_\pi - \mathbf{m}_p\|_2^2 + \text{Tr} \left(\boldsymbol{\Sigma}_\pi + \boldsymbol{\Sigma}_p - 2\sqrt{\boldsymbol{\Sigma}_\pi \boldsymbol{\Sigma}_p} \right).$$

FID is related to moment matching.

Salimans T. et al. *Improved Techniques for Training GANs*, 2016

Heusel M. et al. *GANs Trained by a Two Time-Scale Update Rule Converge to a Local Nash Equilibrium*, 2017

Recap of previous lecture

- ▶ $\mathcal{S}_\pi = \{\mathbf{x}_i\}_{i=1}^n \sim \pi(\mathbf{x})$ – real samples;
- ▶ $\mathcal{S}_p = \{\mathbf{x}_i\}_{i=1}^n \sim p(\mathbf{x}|\boldsymbol{\theta})$ – generated samples.

Embed samples using pretrained classifier network (as previously):

$$\mathcal{G}_\pi = \{\mathbf{g}_i\}_{i=1}^n, \quad \mathcal{G}_p = \{\mathbf{g}_i\}_{i=1}^n.$$

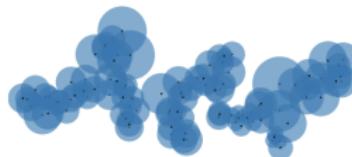
Define binary function:

$$f(\mathbf{g}, \mathcal{G}) = \begin{cases} 1, & \text{if exists } \mathbf{g}' \in \mathcal{G} : \|\mathbf{g} - \mathbf{g}'\|_2 \leq \|\mathbf{g}' - \text{NN}_k(\mathbf{g}', \mathcal{G})\|_2; \\ 0, & \text{otherwise.} \end{cases}$$

$$\text{Precision}(\mathcal{G}_\pi, \mathcal{G}_p) = \frac{1}{n} \sum_{\mathbf{g} \in \mathcal{G}_p} f(\mathbf{g}, \mathcal{G}_\pi); \quad \text{Recall}(\mathcal{G}_\pi, \mathcal{G}_p) = \frac{1}{n} \sum_{\mathbf{g} \in \mathcal{G}_\pi} f(\mathbf{g}, \mathcal{G}_p).$$



(a) True manifold



(b) Approx. manifold

Outline

1. Langevin dynamic
2. Denoising score matching
3. Noise Conditioned Score Network (NCSN)

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Langevin dynamic

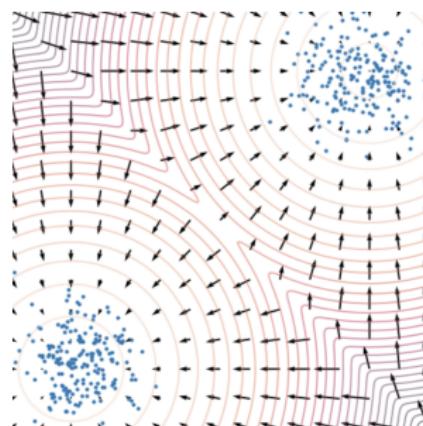
Statement

Let \mathbf{x}_0 be a random vector. Then 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 $p(\mathbf{x} | \theta)$ under mild regularity conditions for small enough η and large enough t .

- ▶ Here we assume that we already have some generative model $p(\mathbf{x} | \theta)$.
- ▶ The density $p(\mathbf{x} | \theta)$ is a **stationary** distribution for this SDE.
- ▶ What do we get if $\epsilon = \mathbf{0}$?



Energy-based models

- ▶ We could sample from the model using Langevin dynamics if we have $\nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta)$.
- ▶ Where is it helpful?

Unnormalized density

$$p(\mathbf{x}|\theta) = \frac{\hat{p}(\mathbf{x}|\theta)}{Z_\theta}, \quad \text{where } Z_\theta = \int \hat{p}(\mathbf{x}|\theta) d\mathbf{x}$$

- ▶ $\hat{p}(\mathbf{x}|\theta)$ is any non-negative function.
- ▶ If we use the reparametrization $\hat{p}(\mathbf{x}|\theta) = \exp(-f_\theta(\mathbf{x}))$, we remove the non-negativite constraint.

$$\nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta) = \nabla_{\mathbf{x}} \log \hat{p}(\mathbf{x}|\theta) - \nabla_{\mathbf{x}} \log Z_\theta = \nabla_{\mathbf{x}} \log \hat{p}(\mathbf{x}|\theta)$$

The gradient of the normalized density equals to the gradient of the unnormalized density.

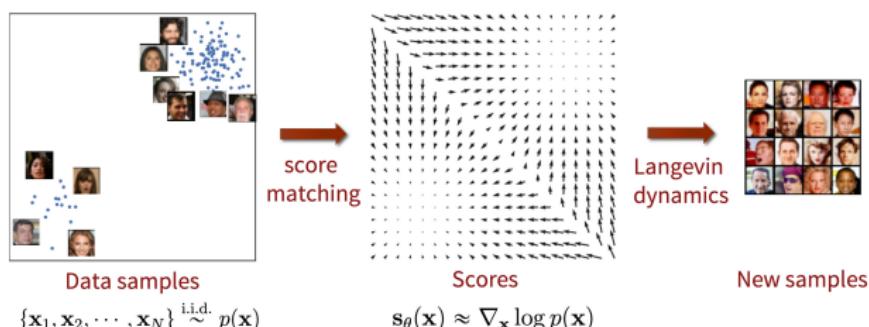
Score matching

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

Fisher divergence

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

Let introduce **score function** $s_{\theta}(\mathbf{x}) = \nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta)$.



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

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3. Noise Conditioned Score Network (NCSN)

Denoising score matching

Let perturb original data $\mathbf{x} \sim \pi(\mathbf{x})$ by random normal noise

$$\mathbf{x}' = \mathbf{x} + \sigma \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}), \quad p(\mathbf{x}' | \mathbf{x}, \sigma) = \mathcal{N}(\mathbf{x}' | \mathbf{x}, \sigma^2 \mathbf{I})$$

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

Assumption

The solution of

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

satisfies $\mathbf{s}_\theta(\mathbf{x}', \sigma) \approx \mathbf{s}_\theta(\mathbf{x}', 0) = \mathbf{s}_\theta(\mathbf{x})$ if σ is small enough.

- ▶ $\mathbf{s}_\theta(\mathbf{x}', \sigma)$ tries to **denoise** a corrupted sample \mathbf{x}' .
- ▶ Score function $\mathbf{s}_\theta(\mathbf{x}', \sigma)$ parametrized by σ .

Denoising score matching

Theorem

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

Proof

$$\begin{aligned}\mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \left\| \mathbf{s}_\theta(\mathbf{x}', \sigma) - \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \right\|_2^2 &= \\ &= \mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \left[\left\| \mathbf{s}_\theta(\mathbf{x}', \sigma) \right\|^2 + \underbrace{\left\| \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \right\|_2^2}_{\text{const}(\theta)} - 2 \mathbf{s}_\theta^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \right] \\ \mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \left\| \mathbf{s}_\theta(\mathbf{x}', \sigma) \right\|^2 &= \int \pi(\mathbf{x}'|\sigma) \left\| \mathbf{s}_\theta(\mathbf{x}', \sigma) \right\|^2 d\mathbf{x}' = \\ &= \int \left(\int p(\mathbf{x}'|\mathbf{x}, \sigma) \pi(\mathbf{x}) d\mathbf{x} \right) \left\| \mathbf{s}_\theta(\mathbf{x}', \sigma) \right\|^2 d\mathbf{x}' = \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{p(\mathbf{x}'|\mathbf{x}, \sigma)} \left\| \mathbf{s}_\theta(\mathbf{x}', \sigma) \right\|^2 d\mathbf{x}'\end{aligned}$$

Denoising score matching

Theorem

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

Proof (continued)

$$\begin{aligned}\mathbb{E}_{\pi(\mathbf{x}'|\sigma)} [\mathbf{s}_\theta^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma)] &= \int \pi(\mathbf{x}'|\sigma) \left[\mathbf{s}_\theta^T(\mathbf{x}', \sigma) \frac{\nabla_{\mathbf{x}'} \pi(\mathbf{x}'|\sigma)}{\pi(\mathbf{x}'|\sigma)} \right] d\mathbf{x}' = \\ &= \int \left[\mathbf{s}_\theta^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} \left(\int p(\mathbf{x}'|\mathbf{x}, \sigma) \pi(\mathbf{x}) d\mathbf{x} \right) \right] d\mathbf{x}' = \\ &= \int \int \pi(\mathbf{x}) [\mathbf{s}_\theta^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} p(\mathbf{x}'|\mathbf{x}, \sigma)] d\mathbf{x}' d\mathbf{x} = \\ &= \int \int \pi(\mathbf{x}) p(\mathbf{x}'|\mathbf{x}, \sigma) [\mathbf{s}_\theta^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} \log p(\mathbf{x}'|\mathbf{x}, \sigma)] d\mathbf{x}' d\mathbf{x} = \\ &= \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{p(\mathbf{x}'|\mathbf{x}, \sigma)} [\mathbf{s}_\theta^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} \log p(\mathbf{x}'|\mathbf{x}, \sigma)]\end{aligned}$$

Denoising score matching

Theorem

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

Proof (continued)

$$\begin{aligned}\mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \left\| \mathbf{s}_\theta(\mathbf{x}', \sigma) - \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \right\|_2^2 &= \\ &= \mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \left[\left\| \mathbf{s}_\theta(\mathbf{x}', \sigma) \right\|^2 - 2 \mathbf{s}_\theta^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \right] + \text{const}(\theta) = \\ &= \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{p(\mathbf{x}'|\mathbf{x}, \sigma)} \left[\left\| \mathbf{s}_\theta(\mathbf{x}', \sigma) \right\|^2 - 2 \mathbf{s}_\theta^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} \log p(\mathbf{x}'|\mathbf{x}, \sigma) \right] + \text{const}(\theta)\end{aligned}$$

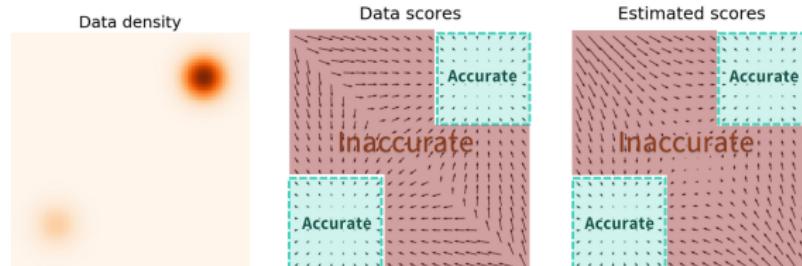
Gradient of the noise kernel

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

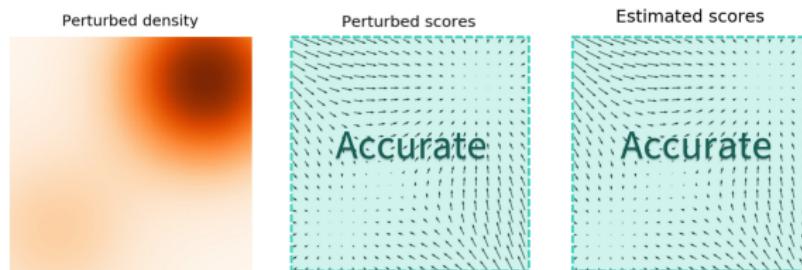
The RHS does not need to compute $\nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma)$ and even $\nabla_{\mathbf{x}'} \log \pi(\mathbf{x}')$.

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.



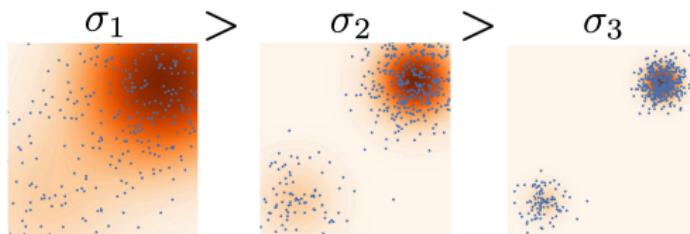
Outline

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Noise Conditioned Score Network (NCSN)

- ▶ Define the sequence of the noise levels: $\sigma_1 > \sigma_2 > \dots > \sigma_L$.
- ▶ Perturb the original data with the different noise levels to obtain $\pi(\mathbf{x}'|\sigma_1), \dots, \pi(\mathbf{x}'|\sigma_L)$.
- ▶ Choose σ_1, σ_L such that:

$$\pi(\mathbf{x}'|\sigma_1) \approx \mathcal{N}(0, \sigma_1^2 \mathbf{I}), \quad \pi(\mathbf{x}'|\sigma_L) \approx \pi(\mathbf{x}).$$



Noise Conditioned Score Network (NCSN)

Train the denoising score function $s_\theta(\mathbf{x}', \sigma)$ for each noise level using unified weighted objective:

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

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

Training

1. Get the sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Sample noise level $l \sim U[1, L]$ and the noise $\epsilon \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}' = \mathbf{x}_0 + \sigma_l \cdot \epsilon$.
4. Compute loss $\mathcal{L} = \|s_\theta(\mathbf{x}', \sigma_l) + \frac{\epsilon}{\sigma_l}\|^2$.

How to sample from this model?

Noise Conditioned Score Network (NCSN)

Sampling (annealed Langevin dynamics)

- ▶ Sample $\mathbf{x}_0 \sim \mathcal{N}(0, \sigma_1 \mathbf{I}) \approx \pi(\mathbf{x} | \sigma_1)$.
- ▶ Apply T steps of Langevin dynamic

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \frac{1}{2}\eta \mathbf{s}_\theta(\mathbf{x}_{t-1}, \sigma_t) + \sqrt{\eta}\epsilon_t.$$

- ▶ Update $\mathbf{x}_0 := \mathbf{x}_T$ and choose the next σ_t .



Summary

- ▶ Langevin dynamics allows to sample from the generative model using the gradient of the log-likelihood.
- ▶ Score matching proposes to minimize Fisher divergence to get the score function.
- ▶ Denoising score matching minimizes Fisher divergence on noisy samples. It allows to estimate Fisher divergence using samples.
- ▶ Noise conditioned score network uses multiple noise levels and annealed Langevin dynamics to fit score function and sample from the model.