

Deep Generative Models

Lecture 8

Roman Isachenko

Moscow Institute of Physics and Technology
Yandex School of Data Analysis

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Recap of previous lecture

f-divergence minimization

$$D_f(\pi || p) = \mathbb{E}_{p(\mathbf{x})} f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) \rightarrow \min_p .$$

Here $f : \mathbb{R}_+ \rightarrow \mathbb{R}$ is a convex, lower semicontinuous function satisfying $f(1) = 0$.

Variational divergence estimation

$$D_f(\pi || p) \geq \sup_{T \in \mathcal{T}} [\mathbb{E}_\pi T(\mathbf{x}) - \mathbb{E}_p f^*(T(\mathbf{x}))],$$

Fenchel conjugate

$$f^*(t) = \sup_{u \in \text{dom}_f} (ut - f(u)), \quad f(u) = \sup_{t \in \text{dom}_{f^*}} (ut - f^*(t))$$

Note: To evaluate lower bound we only need samples from $\pi(\mathbf{x})$ and $p(\mathbf{x})$. Hence, we could fit implicit generative model.

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

Frechet Inception Distance (FID)

In case of Normal distributions $\pi(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_\pi, \boldsymbol{\Sigma}_\pi)$,
 $p(\mathbf{y}) = \mathcal{N}(\boldsymbol{\mu}_p, \boldsymbol{\Sigma}_p)$:

$$\begin{aligned}\text{FID}(\pi, p) &= W_2^2(\pi, p) = \inf_{\gamma \in \Gamma(\pi, p)} \mathbb{E}_{(\mathbf{x}, \mathbf{y}) \sim \gamma} \|\mathbf{x} - \mathbf{y}\|^2 \\ &= \|\boldsymbol{\mu}_\pi - \boldsymbol{\mu}_p\|_2^2 + \text{tr} \left[\boldsymbol{\Sigma}_\pi + \boldsymbol{\Sigma}_p - 2 \left(\boldsymbol{\Sigma}_\pi^{1/2} \boldsymbol{\Sigma}_p \boldsymbol{\Sigma}_\pi^{1/2} \right)^{1/2} \right]\end{aligned}$$

Maximum Mean Discrepancy (MMD)

$\pi(\mathbf{x}) = p(\mathbf{y})$ if and only if $\mathbb{E}_{\pi(\mathbf{x})} f(\mathbf{x}) = \mathbb{E}_{p(\mathbf{y})} f(\mathbf{y})$ for any bounded and continuous f

$$\text{MMD}^2(\pi, p) = \mathbb{E}_{\substack{\mathbf{x} \sim \pi(\mathbf{x}) \\ \mathbf{x}' \sim \pi(\mathbf{x})}} k(\mathbf{x}, \mathbf{x}') + \mathbb{E}_{\substack{\mathbf{y} \sim p(\mathbf{y}) \\ \mathbf{y}' \sim p(\mathbf{y})}} k(\mathbf{y}, \mathbf{y}') - 2 \mathbb{E}_{\substack{\mathbf{x} \sim \pi(\mathbf{x}) \\ \mathbf{y} \sim p(\mathbf{y})}} k(\mathbf{x}, \mathbf{y})$$

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

Jayasumana S. et al. *Rethinking FID: Towards a Better Evaluation Metric for Image Generation*, 2024

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):

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

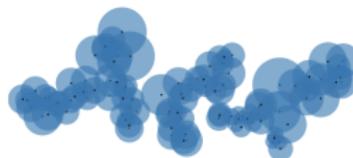
Define binary function:

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

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



(a) True manifold



(b) Approx. manifold

Outline

1. Langevin dynamic
2. Score matching
3. Denoising score matching
4. Noise Conditioned Score Network (NCSN)
5. Forward gaussian diffusion process

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Langevin dynamic

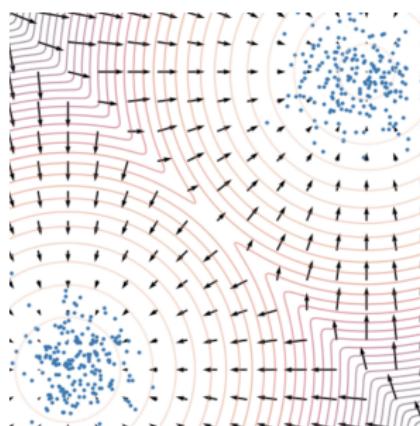
Statement

Let \mathbf{x}_0 be a random vector. Then samples from the following dynamics

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

will come from $p(\mathbf{x} | \theta)$ (under mild regularity conditions, for small enough η and large enough l).

- ▶ 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 the Markov chain.
- ▶ What do we get if $\epsilon = \mathbf{0}$?



Energy-based models

Langevin dynamic

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

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

Unnormalized density

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

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

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

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

Outline

1. Langevin dynamic
2. Score matching
3. Denoising score matching
4. Noise Conditioned Score Network (NCSN)
5. Forward gaussian diffusion process

Score matching

Score function

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

Langevin dynamic

If we find the score function $\mathbf{s}_\theta(\mathbf{x}) = \nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta)$ we will be able to sample from the model using Langevin dynamic.

$$\mathbf{x}_{I+1} = \mathbf{x}_I + \frac{\eta}{2} \cdot \nabla_{\mathbf{x}_I} \log p(\mathbf{x}_I|\theta) + \sqrt{\eta} \cdot \epsilon = \mathbf{x}_I + \frac{\eta}{2} \cdot \mathbf{s}_\theta(\mathbf{x}_I) + \sqrt{\eta} \cdot \epsilon.$$

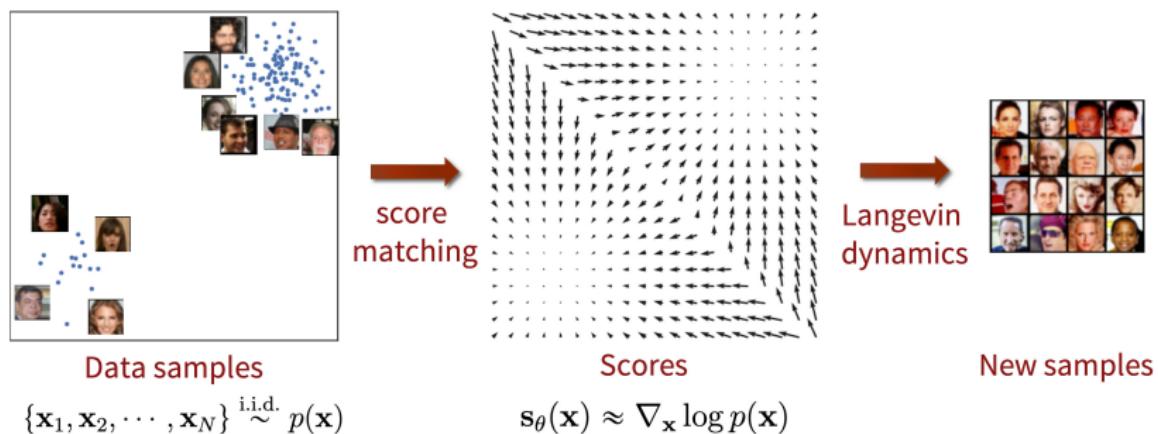
Fisher divergence

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

Score matching

Fisher divergence

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



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

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Denoising score matching

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

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

$$q(\mathbf{x}_\sigma) = \int q(\mathbf{x}_\sigma | \mathbf{x}) \pi(\mathbf{x}) d\mathbf{x}.$$

Assumption

The solution of

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

satisfies $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) \approx \mathbf{s}_{\theta, 0}(\mathbf{x}_0) = \mathbf{s}_\theta(\mathbf{x})$ if σ is small enough.

- ▶ $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma)$ tries to **denoise** a corrupted sample \mathbf{x}_σ .
- ▶ Score function $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma)$ parametrized by σ .
- ▶ **Problem:** We don't know $q(\mathbf{x}_\sigma)$, just like $\pi(\mathbf{x})$.

Denoising score matching

Theorem

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

Proof

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} h(\mathbf{x}_\sigma) &= \int q(\mathbf{x}_\sigma) h(\mathbf{x}_\sigma) d\mathbf{x}_\sigma = \\ &= \int \left(\int q(\mathbf{x}_\sigma|\mathbf{x}) \pi(\mathbf{x}) d\mathbf{x} \right) h(\mathbf{x}_\sigma) d\mathbf{x}_\sigma = \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} h(\mathbf{x}_\sigma) d\mathbf{x}_\sigma \end{aligned}$$

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

Denoising score matching

Theorem

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

Proof (continued)

$$\begin{aligned}\mathbb{E}_{q(\mathbf{x}_\sigma)} [\mathbf{s}_{\theta,\sigma}^T(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)] &= \int q(\mathbf{x}_\sigma) \left[\mathbf{s}_{\theta,\sigma}^T(\mathbf{x}_\sigma) \frac{\nabla_{\mathbf{x}_\sigma} q(\mathbf{x}_\sigma)}{q(\mathbf{x}_\sigma)} \right] d\mathbf{x}_\sigma = \\ &= \int \left[\mathbf{s}_{\theta,\sigma}^T(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \left(\int q(\mathbf{x}_\sigma|\mathbf{x}) \pi(\mathbf{x}) d\mathbf{x} \right) \right] d\mathbf{x}_\sigma = \\ &= \int \int \pi(\mathbf{x}) [\mathbf{s}_{\theta,\sigma}^T(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} q(\mathbf{x}_\sigma|\mathbf{x})] d\mathbf{x}_\sigma d\mathbf{x} = \\ &= \int \int \pi(\mathbf{x}) q(\mathbf{x}_\sigma|\mathbf{x}) [\mathbf{s}_{\theta,\sigma}^T(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})] d\mathbf{x}_\sigma d\mathbf{x} = \\ &= \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} [\mathbf{s}_{\theta,\sigma}^T(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})]\end{aligned}$$

Denoising score matching

Theorem

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

Proof (continued)

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

Gradient of the noise kernel

$$\nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x}) = \nabla_{\mathbf{x}_\sigma} \log \mathcal{N}(\mathbf{x}, \sigma^2 \mathbf{I}) = -\frac{\mathbf{x}_\sigma - \mathbf{x}}{\sigma^2} = -\frac{\boldsymbol{\epsilon}}{\sigma}$$

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

Denoising score matching

Initial objective:

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

Noised objective:

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

This is equivalent to denoising task

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

$$\mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{\mathcal{N}(0, \mathbf{I})} \left\| \mathbf{s}_{\theta,\sigma}(\mathbf{x} + \sigma \cdot \boldsymbol{\epsilon}) + \frac{\boldsymbol{\epsilon}}{\sigma} \right\|_2^2 \rightarrow \min_\theta$$

Langevin dynamic

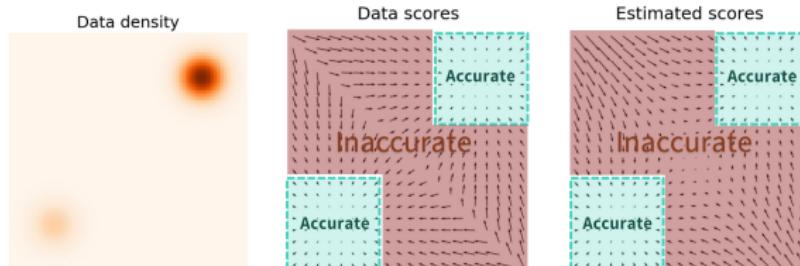
$$\mathbf{x}_{I+1} = \mathbf{x}_I + \frac{\eta}{2} \cdot \mathbf{s}_{\theta,\sigma}(\mathbf{x}_I) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

Outline

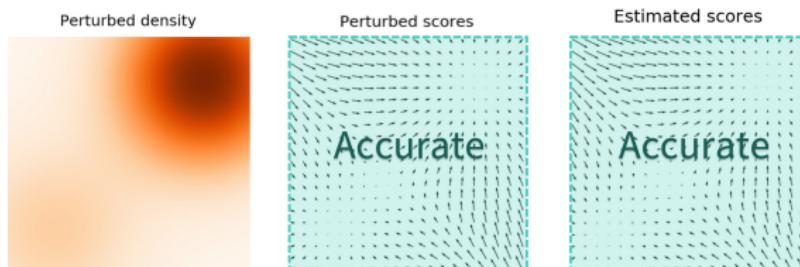
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Denoising score matching

- 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.

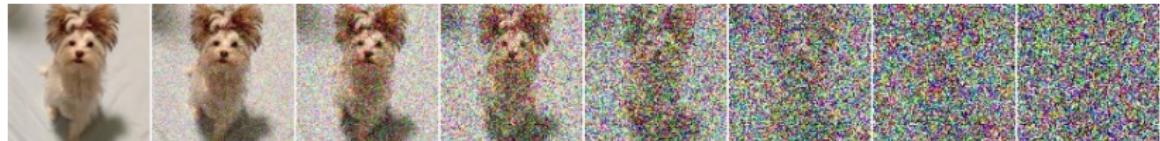
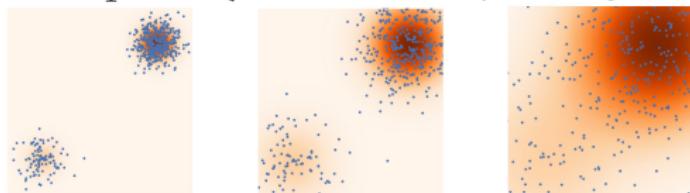


Noise Conditioned Score Network (NCSN)

- ▶ Define the sequence of the noise levels: $\sigma_1 < \sigma_2 < \dots < \sigma_T$.
- ▶ Perturb the original data with the different noise levels to obtain $\mathbf{x}_t = \mathbf{x} + \sigma_t \cdot \epsilon$, $\mathbf{x}_t \sim q(\mathbf{x}_t)$.
- ▶ Choose σ_1, σ_T such that:

$$q(\mathbf{x}_1) \approx \pi(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \sigma_T^2 \cdot \mathbf{I}).$$

$$\sigma_1 \quad < \quad \sigma_2 \quad < \quad \sigma_3$$



Noise Conditioned Score Network (NCSN)

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

$$\sum_{t=1}^T \sigma_t^2 \cdot \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x})} \| s_{\theta, \sigma_t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}) \|_2^2 \rightarrow \min_{\theta}$$

$$\text{Here } \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}) = -\frac{\mathbf{x}_t - \mathbf{x}}{\sigma_t^2} = -\frac{\boldsymbol{\epsilon}}{\sigma_t}.$$

Training

1. Get the sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Sample noise level $t \sim U\{1, T\}$ and the noise $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}$.
4. Compute loss $\mathcal{L} = \sigma_t^2 \cdot \| s_{\theta, \sigma_t}(\mathbf{x}_t) + \frac{\boldsymbol{\epsilon}}{\sigma_t} \|_2^2$.

How to sample from this model?

Noise Conditioned Score Network (NCSN)

Sampling (annealed Langevin dynamics)

- ▶ Sample $\mathbf{x}_0 \sim \mathcal{N}(0, \sigma_T^2 \cdot \mathbf{I}) \approx q(\mathbf{x}_T)$.
- ▶ Apply L steps of Langevin dynamic

$$\mathbf{x}_l = \mathbf{x}_{l-1} + \frac{\eta_t}{2} \cdot \mathbf{s}_{\theta, \sigma_t}(\mathbf{x}_{l-1}) + \sqrt{\eta_t} \cdot \boldsymbol{\epsilon}_l.$$

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



Outline

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Forward gaussian diffusion process

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

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

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

Statement 1

Let denote $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{s=1}^t \alpha_s = \prod_{s=1}^t (1 - \beta_s)$. Then

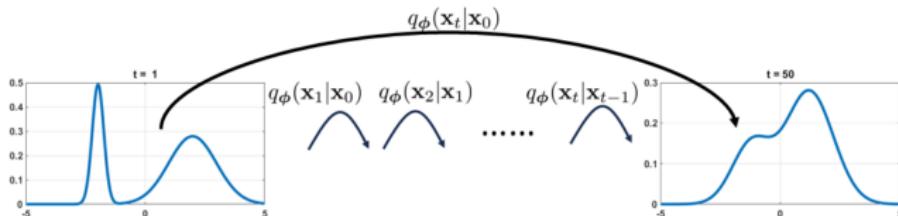
$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_t) \cdot \mathbf{I})$$

We are able to sample from any timestamp using only \mathbf{x}_0 !

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t} \cdot \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \cdot \boldsymbol{\epsilon}_t = \\ &= \sqrt{\alpha_t} (\sqrt{\alpha_{t-1}} \cdot \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \cdot \boldsymbol{\epsilon}_{t-1}) + \sqrt{1 - \alpha_t} \cdot \boldsymbol{\epsilon}_t = \\ &= \sqrt{\alpha_t \alpha_{t-1}} \cdot \mathbf{x}_{t-2} + (\sqrt{\alpha_t (1 - \alpha_{t-1})} \cdot \boldsymbol{\epsilon}_{t-1} + \sqrt{1 - \alpha_t} \cdot \boldsymbol{\epsilon}_t) = \\ &= \sqrt{\alpha_t \alpha_{t-1}} \cdot \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1} \alpha_t} \cdot \boldsymbol{\epsilon}'_t = \\ &= \dots = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).\end{aligned}$$

Forward gaussian diffusion process

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N} \left(\sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I} \right); \quad q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N} \left(\sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I} \right).$$



Statement 2

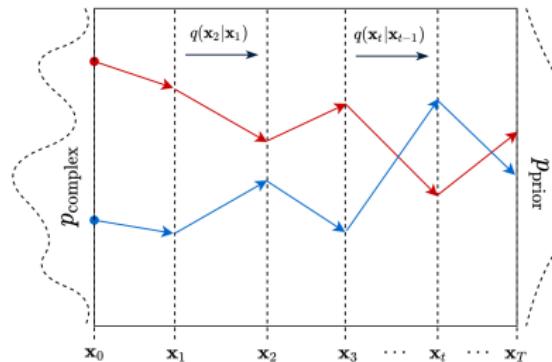
Applying the Markov chain to samples from any $\pi(\mathbf{x})$ we will get $\mathbf{x}_\infty \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$. Here $p_\infty(\mathbf{x})$ is a **stationary** and **limiting** distribution:

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

$$p_\infty(\mathbf{x}) = \int q(\mathbf{x}_\infty | \mathbf{x}_0) \pi(\mathbf{x}_0) d\mathbf{x}_0 \approx \mathcal{N}(0, \mathbf{I}) \int \pi(\mathbf{x}_0) d\mathbf{x}_0 = \mathcal{N}(0, \mathbf{I})$$

Forward gaussian 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. $\mathbf{x}_t = \sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$, $t \geq 1$;
3. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$, where $T \gg 1$.

If we are able to invert this process, we will get the way to sample $\mathbf{x} \sim \pi(\mathbf{x})$ using noise samples $p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$.

Now our goal is to revert this process.

Summary

- ▶ Langevin dynamics allows to sample from the generative model using the gradient of the log-likelihood.
- ▶ Score matching proposes to minimize the 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.
- ▶ Gaussian diffusion process is a Markov chain that injects special form of Gaussian noise to the samples.
- ▶ Denoising score matching is applicable to gaussian diffusion process.