Deep Generative Models

Lecture 13

Roman Isachenko

Moscow Institute of Physics and Technology

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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)

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

Langevin dynamics

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

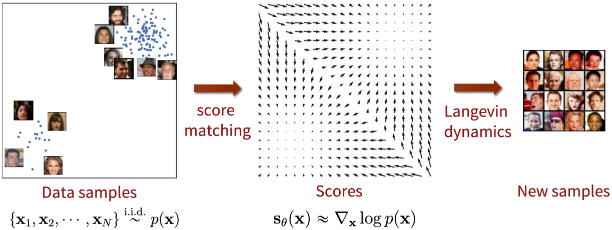
$$\mathbf{x}_{t+1} = \mathbf{x}_t + \eta \frac{1}{2} \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

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

Recap of previous lecture



Theorem (implicit score matching)

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

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 (Hutchinson's trace estimation)**.

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

Recap of previous lecture

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

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

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

Theorem (denoising score matching)

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

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

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 $\nabla_{\mathbf{x}'}\log\pi(\mathbf{x}'|\sigma)$ and even more $\nabla_{\mathbf{x}'}\log\pi(\mathbf{x}')$.
- $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma)$ tries to **denoise** a corrupted sample.
- Score function $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma)$ parametrized by σ.

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

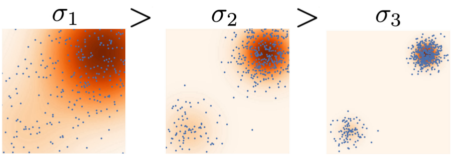
Recap of previous lecture

Noise conditioned score network

- Define the sequence of noise levels: $\sigma_1 > \sigma_2 > \dots > \sigma_L$.
- Train denoised score function $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma)$ for each noise level:

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

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



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

Outline

1. Score matching
   Implicit score matching
   Denoising score matching

2. Noise conditioned score network

3. DDPM vs Score matching

Outline

1. Score matching
    - Implicit score matching
    - Denoising score matching
2. Noise conditioned score network
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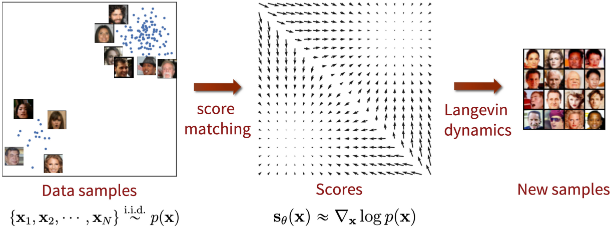
Score matching

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

Fisher divergence

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

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



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

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

Outline

Implicit score matching

Theorem

Under some regularity conditions, it holds

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

Proof (only for 1D)

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

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

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

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

Score matching

Theorem (implicit score matching)

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

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

1. The right hand side is complex due to Hessian matrix – **sliced score matching**.
2. The left hand side is intractable due to unknown $\pi(\mathbf{x})$ – **denoising score matching**.

Sliced score matching (Hutchinson's trace estimation)

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

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

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

Outline

1. Score matching
   - Implicit score matching
   - Denoising score matching

2. Noise conditioned score network

3. DDPM vs Score matching

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

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

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

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

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

Denoising score matching

Theorem

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

Proof

$$\mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \big\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma) - \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \big\|_2^2 =$$
$$= \mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \Big[\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma) \|^2 + \underbrace{\| \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \|_2^2}_{\text{const}(\boldsymbol{\theta})} - 2 \mathbf{s}_{\boldsymbol{\theta}}^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \Big]$$

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

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

Denoising score matching

Theorem

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

Proof (continued)

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

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

Denoising score matching

Theorem

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

Proof (continued)

$$\mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \big\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma) - \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \big\|_2^2 =$$
$$= \mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \Big[\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma) \|^2 - 2 \mathbf{s}_{\boldsymbol{\theta}}^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \Big] + \text{const}(\boldsymbol{\theta}) =$$
$$= \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{p(\mathbf{x}'|\mathbf{x}, \sigma)} \Big[\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma) \|^2 - 2 \mathbf{s}_{\boldsymbol{\theta}}^T(\mathbf{x}', \sigma) \nabla_{\mathbf{x}'} \log p(\mathbf{x}'|\mathbf{x}, \sigma) \Big] + \text{const}(\boldsymbol{\theta})$$

Gradient of the noise kernel

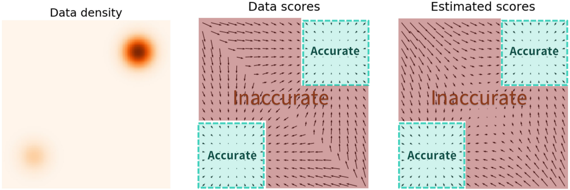
$$\nabla_{\mathbf{x}'} \log p(\mathbf{x}'|\mathbf{x}, \sigma) = \nabla_{\mathbf{x}'} \log \mathcal{N}(\mathbf{x}'|\mathbf{x}, \sigma^2 \mathbf{I}) = - \frac{\mathbf{x}' - \mathbf{x}}{\sigma^2}$$

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

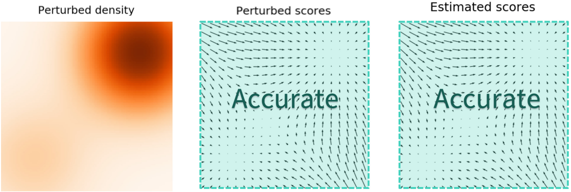
Vincent P. A Connection Between Score Matching and Denoising Autoencoders, 2010

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

Outline

1. Score matching
   - Implicit score matching
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2. Noise conditioned score network
3. DDPM vs Score matching

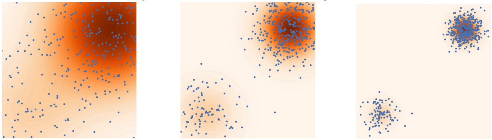
Noise conditioned score network

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

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

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

$\sigma_1 > \sigma_2 > \sigma_3$



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

Noise conditioned score network

Training: loss function

$$\sum_{i=1}^{L} \sigma_l^2 \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{\epsilon} \left\| \mathbf{s}_l + \frac{\epsilon}{\sigma_l} \right\|_2^2,$$

Here

- $\mathbf{s}_l = \mathbf{s}_{\theta}(\mathbf{x} + \sigma_l \cdot \epsilon, \sigma_l)$.
- $\nabla_{\mathbf{x}'} \log p(\mathbf{x}' | \mathbf{x}, \sigma) = -\frac{\mathbf{x}' - \mathbf{x}}{\sigma^2} = -\frac{\epsilon}{\sigma_l}$.

Inference: annealed Langevin dynamic

Algorithm 1 Annealed Langevin dynamics.

Require: $\{\sigma_i\}_{i=1}^L, \epsilon, T$.

```
Initialize x̃_0
for i ← 1 to L do
    α_i ← ε · σ_i^2 / σ_L^2        ▷ α_i is the step size.
    for t ← 1 to T do
        Draw z_t ∼ N(0, I)
        x̃_t ← x̃_{t−1} + (α_i / 2) s_θ(x̃_{t−1}, σ_i) + √α_i z_t
    end for
    x̃_0 ← x̃_T
end for
return x̃_T
```

Samples

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

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DDPM vs Score matching

$$\mathcal{L}_t = \mathbb{E}_{\boldsymbol{\epsilon}} \left[\frac{\beta_t^2}{2\tilde{\beta}_t(1-\beta_t)} \left\| \frac{\boldsymbol{\epsilon}}{\sqrt{1-\bar{\alpha}_t}} - \frac{\boldsymbol{\epsilon}_{\boldsymbol{\theta}}(\mathbf{x}_t, t)}{\sqrt{1-\bar{\alpha}_t}} \right\|^2 \right]$$

- Result from Statement 2

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

- Score of noised distribution

$$\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}_0) = -\frac{\boldsymbol{\epsilon}}{\sqrt{1-\bar{\alpha}_t}}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

- Let reparametrize our model:

$$\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) = -\frac{\boldsymbol{\epsilon}_{\boldsymbol{\theta}}(\mathbf{x}_t, t)}{\sqrt{1-\bar{\alpha}_t}}.$$

Noise conditioned score network

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Summary

- Score matching proposes to minimize Fisher divergence to get score function.
- Implicit score matching tries to avoid the value of original distribution $\pi(\mathbf{x})$. Sliced score matching makes implicit score matching scalable.
- Denoising score matching minimizes Fisher divergence on noisy samples.
- Noise conditioned score network uses multiple noise levels and annealed Langevin dynamics to fit score function.
- Objective of DDPM is closely related to the noise conditioned score network and score matching.