Deep Generative Models

Lecture 13

Roman Isachenko

Moscow Institute of Physics and Technology

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Recap of previous lecture

ELBO of gaussian diffusion model

$$\mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p(\mathbf{x}_0|\mathbf{x}_1, \boldsymbol{\theta}) - KL\big(q(\mathbf{x}_T|\mathbf{x}_0)||p(\mathbf{x}_T)\big) - \\ - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} KL\big(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)||p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta})\big)}_{\mathcal{L}_t}$$

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}),$$
$$p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) = \mathcal{N}\big(\mathbf{x}_{t-1}|\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_t, t), \boldsymbol{\sigma}^2_{\boldsymbol{\theta}}(\mathbf{x}_t, t)\big)$$

Our assumption: $\boldsymbol{\sigma}^2_{\boldsymbol{\theta}}(\mathbf{x}_t, t) = \tilde{\beta}_t \mathbf{I}$.

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[\frac{1}{2\tilde{\beta}_t} \left\| \tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) \right\|^2 \right]$$

Ho J. Denoising Diffusion Probabilistic Models, 2020

Recap of previous lecture

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)}\left[\frac{1}{2\tilde{\beta}_t}\left\|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_t, t)\right\|^2\right]$$

Reparametrization

$$\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{\alpha_t}}\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{\alpha_t(1-\bar{\alpha}_t)}}\boldsymbol{\epsilon}$$

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

$$\mathcal{L}_t = \mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(0,\mathbf{I})}\left[\frac{(1-\alpha_t)^2}{2\tilde{\beta}_t\alpha_t(1-\bar{\alpha}_t)}\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{\theta}}\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t\right)\right\|^2\right]$$

At each step of reverse diffusion process we try to predict the noise $\boldsymbol{\epsilon}$ that we used in the forward diffusion process!

Simplified objective

$$\mathcal{L}_{\text{simple}} = \mathbb{E}_{t\sim U[2,T]}\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(0,\mathbf{I})}\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{\theta}}\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t\right)\right\|^2$$

Ho J. Denoising Diffusion Probabilistic Models, 2020

Recap of previous lecture

Training

1. Get the sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Sample timestamp $t \sim U[1, T]$ and the noise $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}$.
4. Compute loss $\mathcal{L}_{\text{simple}} = \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{\theta}}(\mathbf{x}_t, t)\|^2$.

Sampling

1. Sample $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$.
2. Compute mean of $p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_t, t), \tilde{\beta}_t\mathbf{I})$:

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

3. Get denoised image $\mathbf{x}_{t-1} = \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) + \sqrt{\tilde{\beta}_t} \cdot \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.

Ho J. Denoising Diffusion Probabilistic Models, 2020

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

Outline

1. Score matching
   - Implicit score matching
   - Denoising score matching
2. Noise conditioned score network (NCSN)
3. DDPM vs Score matching

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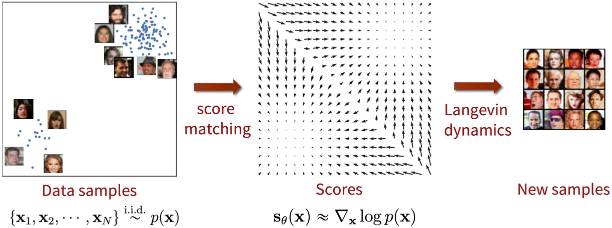
Score matching

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

1. Score matching
   Implicit score matching
   Denoising score matching

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3. DDPM vs Score matching

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)

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

$$\mathbb{E}_\pi[s(x)\nabla_x\log\pi(x)]=\int\pi(x)s(x)\nabla_x\log\pi(x)dx=\int\underbrace{\nabla_x\log p(x)}_{g}\underbrace{\nabla_x\pi(x)}_{\nabla f}dx$$

$$=\underbrace{\nabla_x\log p(x)}_{g}\underbrace{\pi(x)}_{f}\Big|_{-\infty}^{+\infty}-\int\underbrace{\nabla_x\big(\nabla_x\log p(x)\big)}_{\nabla g}\underbrace{\pi(x)}_{f}dx$$

$$=-\mathbb{E}_\pi\nabla_x s(x)$$

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

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

Score matching

Theorem (implicit score matching)

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

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

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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

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

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)

$$\mathbb{E}_{\pi(\mathbf{x}'|\sigma)}\left[\mathbf{s}^T_{\boldsymbol{\theta}}(\mathbf{x}',\sigma)\nabla_{\mathbf{x}'}\log\pi(\mathbf{x}'|\sigma)\right] = \int \pi(\mathbf{x}'|\sigma)\left[\mathbf{s}^T_{\boldsymbol{\theta}}(\mathbf{x}',\sigma)\frac{\nabla_{\mathbf{x}'}\pi(\mathbf{x}'|\sigma)}{\pi(\mathbf{x}'|\sigma)}\right]d\mathbf{x}' =$$
$$= \int\left[\mathbf{s}^T_{\boldsymbol{\theta}}(\mathbf{x}',\sigma)\nabla_{\mathbf{x}'}\left(\int p(\mathbf{x}'|\mathbf{x},\sigma)\pi(\mathbf{x})d\mathbf{x}\right)\right]d\mathbf{x}' =$$
$$= \int\int \pi(\mathbf{x})\left[\mathbf{s}^T_{\boldsymbol{\theta}}(\mathbf{x}',\sigma)\nabla_{\mathbf{x}'}p(\mathbf{x}'|\mathbf{x},\sigma)\right]d\mathbf{x}'d\mathbf{x} =$$
$$= \int\int \pi(\mathbf{x})p(\mathbf{x}'|\mathbf{x},\sigma)\left[\mathbf{s}^T_{\boldsymbol{\theta}}(\mathbf{x}',\sigma)\nabla_{\mathbf{x}'}\log p(\mathbf{x}'|\mathbf{x},\sigma)\right]d\mathbf{x}'d\mathbf{x} =$$
$$= \mathbb{E}_{\pi(\mathbf{x})}\mathbb{E}_{p(\mathbf{x}'|\mathbf{x},\sigma)}\left[\mathbf{s}^T_{\boldsymbol{\theta}}(\mathbf{x}',\sigma)\nabla_{\mathbf{x}'}\log p(\mathbf{x}'|\mathbf{x},\sigma)\right]$$

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

Denoising score matching

Theorem

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

Proof (continued)

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

Gradient of the noise kernel

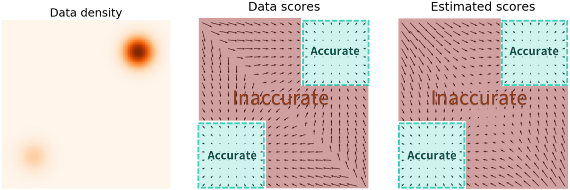
$$\nabla_{\mathbf{x}'} \log p(\mathbf{x}'|\mathbf{x}, \sigma) = \nabla_{\mathbf{x}'} \log \mathcal{N}(\mathbf{x}'|\mathbf{x}, \sigma^2\mathbf{I}) = -\frac{\mathbf{x}' - \mathbf{x}}{\sigma^2}$$

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

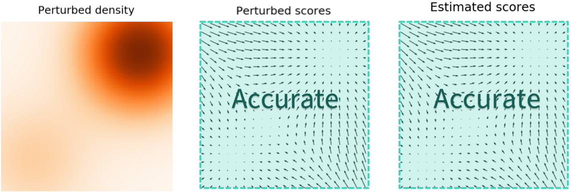
Vincent P. A Connection Between Score Matching and Denoising Autoencoders, 2010

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

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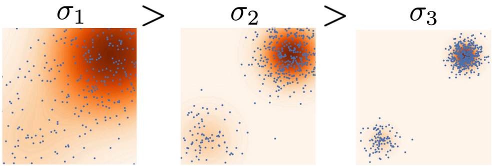
Noise conditioned score network

- 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 $l = 1, \dots, L$).



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 $\tilde{\mathbf{x}}_0$
for $i \leftarrow 1$ to L **do**
  $\alpha_i \leftarrow \epsilon \cdot \sigma_i^2 / \sigma_L^2$ ▷ α_i is the step size.
  for $t \leftarrow 1$ to T **do**
    Draw $\mathbf{z}_t \sim \mathcal{N}(0, I)$
    $\tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_{t-1} + \frac{\alpha_i}{2} \mathbf{s}_{\theta}(\tilde{\mathbf{x}}_{t-1}, \sigma_i) + \sqrt{\alpha_i}\, \mathbf{z}_t$
  end for
  $\tilde{\mathbf{x}}_0 \leftarrow \tilde{\mathbf{x}}_T$
end for
return $\tilde{\mathbf{x}}_T$

Samples

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

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DDPM vs Score matching

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

- 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

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

- Let reparametrize our model:

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

Noise conditioned score network

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

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.