Deep Generative Models

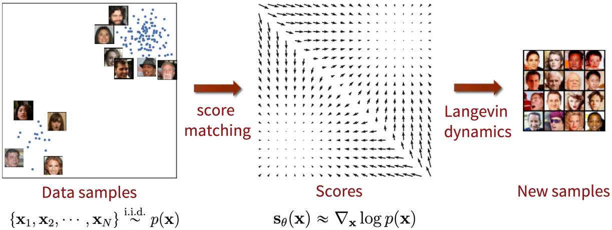
Lecture 12

Roman Isachenko

Moscow Institute of Physics and Technology

2023, Autumn

Recap of previous lecture



Theorem (implicit score matching)

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

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 (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

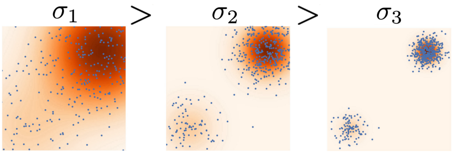
Recap of previous lecture

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

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. Overview of DDPM
2. Langevin dynamic and SDE basics
3. Score matching
4. Noise conditioned score network
5. The worst course overview

Outline

Denoising diffusion probabilistic model (DDPM)

DDPM is a VAE model

- Encoder is a fixed Gaussian Markov chain.
- Latent variable is a hierarchical (in each step the dim. of the latent equals to the dim of the input).
- Decoder is a simple Gaussian model.
- Prior distribution is given by parametric Gaussian Makov chain.

Forward process

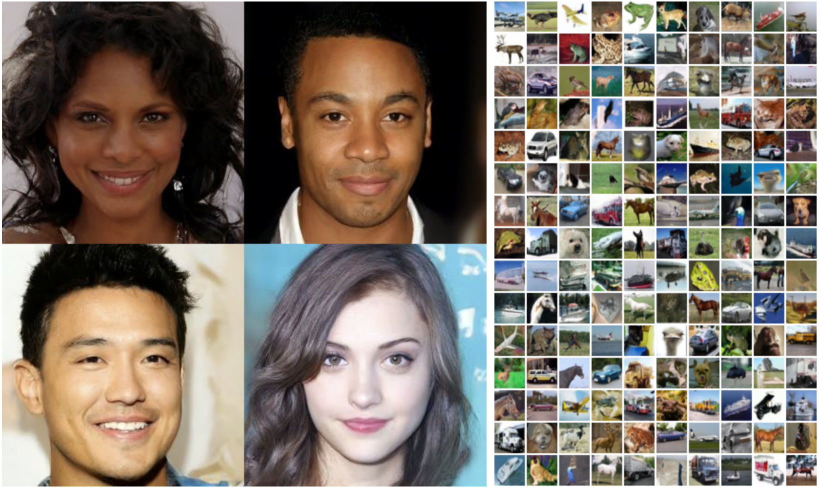
1. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$;
2. $\mathbf{x}_t = \sqrt{1-\beta} \cdot \mathbf{x}_{t-1} + \sqrt{\beta} \cdot \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, 1)$, $t \geq 1$;
3. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, 1)$.

Reverse process

1. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, 1)$;
2. $\mathbf{x}_{t-1} = \boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_t, t)$;
3. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$;

Denoising diffusion probabilistic model (DDPM)

Samples



Ho J. Denoising Diffusion Probabilistic Models, 2020

Outline

1. Overview of DDPM
2. Langevin dynamic and SDE basics
3. Score matching
4. Noise conditioned score network
5. The worst course overview

Langevin dynamic

Imagine that we have some generative model $p(\mathbf{x}|\boldsymbol{\theta})$.

Statement

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

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

will comes from $p(\mathbf{x}|\boldsymbol{\theta})$.

What do we get if $\boldsymbol{\epsilon} = \mathbf{0}$?

Energy-based model

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

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

Gradient of normalized density equals to gradient of unnormalized density.

Welling M. Bayesian Learning via Stochastic Gradient Langevin Dynamics, 2011

Stochastic differential equation (SDE)

Let define stochastic process $\mathbf{x}(t)$ with initial condition $\mathbf{x}(0) \sim p_0(\mathbf{x})$:

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$$

- $\mathbf{f}(\mathbf{x}, t)$ is the **drift** function of $\mathbf{x}(t)$.
- $g(t)$ is the **diffusion** coefficient of $\mathbf{x}(t)$.
- If $g(t) = 0$ we get standard ODE.
- $\mathbf{w}(t)$ is the standard Wiener process (Brownian motion)

$$\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, t - s), \quad d\mathbf{w} = \boldsymbol{\epsilon} \cdot \sqrt{dt}, \text{ where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1).$$

How to get distribution $p(\mathbf{x}, t)$ for $\mathbf{x}(t)$?

Theorem (Kolmogorov-Fokker-Planck)

Evolution of the distribution $p(\mathbf{x}, t)$ is given by the following ODE:

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\bigl[\mathbf{f}(\mathbf{x}, t)p(\mathbf{x}, t)\bigr] + \frac{1}{2}g^2(t)\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right)$$

Langevin SDE (special case)

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}, \quad d\mathbf{w} = \boldsymbol{\epsilon} \cdot \sqrt{dt}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1).$$

$$d\mathbf{x} = \frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t)dt + 1 d\mathbf{w}$$

$$\mathbf{x}_{t+1} - \mathbf{x}_t = \eta \frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \eta \approx dt.$$

Let apply KFP theorem.

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = \operatorname{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[p(\mathbf{x}, t)\frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t)\right] + \frac{1}{2}\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right) =$$

$$= \operatorname{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\frac{1}{2}\frac{\partial}{\partial \mathbf{x}} p(\mathbf{x}, t)\right] + \frac{1}{2}\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right) = 0$$

The density $p(\mathbf{x}, t) = \text{const}$.

Langevin dynamic

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

Stochastic differential equation (SDE)

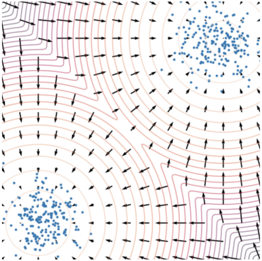
Statement

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

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

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

The density $p(\mathbf{x}|\boldsymbol{\theta})$ is a **stationary** distribution for this SDE.



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

Outline

1. Overview of DDPM
2. Langevin dynamic and SDE basics
3. Score matching
4. Noise conditioned score network
5. The worst course overview

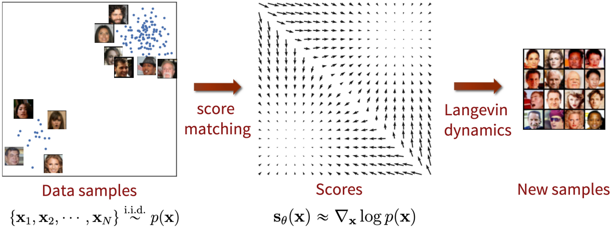
Score matching

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

Fisher divergence

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

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

Score matching

Theorem (implicit score matching)

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)

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

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

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

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

Score matching

Theorem (implicit score matching)

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

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 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**.

Sliced score matching (Hutchinson's trace estimation)

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

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

Denoising score matching

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

$$\mathbf{x}' = \mathbf{x} + \sigma \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1), \quad p(\mathbf{x}'|\mathbf{x}, \sigma) = \mathcal{N}(\mathbf{x}'|\mathbf{x}, \sigma^2 \mathbf{I})$$

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

Then the solution of

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

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.

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

Denoising score matching

Theorem

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

Gradient of the noise kernel

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

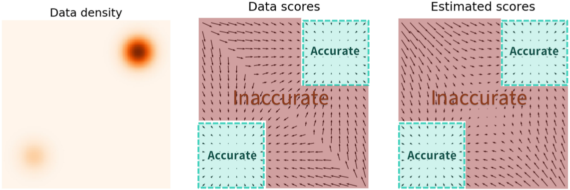
- The RHS does not need to compute $\nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma)$ and even $\nabla_{\mathbf{x}'} \log \pi(\mathbf{x}')$.
- $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma)$ tries to **denoise** a corrupted sample $\mathbf{x}'$.
- Score function $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma)$ parametrized by σ. How to make it?

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

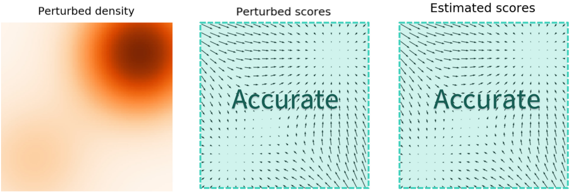
Outline

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.

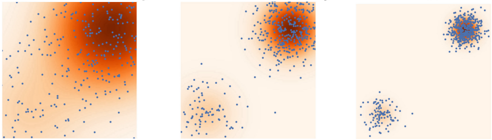


Song Y. Generative Modeling by Estimating Gradients of the Data Distribution, blog post, 2021

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

Samples

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

Gaussian diffusion model 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

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

- 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

Outline

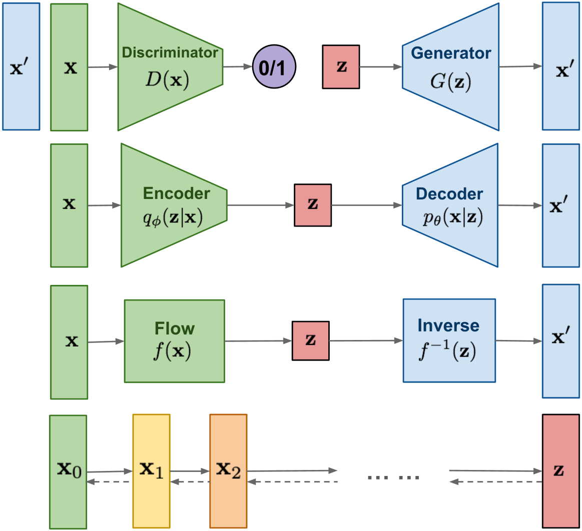
The worst course overview :)

GAN: Adversarial training

VAE: maximize variational lower bound

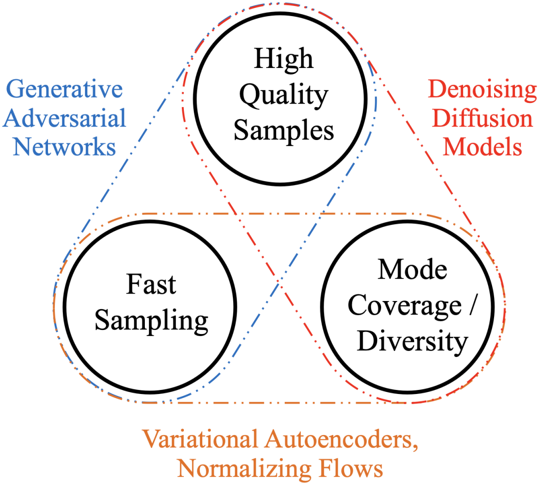
Flow-based models: Invertible transform of distributions

Diffusion models: Gradually add Gaussian noise and then reverse



Weng L. What are Diffusion Models?, blog post, 2021

The worst course overview :)



Xiao Z., Kreis K., Vahdat A. Tackling the generative learning trilemma with denoising diffusion GANs, 2021

Summary

- Langevin dynamics allows to sample from the model using the score function (due to the existence of stationary distribution for SDE).
- Score matching proposes to minimize Fisher divergence to get score function.
- Sliced score matching and denoising score matching are two techniques to get scalable algorithm for fitting Fisher divergence.
- 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.