

Deep Generative Models

Lecture 10

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2024, Spring

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

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

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):

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

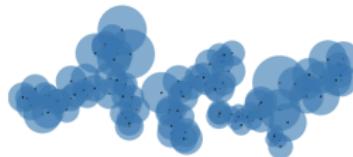
Define binary function:

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

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



(a) True manifold



(b) Approx. manifold

Recap of previous lecture

Langevin dynamic

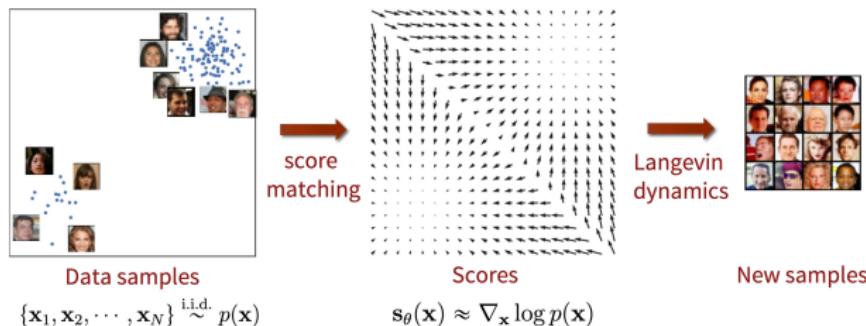
$$\mathbf{x}_{I+1} = \mathbf{x}_I + \frac{\eta}{2} \cdot \nabla_{\mathbf{x}_I} \log p(\mathbf{x}_I | \boldsymbol{\theta}) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

Fisher divergence

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

Score function

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



Outline

1. Denoising score matching
2. Noise Conditioned Score Network (NCSN)
3. Gaussian diffusion process
 - Forward gaussian diffusion process
 - Denoising score matching
 - Reverse gaussian diffusion process

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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

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

Proof

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

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)

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

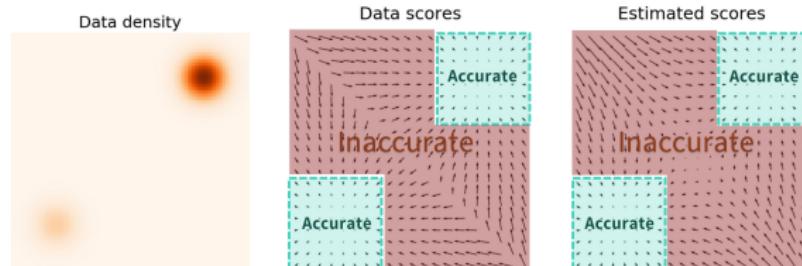
Gradient of the noise kernel

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

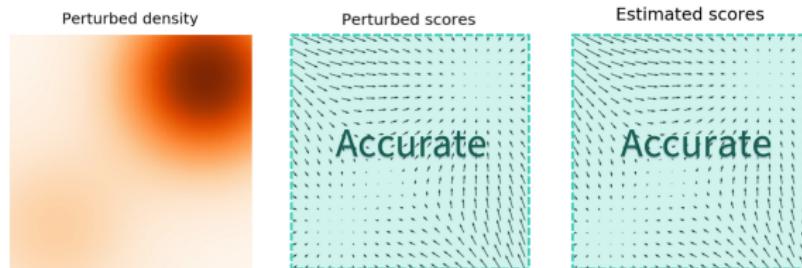
The RHS does not need to compute $\nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)$ and even $\nabla_{\mathbf{x}_\sigma} \log \pi(\mathbf{x}_\sigma)$.

Denoising score matching

- 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

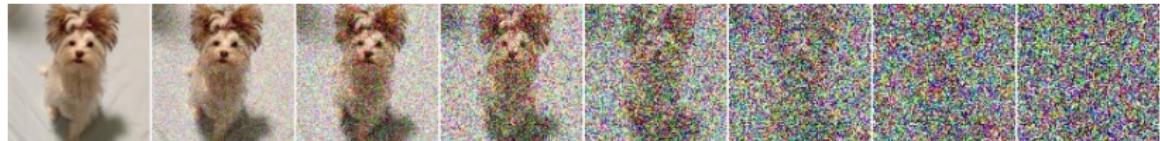
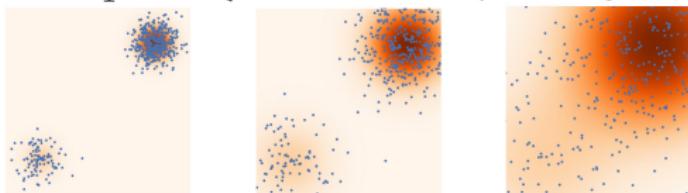
1. Denoising score matching
2. Noise Conditioned Score Network (NCSN)
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 - Forward gaussian diffusion process
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Noise Conditioned Score Network (NCSN)

- ▶ 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:

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

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 $\mathcal{L} = \|s_{\theta, \sigma_t}(\mathbf{x}_t) + \frac{\boldsymbol{\epsilon}}{\sigma_t}\|^2$.

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 .



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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

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

Statement 1

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

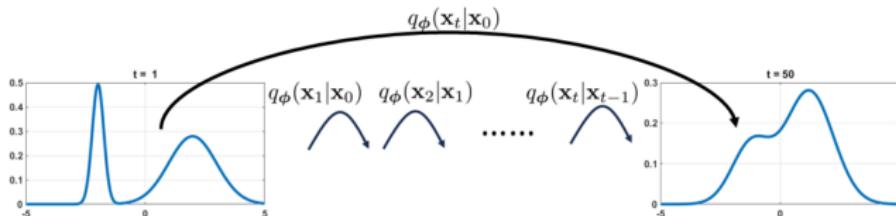
$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_t) \cdot \mathbf{I})$$

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

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

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

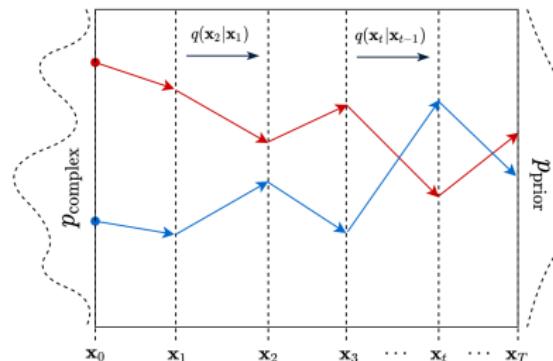
Applying the Markov chain to samples from any $\pi(\mathbf{x})$ we will get $\mathbf{x}_\infty \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$. Here $p_\infty(\mathbf{x})$ is a **stationary** and **limiting** distribution:

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

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

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.

Outline

1. Denoising score matching
2. Noise Conditioned Score Network (NCSN)
3. **Gaussian diffusion process**
 - Forward gaussian diffusion process
 - Denoising score matching**
 - Reverse gaussian diffusion process

Denoising score matching

NCSN

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\mathbf{x}, \sigma_t^2 \cdot \mathbf{I}), \quad q(\mathbf{x}_1) \approx \pi(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \sigma_T^2 \cdot \mathbf{I}).$$

$$\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}) = -\frac{\mathbf{x}_t - \mathbf{x}}{\sigma_t^2}$$

Gaussian diffusion

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_t) \cdot \mathbf{I}), \quad q(\mathbf{x}_1) \approx \pi(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \mathbf{I})$$

$$\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}) = -\frac{\mathbf{x}_t - \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0}{1 - \bar{\alpha}_t}$$

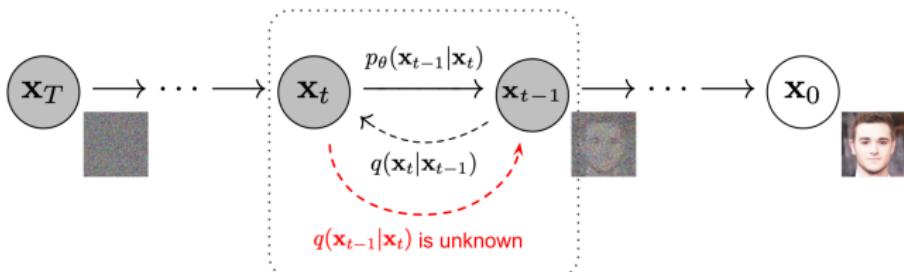
Theorem (denoising score matching)

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

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Reverse gaussian diffusion process



Forward process

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

Reverse process

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)} \approx p(\mathbf{x}_{t-1}|\mathbf{x}_t, \theta)$$

- ▶ $q(\mathbf{x}_{t-1})$, $q(\mathbf{x}_t)$ are intractable.
- ▶ If β_t is small enough, $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ will be Gaussian (Feller, 1949).

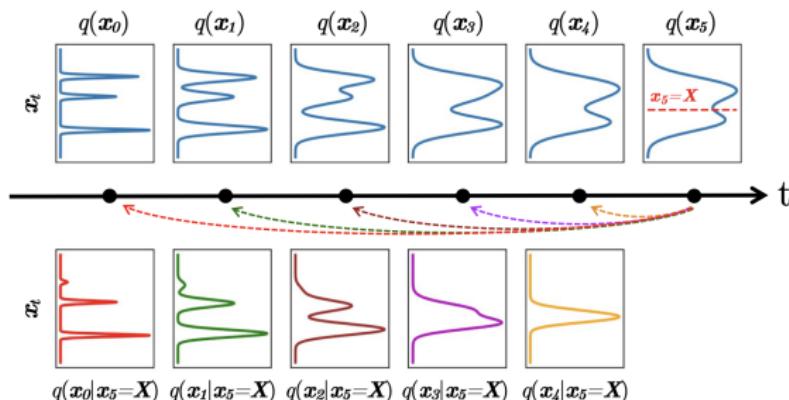
Feller W. On the theory of stochastic processes, with particular reference to applications, 1949

Reverse gaussian diffusion process

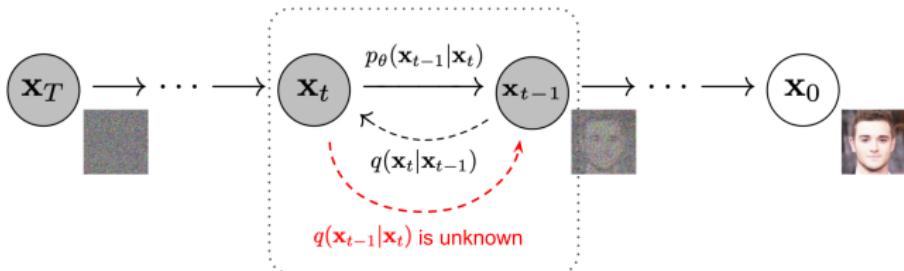
$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)}$$

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} = \mathcal{N}(\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I})$$

- ▶ $q(\mathbf{x}_{t-1})$, $q(\mathbf{x}_t)$ are intractable.
- ▶ If β_t is small enough, $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ will be Gaussian (Feller, 1949).



Reverse gaussian diffusion process



Let define the reverse process

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) \approx p(\mathbf{x}_{t-1}|\mathbf{x}_t, \theta) = \mathcal{N}(\mu_\theta(\mathbf{x}_t, t), \sigma_\theta^2(\mathbf{x}_t, t))$$

Forward process

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. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I}).$

Reverse process

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

Note: The forward process does not have any learnable parameters!

Summary

- ▶ 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.
- ▶ Reverse process allows to sample from the real distribution $\pi(\mathbf{x})$ using samples from noise.