Deep Generative Models

Lecture 13

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Recap of previous lecture

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

Variance Exploding SDE (NCSN)

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}, \quad \mathbf{f}(\mathbf{x}, t) = 0, \quad g(t) = \sqrt{\frac{d[\sigma^2(t)]}{dt}}$$

Variance grows since $\sigma(t)$ is a monotonically increasing function.

Variance Preserving SDE (DDPM)

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}$$

$$\mathbf{f}(\mathbf{x}, t) = -\frac{1}{2}\beta(t)\mathbf{x}(t), \quad g(t) = \sqrt{\beta(t)}$$

Variance is preserved if $\mathbf{x}(0)$ has a unit variance.

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Outline

Outline

1. Conditional Flow Matching
   Conical gaussian paths

Conditional Flow Matching

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \left\| \mathbf{f}(\mathbf{x}, \mathbf{z}, t) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t) \right\|^2 \rightarrow \min_{\boldsymbol{\theta}}$$

What is left?

- How to choose the conditioning latent variable $\mathbf{z}$?
- How to define $p_t(\mathbf{x}|\mathbf{z})$ which follows the constraints?

Gaussian conditional probability path

$$p_t(\mathbf{x}|\mathbf{z}) = \mathcal{N}\left(\boldsymbol{\mu}_t(\mathbf{z}), \boldsymbol{\sigma}_t^2(\mathbf{z})\right)$$

- There is an infinite number of vector fields that generate any particular probability path.
- Let consider the following dynamics:

$$\mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{z}) + \boldsymbol{\sigma}_t(\mathbf{z}) \odot \mathbf{x}_0, \quad \mathbf{x}_0 \sim p_0(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$$

Tong A., et al. Improving and Generalizing Flow-Based Generative Models with Minibatch Optimal Transport, 2023

Flow Matching

Gaussian conditional probability path

$$p_t(\mathbf{x}|\mathbf{z}) = \mathcal{N}\left(\boldsymbol{\mu}_t(\mathbf{z}), \boldsymbol{\sigma}_t^2(\mathbf{z})\right); \quad \mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{z}) + \boldsymbol{\sigma}_t(\mathbf{z}) \odot \mathbf{x}_0$$

Theorem

$$\mathbf{f}(\mathbf{x}, \mathbf{z}, t) = \boldsymbol{\mu}'_t(\mathbf{z}) + \frac{\boldsymbol{\sigma}'_t(\mathbf{z})}{\boldsymbol{\sigma}_t(\mathbf{z})} \odot (\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{z}))$$

Proof

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{z}, t); \quad \mathbf{x}_0 = \frac{1}{\boldsymbol{\sigma}_t(\mathbf{z})} \odot (\mathbf{x}_t - \boldsymbol{\mu}_t(\mathbf{z}))$$

$$\frac{d\mathbf{x}}{dt} = \boldsymbol{\mu}'_t(\mathbf{z}) + \boldsymbol{\sigma}'_t(\mathbf{z}) \odot \mathbf{x}_0 = \boldsymbol{\mu}'_t(\mathbf{z}) + \frac{\boldsymbol{\sigma}'_t(\mathbf{z})}{\boldsymbol{\sigma}_t(\mathbf{z})} \odot (\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{z}))$$

Tong A., et al. Improving and Generalizing Flow-Based Generative Models with Minibatch Optimal Transport, 2023

Outline

1. Conditional Flow Matching
   Conical gaussian paths

Endpoint conditioning

Conditional Flow Matching

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \left\| \mathbf{f}(\mathbf{x}, \mathbf{z}, t) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t) \right\|^2 \to \min_{\boldsymbol{\theta}}$$

Conditioning latent variable

Let choose $\mathbf{z} = \mathbf{x}_1$. Then $p(\mathbf{z}) = p_1(\mathbf{x}_1)$.

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x}|\mathbf{x}_1) p_1(\mathbf{x}_1) d\mathbf{x}_1$$

We need to ensure boundary constraints:

$$\begin{cases} p(\mathbf{x}) = \mathbb{E}_{p(\mathbf{z})} p_0(\mathbf{x}|\mathbf{z}); (= \mathcal{N}(0, \mathbf{I})) \\ \pi(\mathbf{x}) = \mathbb{E}_{p(\mathbf{z})} p_1(\mathbf{x}|\mathbf{z}). \end{cases} \Rightarrow \begin{cases} p_0(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(0, \mathbf{I}); \\ p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \end{cases}$$

Lipman Y., et al. Flow Matching for Generative Modeling, 2022

Conical gaussian paths

$$p_0(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(0, \mathbf{I}); \quad p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1).$$

Gaussian conditional probability path

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(\boldsymbol{\mu}_t(\mathbf{x}_1), \boldsymbol{\sigma}_t^2(\mathbf{x}_1)\right); \quad \mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{x}_1) + \boldsymbol{\sigma}_t(\mathbf{x}_1) \odot \mathbf{x}_0.$$

Let consider straight conditional paths

$$\begin{cases} \boldsymbol{\mu}_t(\mathbf{x}_1) = t\mathbf{x}_1; \\ \boldsymbol{\sigma}_t(\mathbf{x}_1) = 1 - t. \end{cases} \quad \Rightarrow \quad \begin{cases} p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(t\mathbf{x}_1, (1-t)^2 \cdot \mathbf{I}\right); \\ \mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0. \end{cases}$$

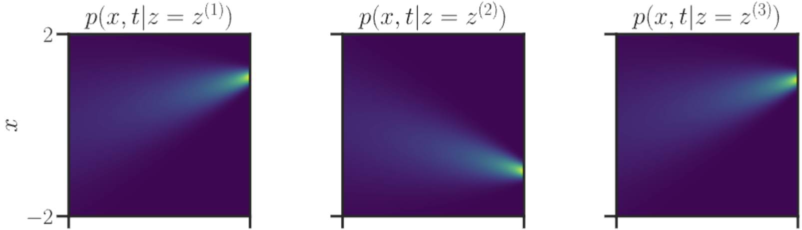

image credit: A Visual Dive into Conditional Flow Matching

Summary

- Conditional flow matching allows to make the FM objective tractable.