Deep Generative Models

Lecture 13

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Outline

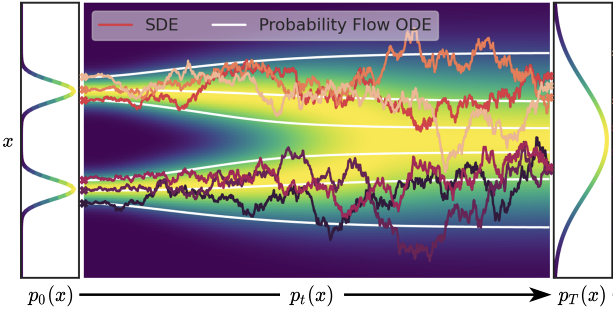
Recap of previous lecture

$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ – SDE with the probability path $p_t(\mathbf{x})$

Probability flow ODE

There exists ODE with identical the probability path $p_t(\mathbf{x})$ of the form

$$d\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right] dt$$



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

Recap of previous lecture

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

Reverse ODE

Let $\tau = 1 - t$ $(d\tau = -dt)$.

$$d\mathbf{x} = -\mathbf{f}(\mathbf{x}, 1 - \tau)d\tau$$

Reverse SDE

There exists the reverse SDE for the SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ that has the following form

$$d\mathbf{x} = \left(\mathbf{f}(\mathbf{x}, t) - g^2(t)\frac{\partial \log p_t(\mathbf{x})}{\partial \mathbf{x}}\right) dt + g(t)d\mathbf{w}, \quad dt < 0$$

Sketch of the proof

- Convert initial SDE to probability flow ODE.
- Revert probability flow ODE.
- Convert reverse probability flow ODE to reverse SDE.

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

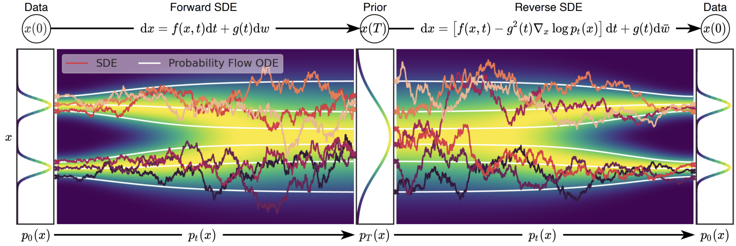
Recap of previous lecture

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

$$d\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right] dt \text{ -- probability flow ODE}$$

$$d\mathbf{x} = \left(\mathbf{f}(\mathbf{x}, t) - g^2(t)\frac{\partial \log p_t(\mathbf{x})}{\partial \mathbf{x}}\right) dt + g(t)d\mathbf{w} \text{ -- reverse SDE}$$

- We got the way to transform one distribution to another via SDE with some probability path $p_t(\mathbf{x})$.
- We are able to revert this process with the score function.



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

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

1. Flow Matching

Flow Matching

Let consider ODE dynamic $x_t = x(t)$ in time interval $t \in [0, 1]$ with boundaries $\mathbf{x}_0 \sim p_0(\mathbf{x}) = p(\mathbf{x})$, $\mathbf{x}_1 \sim p_1(\mathbf{x}) = \pi(\mathbf{x})$. Here $p(\mathbf{x})$ is a base distribution ($\mathcal{N}(0, \mathbf{I})$) and $\pi(\mathbf{x})$ is a true data distribution.

$$d\mathbf{x} = \mathbf{u}(\mathbf{x}, t)dt$$

$\mathbf{u}(\mathbf{x}, t) : \mathbb{R}^m \times [0, 1] \to \mathbb{R}^m$ is a vector field.

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = -\mathrm{div}\left(\mathbf{u}(\mathbf{x}, t)p_t(\mathbf{x})\right)$$

If we know the true vector field $\mathbf{u}(\mathbf{x}, t)$, then KFP equation gives us the way to compute the density $p_t(\mathbf{x})$.

Flow Matching

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

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

Flow Matching

There exists infinite number of possible $\mathbf{u}(\mathbf{x}, t)$ between $\pi(\mathbf{x})$ and $p(\mathbf{x})$.

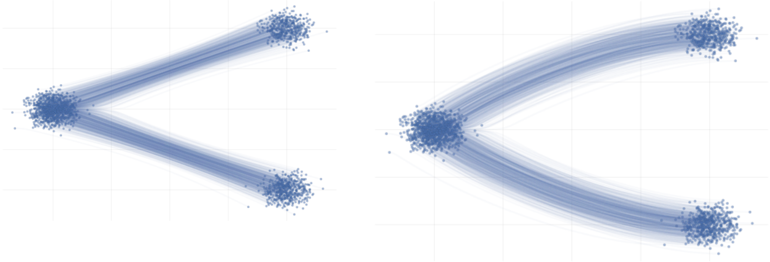
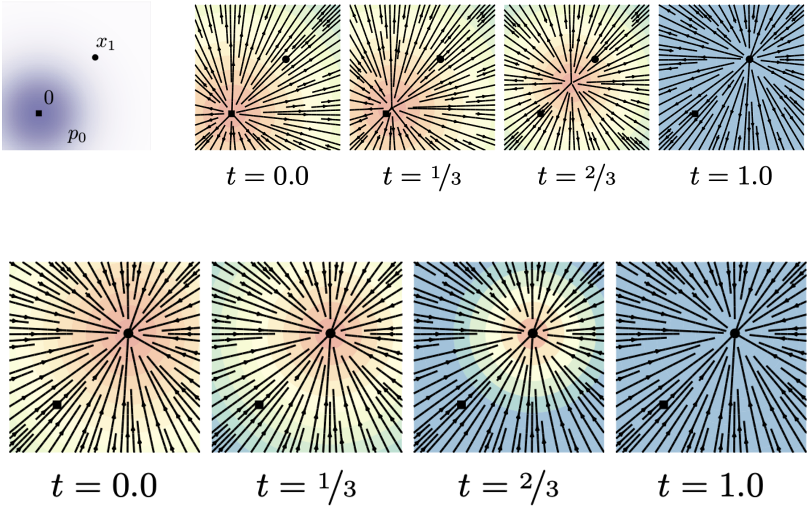


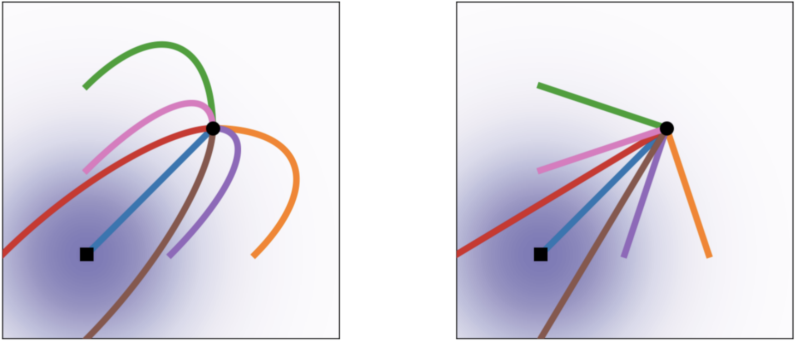
image credit: https://mlg.eng.cam.ac.uk/blog/2024/01/20/flow-matching.html

Flow Matching



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

Flow Matching



Diffusion OT

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

Summary

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