Deep Generative Models

Lecture 13

Roman Isachenko

Moscow Institute of Physics and Technology
Yandex School of Data Analysis

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Outline

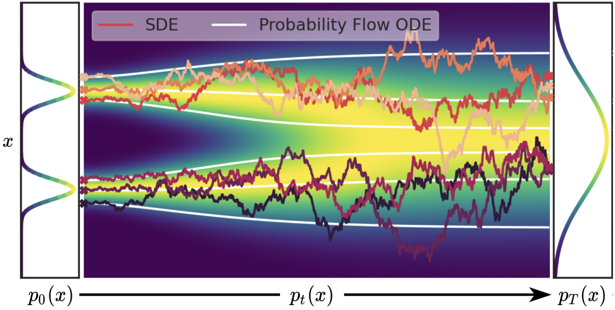
Recap of previous lecture

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

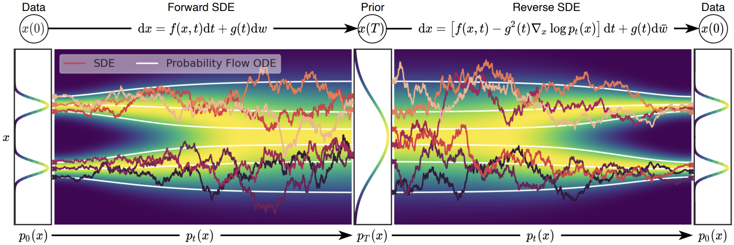
Recap of previous lecture

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

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

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

- 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

Flow Matching

Let consider ODE dynamic $\mathbf{x}_t = \mathbf{x}(t)$ 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.

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

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

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

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

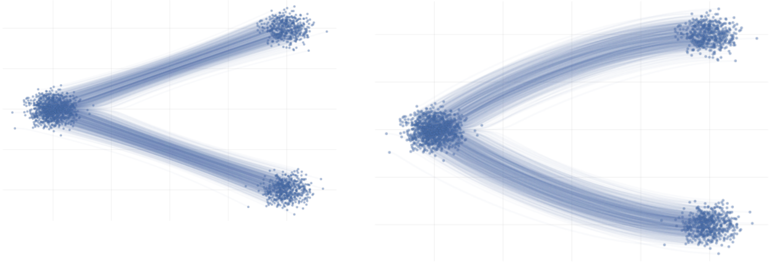
Flow Matching

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

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 $p(\mathbf{x})$.



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Flow Matching

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$$

Here $p_t(\mathbf{x}|\mathbf{z})$ is a **conditional probability path**.
The conditional probability path $p_t(\mathbf{x}|\mathbf{z})$ satisfies KFP theorem

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

where $\mathbf{u}(\mathbf{x}, \mathbf{z}, t)$ is a **conditional vector field**.

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t) \quad \Rightarrow \quad \frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, \mathbf{z}, t)$$

Gaussian conditional probability path

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

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

Flow Matching

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

Theorem

$$\mathbf{u}(\mathbf{x}, t) = \int \mathbf{u}(\mathbf{x}, \mathbf{z}, t) \frac{p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z})}{p_t(\mathbf{x})} d\mathbf{z}$$

Proof

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = \frac{\partial}{\partial t} \int p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} = \int \left(\frac{\partial p_t(\mathbf{x}|\mathbf{z})}{\partial t} \right) p(\mathbf{z}) d\mathbf{z} =$$

$$= \int \left(-\operatorname{div}\left(\mathbf{u}(\mathbf{x}, \mathbf{z}, t) p_t(\mathbf{x}|\mathbf{z})\right) \right) p(\mathbf{z}) d\mathbf{z} =$$

$$= -\operatorname{div}\left(\int \mathbf{u}(\mathbf{x}, \mathbf{z}, t) p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} \right) = -\operatorname{div}\left(\mathbf{u}(\mathbf{x}, t) p_t(\mathbf{x})\right)$$

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

Flow Matching

Flow Matching

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

Conditional Flow Matching

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

Theorem

If $\text{supp}(p_t(\mathbf{x})) = \mathbb{R}^m$, then the optimal value of FM objective is equal to the optimal value of CFM objective.

Proof

It is proved similarly with the denoising score matching theorem.

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Outline

Flow Matching

Conditional Flow Matching

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

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 conditions:

$$p_0(\mathbf{x}|\mathbf{x}_1) = p_0(\mathbf{x}); \quad p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1)$$

Gaussian conditional probability path

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(\boldsymbol{\mu}_t(\mathbf{x}_1), \boldsymbol{\sigma}_t^2(\mathbf{x}_1)\right)$$

$$\boldsymbol{\mu}_0(\mathbf{x}_1) = 0, \quad \boldsymbol{\sigma}_0(\mathbf{x}_1) = 1, \quad \boldsymbol{\mu}_1(\mathbf{x}_1) = \mathbf{x}_1, \quad \boldsymbol{\sigma}_1(\mathbf{x}_1) = 0$$

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

Flow Matching

Theorem

$$\mathbf{u}(\mathbf{x}, \mathbf{x}_1, t) = \boldsymbol{\mu}'_t(\mathbf{x}_1) + \frac{\boldsymbol{\sigma}'_t(\mathbf{x}_1)}{\boldsymbol{\sigma}_t(\mathbf{x}_1)} \odot (\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{x}_1))$$

Proof

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(\boldsymbol{\mu}_t(\mathbf{x}_1), \boldsymbol{\sigma}_t^2(\mathbf{x}_1)\right)$$

$$\mathbf{x} = \boldsymbol{\mu}_t(\mathbf{x}_1) + \boldsymbol{\sigma}_t(\mathbf{x}_1) \odot \boldsymbol{\epsilon}, \quad \Rightarrow \quad \boldsymbol{\epsilon} = \frac{1}{\boldsymbol{\sigma}_t(\mathbf{x}_1)} \odot (\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{x}_1))$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, \mathbf{x}_1, t)$$

$$\frac{d\mathbf{x}}{dt} = \boldsymbol{\mu}'_t(\mathbf{x}_1) + \boldsymbol{\sigma}'_t(\mathbf{x}_1) \odot \boldsymbol{\epsilon} = \boldsymbol{\mu}'_t(\mathbf{x}_1) + \frac{\boldsymbol{\sigma}'_t(\mathbf{x}_1)}{\boldsymbol{\sigma}_t(\mathbf{x}_1)} \odot (\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{x}_1))$$

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Flow Matching

$$\mathbf{u}(\mathbf{x}, \mathbf{x}_1, t) = \boldsymbol{\mu}'_t(\mathbf{x}_1) + \frac{\boldsymbol{\sigma}'_t(\mathbf{x}_1)}{\boldsymbol{\sigma}_t(\mathbf{x}_1)} \odot (\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{x}_1))$$

$$\boldsymbol{\mu}_0(\mathbf{x}_1) = 0, \quad \boldsymbol{\sigma}_0(\mathbf{x}_1) = 1, \quad \boldsymbol{\mu}_1(\mathbf{x}_1) = \mathbf{x}_1, \quad \boldsymbol{\sigma}_1(\mathbf{x}_1) = 0$$

$$\boldsymbol{\mu}_t(\mathbf{x}_1) = t\mathbf{x}_1; \quad \boldsymbol{\sigma}_t(\mathbf{x}_1) = (1 - t); \quad \mathbf{u}(\mathbf{x}, \mathbf{x}_1, t) = \frac{\mathbf{x}_1 - \mathbf{x}}{1 - t}$$

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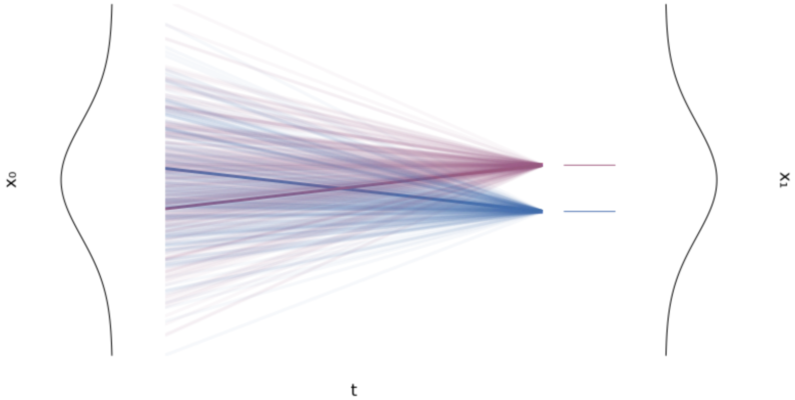
Flow Matching



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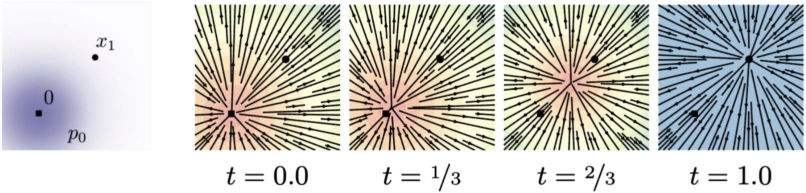
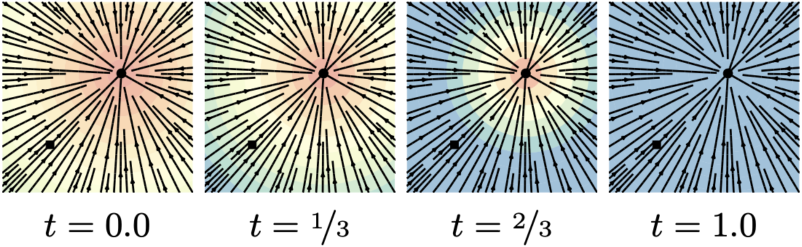
Flow Matching





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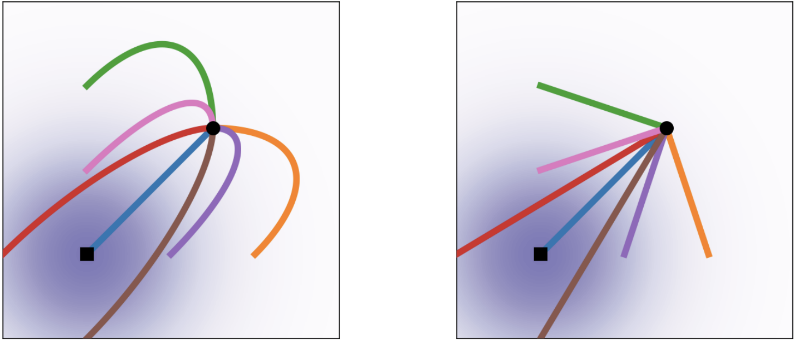
Flow Matching



Diffusion OT

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Outline

Summary

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