Deep Generative Models

Lecture 13

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AI Masters

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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

Recap of previous lecture

Discrete-in-time objective

$$\mathbb{E}_{\pi(\mathbf{x}_0)}\mathbb{E}_{t\sim U\{1,T\}}\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)}\left\|\mathbf{s}_{\boldsymbol{\theta},t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t}\log q(\mathbf{x}_t|\mathbf{x}_0)\right\|_2^2$$

Continuous-in-time objective

$$\mathbb{E}_{\pi(\mathbf{x}(0))}\mathbb{E}_{t\sim U[0,1]}\mathbb{E}_{q(\mathbf{x}(t)|\mathbf{x}(0))}\left\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}(t), t) - \nabla_{\mathbf{x}(t)}\log q(\mathbf{x}(t)|\mathbf{x}(0))\right\|_2^2$$

NCSN

$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\left(\mathbf{x}(0), \left[\sigma^2(t) - \sigma^2(0)\right]\cdot\mathbf{I}\right)$$

DDPM

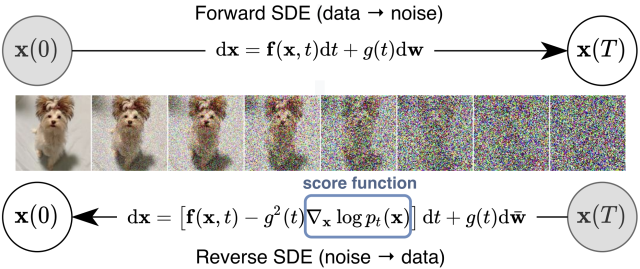
$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\left(\mathbf{x}(0)e^{-\frac{1}{2}\int_0^t\beta(s)ds}, \left(1 - e^{-\int_0^t\beta(s)ds}\right)\cdot\mathbf{I}\right)$$

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

Recap of previous lecture

Sampling

Solve reverse SDE using numerical solvers (SDESolve).



- Discretization of the reverse SDE gives us the ancestral sampling.
- If we use probability flow instead of SDE than the reverse ODE gives us the DDIM sampling.

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

Recap of previous lecture

Let consider ODE dynamic $\mathbf{x}(t)$ in time interval $t \in [0, 1]$ with $\mathbf{x}_0 \sim p_0(\mathbf{x}) = p(\mathbf{x})$, $\mathbf{x}_1 \sim p_1(\mathbf{x}) = \pi(\mathbf{x})$.

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t), \quad \text{with initial condition } \mathbf{x}(0) = \mathbf{x}_0.$$

KFP theorem (continuity equation)

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = -\text{div}\left(\mathbf{f}(\mathbf{x}, t) p_t(\mathbf{x})\right) \Leftrightarrow \frac{d \log p_t(\mathbf{x}(t))}{dt} = -\text{tr}\left(\frac{\partial \mathbf{f}(\mathbf{x}(t), t)}{\partial \mathbf{x}(t)}\right)$$

Solving the continuity equation using the adjoint method is complicated and unstable process.

Flow Matching

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

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

Recap of previous lecture

Let introduce the latent variable $\mathbf{z}$:

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

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

- $p_t(\mathbf{x}|\mathbf{z})$ is a **conditional probability path**;
- $\mathbf{f}(\mathbf{x}, \mathbf{z}, t)$ is a **conditional vector field**.

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

Theorem

The following vector field generates the probability path $p_t(\mathbf{x})$.

$$\mathbf{f}(\mathbf{x}, t) = \mathbb{E}_{p_t(\mathbf{z}|\mathbf{x})}\mathbf{f}(\mathbf{x}, \mathbf{z}, t) = \int \mathbf{f}(\mathbf{x}, \mathbf{z}, t)\frac{p_t(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{p_t(\mathbf{x})}d\mathbf{z}$$

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

Recap of previous lecture

Flow Matching (FM)

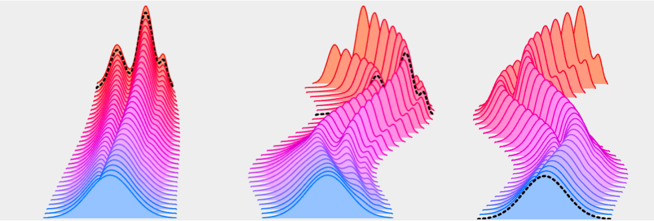
$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x})} \left\| \mathbf{f}(\mathbf{x}, t) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t) \right\|^2 \to \min_{\boldsymbol{\theta}}$$

Conditional Flow Matching (CFM)

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

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.



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

Outline

Outline

Conditional Flow Matching

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

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
   - Linear interpolation
   - Link with score-based models

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

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

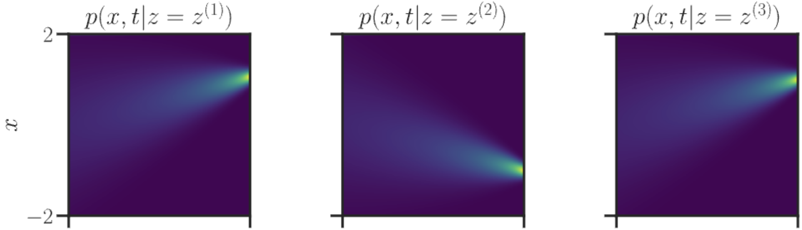


image credit: A Visual Dive into Conditional Flow Matching

Conical gaussian paths

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(t\mathbf{x}_1, (1-t)^2\mathbf{I}\right); \quad \mathbf{x} = t\mathbf{x}_1 + (1-t)\mathbf{x}_0.$$

Conditional vector field

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

$$\mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) = \mathbf{x}_1 - \frac{1}{1-t} \cdot (\mathbf{x} - t\mathbf{x}_1) = \frac{\mathbf{x}_1 - \mathbf{x}}{1-t} =$$

$$= \frac{\mathbf{x}_1 - t\mathbf{x}_1 - (1-t)\mathbf{x}_0}{1-t} = \mathbf{x}_1 - \mathbf{x}_0$$

Conditional Flow Matching

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

$$\mathbb{E}_{t\sim U[0,1]}\mathbb{E}_{\mathbf{x}_1\sim \pi(\mathbf{x})}\mathbb{E}_{\mathbf{x}\sim p_t(\mathbf{x}|\mathbf{x}_1)}\left\|\left(\frac{\mathbf{x}_1 - \mathbf{x}}{1-t}\right) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t)\right\|^2 =$$

$$\mathbb{E}_{t\sim U[0,1]}\mathbb{E}_{\mathbf{x}_1\sim \pi(\mathbf{x})}\mathbb{E}_{\mathbf{x}_0\sim \mathcal{N}(0,\mathbf{I})}\left\|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_{\boldsymbol{\theta}}\left(t\mathbf{x}_1 + (1-t)\mathbf{x}_0, t\right)\right\|^2$$

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

Conditional Flow Matching

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x}_1 \sim \pi(\mathbf{x})} \mathbb{E}_{\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})} \left\| (\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t) \right\|^2 \to \min_{\boldsymbol{\theta}}$$

We fit straight lines between noise distribution $p(\mathbf{x})$ and the data distribution $\pi(\mathbf{x})$.

Training

1. Get the sample $\mathbf{x}_1 \sim \pi(\mathbf{x})$.
2. Sample timestamp $t \sim U[0, 1]$ and $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}_t = t\mathbf{x}_1 + (1 - t)\mathbf{x}_0$.
4. Compute loss $\mathcal{L} = \left\| (\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t) \right\|^2$.

Sampling

1. Sample $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$.
2. Solve the ODE to get $\mathbf{x}_1$:

$$\mathbf{x}_1 = \text{ODESolve}_f(\mathbf{x}_0, \boldsymbol{\theta}, t_0 = 0, t_1 = 1).$$

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

Flow Matching

$$\mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0$$

- The conditional probability path $p_t(\mathbf{x}|\mathbf{z})$ is an **optimal transport path** from $p_0(\mathbf{x}|\mathbf{z})$ to $p_1(\mathbf{x}|\mathbf{z})$ (in terms of the conditional trajectories straightness).
- The marginal path $p_t(\mathbf{x})$ is not in general an optimal transport path from the standard normal $p_0(\mathbf{x})$ to the data distribution $p_1(\mathbf{x})$.

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

Outline

Pair 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 $\mathbf{z} = (\mathbf{x}_0, \mathbf{x}_1)$. Then $p(\mathbf{z}) = p(\mathbf{x}_0, \mathbf{x}_1) = p_0(\mathbf{x}_0)p_1(\mathbf{x}_1)$.

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) p_0(\mathbf{x}_0) p_1(\mathbf{x}_1) d\mathbf{x}_0 d\mathbf{x}_1$$

We need to ensure boundary constraints:

$$\begin{cases} p(\mathbf{x}) = \mathbb{E}_{p(\mathbf{z})} p_0(\mathbf{x}|\mathbf{z}); (= \mathcal{N}(0, \mathbf{I})) \\ \pi(\mathbf{x}) = \mathbb{E}_{p(\mathbf{z})} p_1(\mathbf{x}|\mathbf{z}). \end{cases} \Rightarrow \begin{cases} p_0(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_0); \\ p_1(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \end{cases}$$

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

Linear interpolation

$$p_0(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_0); \quad p_1(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1).$$

Gaussian conditional probability path

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

Let consider straight conditional paths

$$\begin{cases} \boldsymbol{\mu}_t(\mathbf{x}_1) = t\mathbf{x}_1 + (1-t)\mathbf{x}_0; \\ \boldsymbol{\sigma}_t(\mathbf{x}_1) = \epsilon. \end{cases} \Rightarrow \quad \begin{cases} p_0(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_0); \\ p_1(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \end{cases}$$

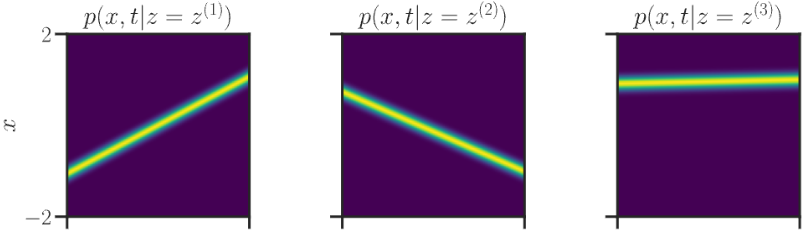
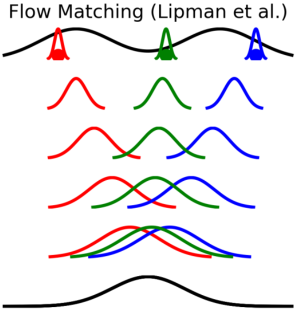


image credit: A Visual Dive into Conditional Flow Matching

Flow Matching: conical paths vs linear interpolation

$$\mathbf{z} = \mathbf{x}_1$$
$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(t\mathbf{x}_1, (1-t)^2\mathbf{I}\right)$$
$$\mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0.$$

$$\mathbf{z} = (\mathbf{x}_0, \mathbf{x}_1)$$
$$p_t(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \mathcal{N}\left(t\mathbf{x}_1 + (1-t)\mathbf{x}_0, \epsilon^2\mathbf{I}\right)$$
$$\mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0.$$



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

Linear interpolation

$$p_t(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \mathcal{N}\left(t\mathbf{x}_1 + (1-t)\mathbf{x}_0, \epsilon^2\mathbf{I}\right); \quad \mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0.$$

Conditional vector field

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{x}_0, \mathbf{x}_1, t) = \boldsymbol{\mu}'_t(\mathbf{x}_0, \mathbf{x}_1) + \frac{\boldsymbol{\sigma}'_t(\mathbf{x}_0, \mathbf{x}_1)}{\boldsymbol{\sigma}_t(\mathbf{x}_0, \mathbf{x}_1)} \odot (\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{x}_0, \mathbf{x}_1))$$

$$\mathbf{f}(\mathbf{x}, \mathbf{x}_0, \mathbf{x}_1, t) = \mathbf{x}_1 - \mathbf{x}_0$$

Conditional Flow Matching

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \left\| \mathbf{f}(\mathbf{x}, \mathbf{z}, t) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t) \right\|^2 =$$
$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{(\mathbf{x}_0, \mathbf{x}_1) \sim p(\mathbf{x}_0, \mathbf{x}_1)} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1)} \left\| (\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) \right\|^2$$

- We got the same procedure as for conical paths!
- Now we do not have the constraint that $p_0(\mathbf{x})$ should be $\mathcal{N}(0, \mathbf{I})$.

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

Conditional Flow Matching

- We could use this conditioning for transferring any distribution $p_0(\mathbf{x})$ to any distribution $p_1(\mathbf{x})$.
- It is possible to use this approach for paired problems (style transfer).

Training

1. Get the sample $(\mathbf{x}_0, \mathbf{x}_1) \sim p(\mathbf{x}_0, \mathbf{x}_1)$.
2. Sample timestamp $t \sim U[0, 1]$.
3. Get noisy image $\mathbf{x}_t = t\mathbf{x}_1 + (1 - t)\mathbf{x}_0$.
4. Compute loss $\mathcal{L} = \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t)\|^2$.

Sampling

1. Sample $\mathbf{x}_0 \sim p_0(\mathbf{x})$.
2. Solve the ODE to get $\mathbf{x}_1$:

$$\mathbf{x}_1 = \text{ODESolve}_f(\mathbf{x}_0, \boldsymbol{\theta}, t_0 = 0, t_1 = 1).$$

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

Stable Diffusion 3: scalable flow matching

Esser P., et al. Scaling Rectified Flow Transformers for High-Resolution Image Synthesis, 2024

Outline

Score-based generative models through SDEs

Training

$$\mathbb{E}_{\pi(\mathbf{x}(0))}\mathbb{E}_{t\sim U[0,1]}\mathbb{E}_{q(\mathbf{x}(t)|\mathbf{x}(0))}\left\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}(t), t) - \nabla_{\mathbf{x}(t)} \log q(\mathbf{x}(t)|\mathbf{x}(0))\right\|_2^2$$

Variance Exploding SDE (NCSN)

$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\left(\mathbf{x}(0), \left[\sigma^2(t) - \sigma^2(0)\right] \cdot \mathbf{I}\right), \quad \sigma(0) = 0.$$

Variance Preserving SDE (DDPM)

$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\left(\mathbf{x}(0)\alpha(t), \left(1 - \alpha(t)^2\right) \cdot \mathbf{I}\right); \quad \alpha(t) = e^{-\frac{1}{2}\int_0^t \beta(s)ds}$$

Flow matching uses the reverse time direction.

$$\textbf{NCSN: } p(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(\mathbf{x}_1, \sigma_{1-t}^2 \cdot \mathbf{I}\right)$$

$$\textbf{DDPM: } p(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(\alpha_{1-t}\mathbf{x}_1, \left(1 - \alpha_{1-t}^2\right) \cdot \mathbf{I}\right)$$

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

Flow matching vs score-based SDE models

Flow matching probability path

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(t\mathbf{x}_1, (1-t)^2\mathbf{I}\right); \quad \mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) = \frac{\mathbf{x}_1 - \mathbf{x}}{1-t}$$

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

Variance Exploding SDE probability path

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(\mathbf{x}_1, \sigma_{1-t}^2\mathbf{I}\right) \quad \Rightarrow \quad \mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) = -\frac{\sigma'_{1-t}}{\sigma_{1-t}} \cdot (\mathbf{x} - \mathbf{x}_1)$$

Variance Preserving SDE probability path

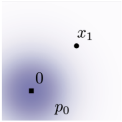
$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}\left(\alpha_{1-t}\mathbf{x}_1, (1-\alpha_{1-t}^2)\mathbf{I}\right) \Rightarrow \mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) = \frac{\alpha'_{1-t}}{1-\alpha_{1-t}^2} \cdot (\alpha_{1-t}\mathbf{x} - \mathbf{x}_1)$$

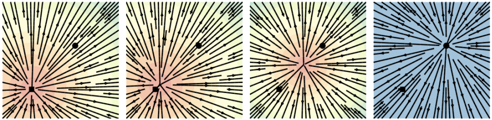
Lipman Y., et al. Flow Matching for Generative Modeling, 2022

Flow matching vs score-based SDE models

SDE vector field

$$\mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) = \frac{\alpha'_{1-t}}{1 - \alpha^2_{1-t}} \cdot (\alpha_{1-t}\mathbf{x} - \mathbf{x}_1)$$

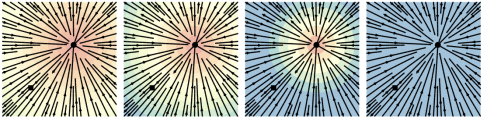




$t = 0.0$ $t = 1/3$ $t = 2/3$ $t = 1.0$

FM vector field

$$\mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) = \frac{\mathbf{x}_1 - \mathbf{x}}{1 - t}$$



$t = 0.0$ $t = 1/3$ $t = 2/3$ $t = 1.0$

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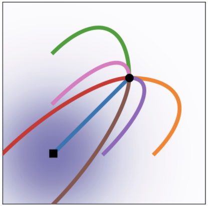
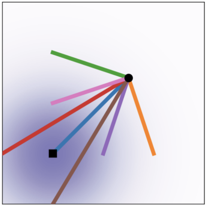
Flow matching vs score-based SDE models

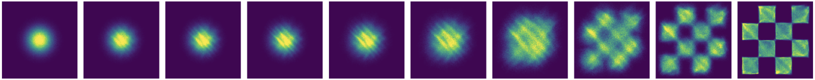
Trajectories



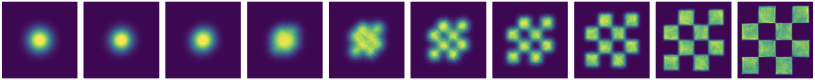
Diffusion



OT



Score matching w/ Diffusion



Flow Matching w/ OT

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Summary

- Conditional flow matching allows to make the FM objective tractable.
- Conical gaussian paths is the example of the effective FM technique.
- Pair conditioning gives the same procedure, but it is more general.
- Diffusion and score-based model are the special case of flow matching approach with curved trajectories.