

Deep Generative Models

Lecture 13

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Recap of previous lecture

SDE basics

Let define stochastic process $\mathbf{x}(t)$ with initial condition $\mathbf{x}(0) \sim p_0(\mathbf{x})$:

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

where $\mathbf{w}(t)$ is the standard Wiener process (Brownian motion)

$$\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, (t-s)\mathbf{I}), \quad d\mathbf{w} = \boldsymbol{\epsilon} \cdot \sqrt{dt}, \text{ where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

Discretization of SDE (Euler method)

$$\mathbf{x}(t + dt) = \mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t), t) \cdot dt + g(t) \cdot \boldsymbol{\epsilon} \cdot \sqrt{dt}$$

- ▶ At each moment t we have the density $p_t(\mathbf{x}) = p(\mathbf{x}, t)$.
- ▶ $p : \mathbb{R}^m \times [0, 1] \rightarrow \mathbb{R}_+$ is a **probability path** between $p_0(\mathbf{x})$ and $p_1(\mathbf{x})$.

Recap of previous lecture

Theorem (Kolmogorov-Fokker-Planck)

Evolution of the distribution $p_t(\mathbf{x})$ is given by the following equation:

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = -\operatorname{div}(\mathbf{f}(\mathbf{x}, t)p_t(\mathbf{x})) + \frac{1}{2}g^2(t)\Delta_{\mathbf{x}}p_t(\mathbf{x})$$

Langevin SDE (special case)

$$d\mathbf{x} = \frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x}) dt + \mathbf{1} \cdot d\mathbf{w}$$

The density $p(\mathbf{x}|\theta)$ is a **stationary** distribution for the SDE.

Langevin dynamics

Samples from the following dynamics will come from $p(\mathbf{x}|\theta)$ under mild regularity conditions for small enough η .

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

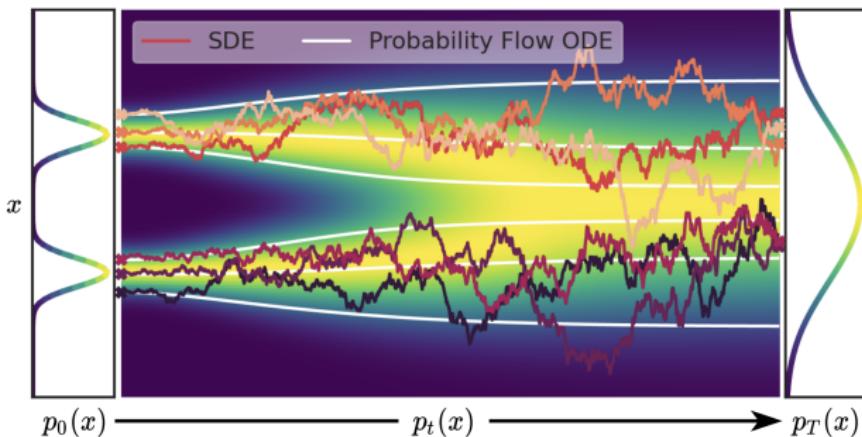
Recap of previous lecture

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

Probability flow ODE

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

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



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

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

Sketch of the proof

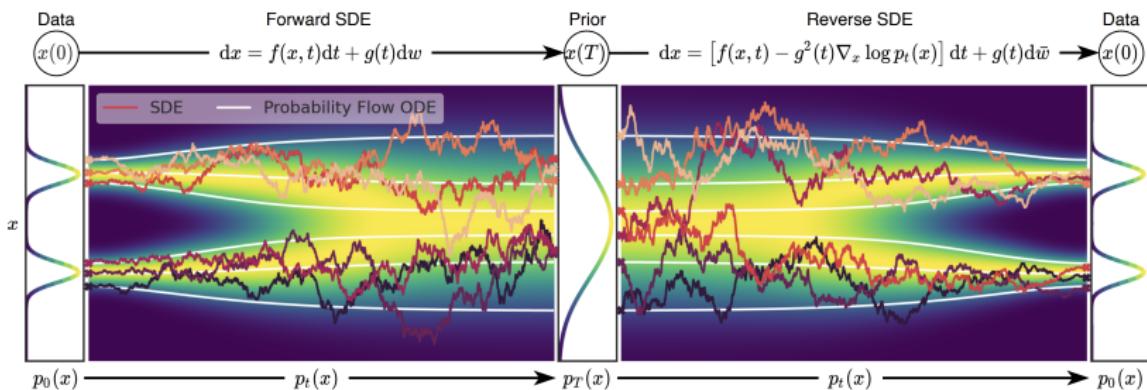
- ▶ Convert initial SDE to probability flow ODE.
- ▶ Revert probability flow ODE.
- ▶ Convert reverse probability flow ODE to reverse SDE.

Recap of previous lecture

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

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

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



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.

Outline

1. Score-based generative models through SDEs
2. Flow Matching
3. Conditional Flow Matching
 - Conical gaussian paths
 - Link with score-based models

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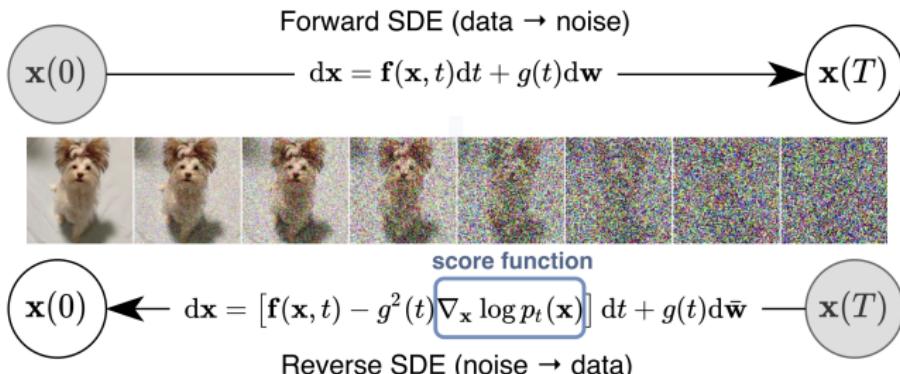
Score-based generative models through SDEs

Discrete-in-time objective

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

Continuous-in-time objective

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



Score-based generative models through SDEs

Continuous-in-time objective

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

$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\left(\boldsymbol{\mu}(\mathbf{x}(t), \mathbf{x}(0)), \boldsymbol{\Sigma}(\mathbf{x}(t), \mathbf{x}(0))\right)$$

Theorem

Moments of the SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ satisfies the equations

$$\frac{d\boldsymbol{\mu}(\mathbf{x}(t), \mathbf{x}(0))}{dt} = \mathbb{E} [\mathbf{f}(\mathbf{x}(t), t)|\mathbf{x}(0)]$$

$$\frac{d\boldsymbol{\Sigma}(\mathbf{x}(t), \mathbf{x}(0))}{dt} = \mathbb{E} \left[\mathbf{f} \cdot (\mathbf{x}(t) - \boldsymbol{\mu})^T + (\mathbf{x}(t) - \boldsymbol{\mu}) \cdot \mathbf{f}^T | \mathbf{x}(0) \right] + g^2(t) \cdot \mathbf{I}$$

Let prove the first one.

Score-based generative models through SDEs

Theorem

$$\frac{d\mu(\mathbf{x}(t), \mathbf{x}(0))}{dt} = \mathbb{E} [\mathbf{f}(\mathbf{x}(t), t) | \mathbf{x}(0)]$$

Proof

$$\begin{aligned}\mathbb{E} [d\mathbf{x} | \mathbf{x}(0)] &= \mathbb{E} [\mathbf{f}(\mathbf{x}, t) dt | \mathbf{x}(0)] + \mathbb{E} [g(t) d\mathbf{w} | \mathbf{x}(0)] \\ &= \mathbb{E} [\mathbf{f}(\mathbf{x}, t) | \mathbf{x}(0)] dt + g(t) \mathbb{E} [d\mathbf{w} | \mathbf{x}(0)] \\ &= \mathbb{E} [\mathbf{f}(\mathbf{x}, t) | \mathbf{x}(0)] dt\end{aligned}$$

$$\frac{d\mathbb{E} [\mathbf{x} | \mathbf{x}(0)]}{dt} = \frac{d\mu(\mathbf{x}(t), \mathbf{x}(0))}{dt} = \mathbb{E} [\mathbf{f}(\mathbf{x}, t) | \mathbf{x}(0)]$$

Examples

NCSN: $\mathbf{f}(\mathbf{x}, t) = 0 \quad \Rightarrow \quad \mu = \mathbf{x}(0)$

DDPM: $\mathbf{f}(\mathbf{x}, t) = -\frac{1}{2}\beta(t)\mathbf{x}(t) \quad \Rightarrow \quad \mu = \mathbf{x}(0) \exp\left(-\frac{1}{2} \int_0^t \beta(s) ds\right)$

Score-based generative models through SDEs

Training

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

$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\left(\boldsymbol{\mu}(\mathbf{x}(t), \mathbf{x}(0)), \boldsymbol{\Sigma}(\mathbf{x}(t), \mathbf{x}(0))\right)$$

NCSN

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

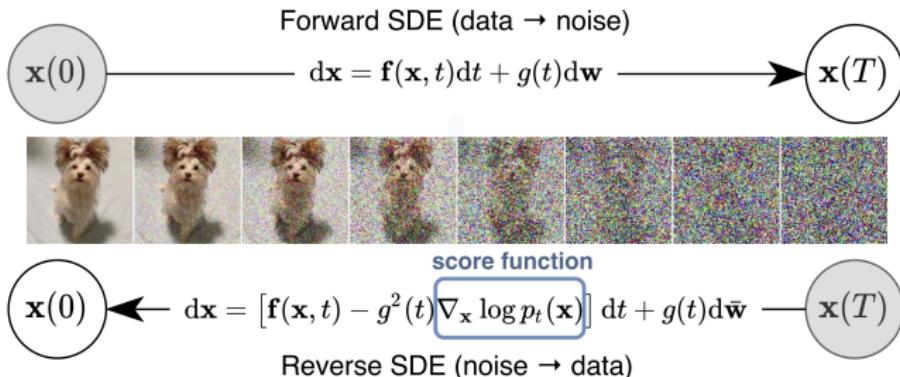
DDPM

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

Score-based generative models through SDEs

Sampling

Solve reverse SDE using numerical solvers (ODESolve).



- ▶ 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.

Outline

1. Score-based generative models through SDEs

2. Flow Matching

3. Conditional Flow Matching

Conical gaussian paths

Link with score-based models

Continuous-in-time NF

Let consider ODE dynamic $\mathbf{x}(t)$ in time interval $t \in [0, 1]$

- ▶ $\mathbf{x}_0 \sim p_0(\mathbf{x}) = p(\mathbf{x})$, $\mathbf{x}_1 \sim p_1(\mathbf{x}) = \pi(\mathbf{x})$;
- ▶ $p(\mathbf{x})$ is a base distribution ($\mathcal{N}(0, \mathbf{I})$) and $\pi(\mathbf{x})$ is a true data distribution.

Note: the time direction is the same as for CNF (opposite to score-based SDE models).

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

KFP theorem (continuity equation)

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

Continuous-in-time NF

KFP theorem (continuity equation)

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

- ▶ If we know the true vector field $\mathbf{f}(\mathbf{x}, t)$, then KFP equation (or continuity equation) gives us the way to compute the density $p_t(\mathbf{x})$.
- ▶ Solving the continuity equation using the adjoint method is complicated and unstable process.
- ▶ **Flow matching** generalizes these models and gives the alternative way to solve the Neural ODE.

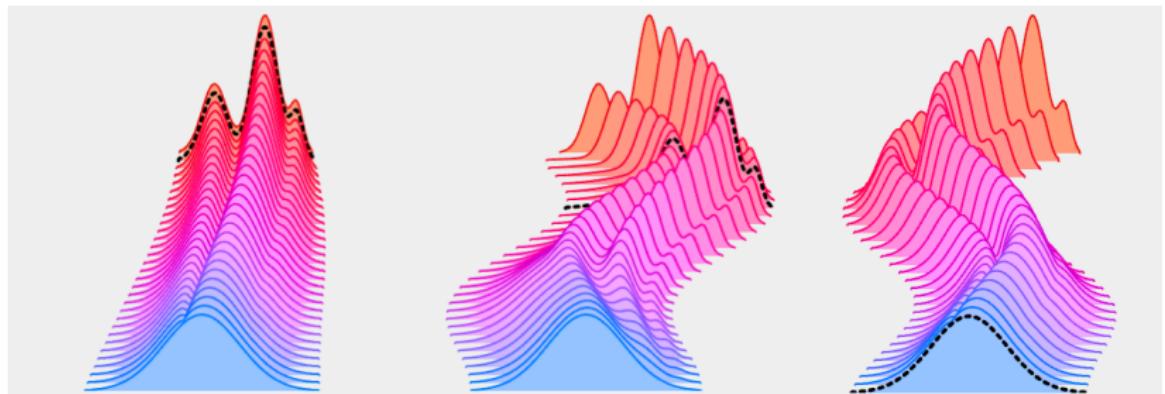
Flow Matching

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

Flow Matching

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

- ▶ There exists infinite number of possible $\mathbf{f}(\mathbf{x}, t)$ between $\pi(\mathbf{x})$ and $p(\mathbf{x})$.
- ▶ The true vector field $\mathbf{f}(\mathbf{x}, t)$ is **unknown**.
- ▶ We need to select the "best" $\mathbf{f}(\mathbf{x}, t)$ and makes the objective tractable.



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Flow Matching

Latent variable model

Let's introduce the latent variable \mathbf{z} :

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

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

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

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

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

What is the relationship between $\mathbf{f}(\mathbf{x}, t)$ and $\mathbf{f}(\mathbf{x}, \mathbf{z}, t)$?

Flow Matching

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

Theorem

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

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

Proof

$$\begin{aligned}\frac{\partial p_t(\mathbf{x})}{\partial t} &= \frac{\partial}{\partial t} \int p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} = \int \left(\frac{\partial p_t(\mathbf{x}|\mathbf{z})}{\partial t} \right) p(\mathbf{z}) d\mathbf{z} = \\ &= \int (-\operatorname{div}(\mathbf{f}(\mathbf{x}, \mathbf{z}, t) p_t(\mathbf{x}|\mathbf{z}))) p(\mathbf{z}) d\mathbf{z} = \\ &= -\operatorname{div} \left(\int \mathbf{f}(\mathbf{x}, \mathbf{z}, t) p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} \right) = -\operatorname{div}(\mathbf{f}(\mathbf{x}, t) p_t(\mathbf{x}))\end{aligned}$$

Flow Matching

Flow Matching (FM)

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

Conditional Flow Matching (CFM)

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

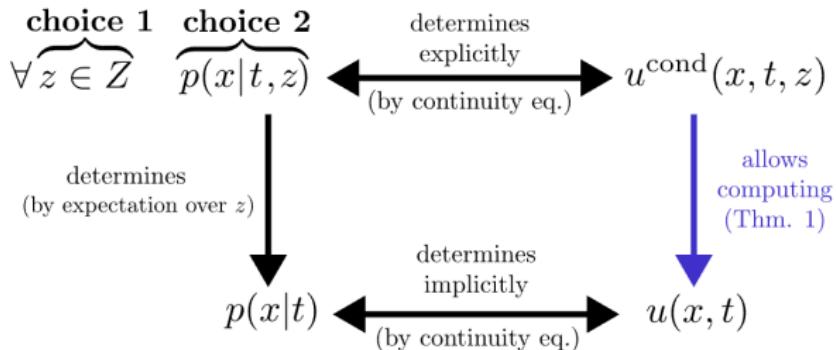
Theorem

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.

Conditional Flow Matching



- ▶ We do not want to model $p_t(\mathbf{x})$ because it is complex.
- ▶ We showed that it is possible to solve CFM task instead of FM task.
- ▶ Let choose the convenient conditioning latent variable \mathbf{z} .
- ▶ Let parametrize $p_t(\mathbf{x}|\mathbf{z})$ instead of $p_t(\mathbf{x})$. It must satisfy the following constraints

$$p(\mathbf{x}) = \mathcal{N}(0, \mathbf{I}) = \mathbb{E}_{p(\mathbf{z})} p_0(\mathbf{x}|\mathbf{z}); \quad \pi(\mathbf{x}) = \mathbb{E}_{p(\mathbf{z})} p_1(\mathbf{x}|\mathbf{z}).$$

Conditional Flow Matching

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

What is left?

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

Gaussian conditional probability path

$$p_t(x|z) = \mathcal{N}(\mu_t(z), \sigma_t^2(z))$$

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

$$x_t = \mu_t(z) + \sigma_t(z) \odot x_0, \quad x_0 \sim p_0(x) = \mathcal{N}(0, I)$$

Flow Matching

Gaussian conditional probability path

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

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

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

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

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3. **Conditional Flow Matching**
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Endpoint conditioning

Conditional Flow Matching

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

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:

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

Conical gaussian paths

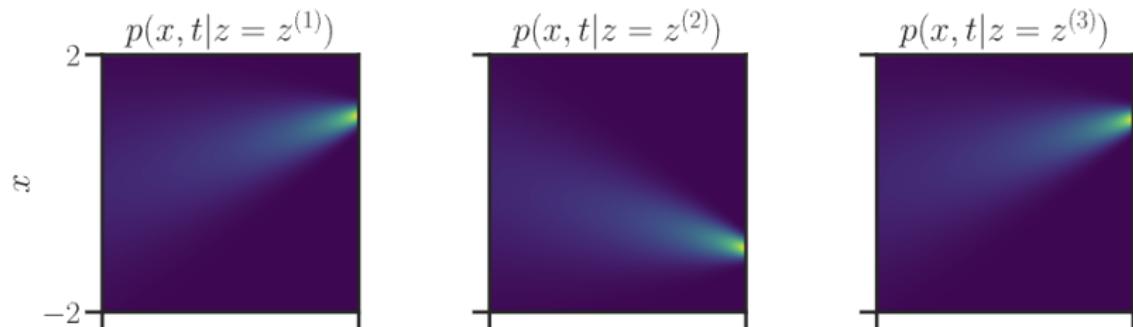
$$p_0(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(0, \mathbf{I}); \quad p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1).$$

Gaussian conditional probability path

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

Let consider straight conditional paths

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



Conical gaussian paths

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

Conditional vector field

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

$$\begin{aligned} \mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) &= \mathbf{x}_1 - \frac{1}{1-t} \cdot (\mathbf{x} - t\mathbf{x}_1) = \frac{\mathbf{x}_1 - \mathbf{x}}{1-t} = \\ &= \frac{\mathbf{x}_1 - t\mathbf{x}_1 + (1-t)\mathbf{x}_0}{1-t} = \mathbf{x}_1 - \mathbf{x}_0 \end{aligned}$$

Conditional Flow Matching

$$\begin{aligned} \mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \|\mathbf{f}(\mathbf{x}, \mathbf{z}, t) - \mathbf{f}_\theta(\mathbf{x}, t)\|^2 &= \\ \mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x}_1 \sim \pi(\mathbf{x})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{x}_1)} \left\| \left(\frac{\mathbf{x}_1 - \mathbf{x}}{1-t} \right) - \mathbf{f}_\theta(\mathbf{x}, t) \right\|^2 &= \\ \mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x}_1 \sim \pi(\mathbf{x})} \mathbb{E}_{\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})} \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_\theta(t\mathbf{x}_1 + (1-t)\mathbf{x}_0, t)\|^2 \end{aligned}$$

Conditional Flow Matching

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

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 $t \sim U\{1, T\}$ and $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$.
4. Compute loss $\mathcal{L} = \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_\theta(\mathbf{x}, t)\|^2$.

Sampling

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

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

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

1. Score-based generative models through SDEs
2. Flow Matching
3. Conditional Flow Matching
 - Conical gaussian paths
 - Link with score-based models

Flow matching vs score-based SDE models

Flow matching probability path

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

Variance Exploding SDE probability path

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}; \quad \Rightarrow \quad \begin{cases} p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(\mathbf{x}_1, \sigma_{1-t}^2 \mathbf{I}) \\ \mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) = -\frac{\sigma'_{1-t}}{\sigma_{1-t}} \cdot (\mathbf{x} - \mathbf{x}_1) \end{cases}$$

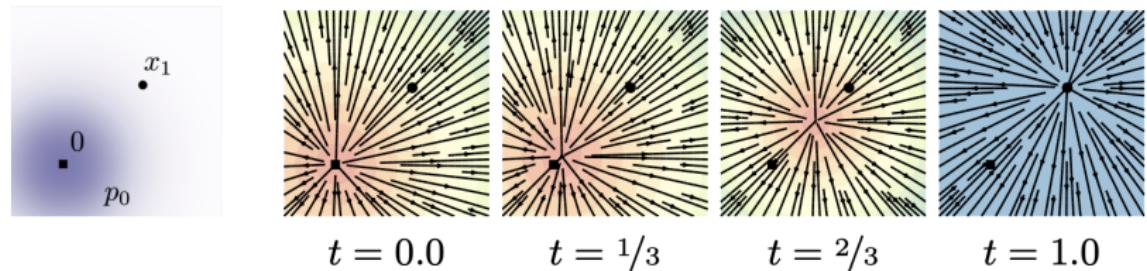
Variance Preserving SDE probability path

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)}d\mathbf{w}; \Rightarrow \begin{cases} p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(\alpha_{1-t}\mathbf{x}_1, (1-\alpha_{1-t}^2)\mathbf{I}) \\ \mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) = \frac{\alpha'_{1-t}}{1-\alpha_{1-t}^2} \cdot (\alpha_{1-t}\mathbf{x} - \mathbf{x}_1) \end{cases}$$

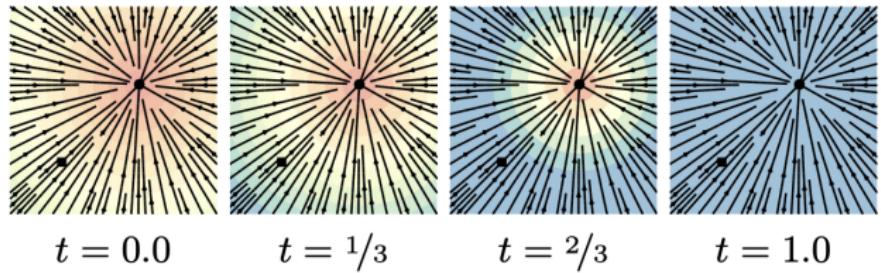
Here $\alpha_t = \exp\left(-\frac{1}{2} \int_0^t \beta(s)ds\right)$.

Flow matching vs score-based SDE models

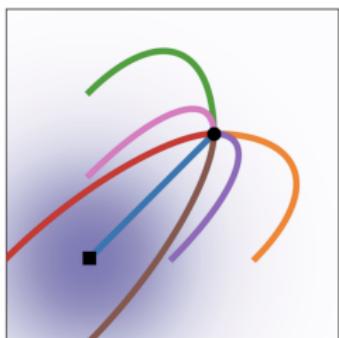
Diffusion vector field



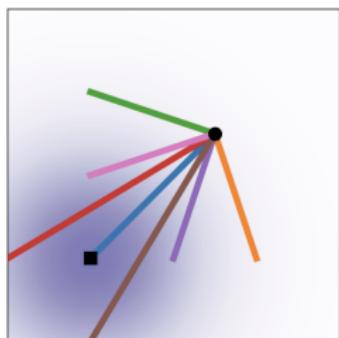
Flow matching vector field



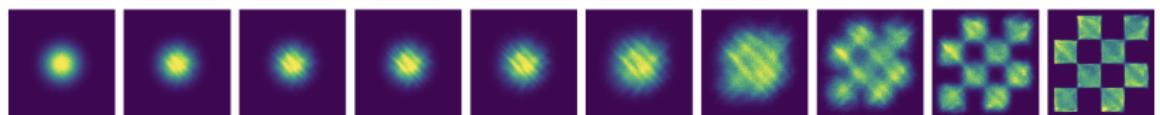
Flow matching vs score-based SDE models



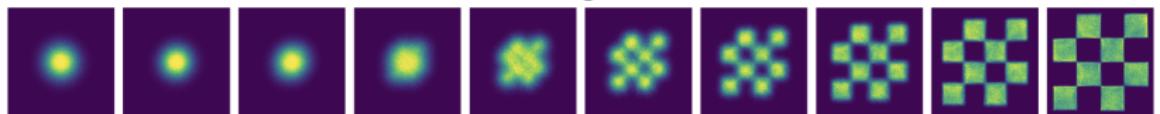
Diffusion



OT



Score matching w/ Diffusion



Flow Matching w/ OT

Summary

- ▶ It is possible to train the continuous-in-time score-based generative models through forward and reverse SDEs.
- ▶ Discretization of the reverse SDE gives the ancestral sampling of the DDPM.
- ▶ Flow matching suggests to fit the vector field directly.
- ▶ Conditional flow matching allows to make the FM objective tractable.
- ▶ Conical gaussian paths is the example of the effective FM technique.