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 $p_t(\mathbf{x}) = p(\mathbf{x}, t)$.
- $p : \mathbb{R}^m \times [0, 1] \to \mathbb{R}_+$ 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:

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

Langevin SDE (special case)

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

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

Langevin dynamics

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

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

Welling M. Bayesian Learning via Stochastic Gradient Langevin Dynamics, 2011

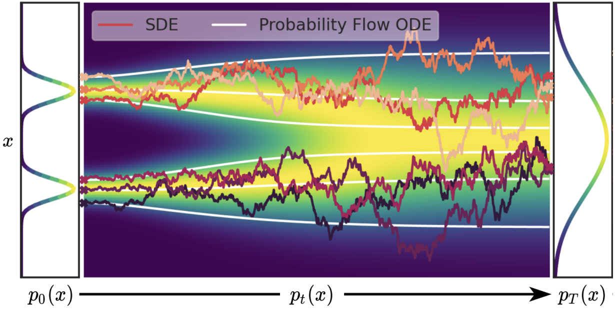
Recap of previous lecture

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

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

Sketch of the proof

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

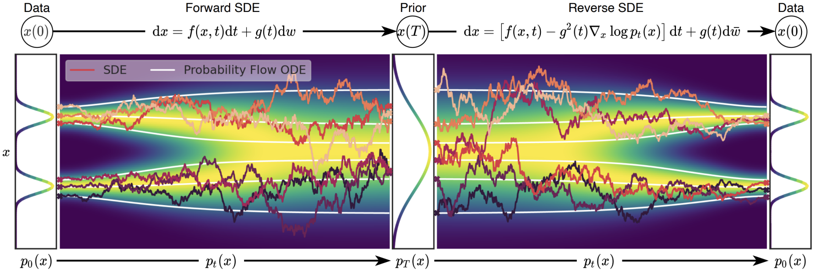
Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Recap of previous lecture

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

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

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



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

Recap of previous lecture

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

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. Score-based generative models through SDEs

2. Flow Matching
   - Endpoint conditioning
   - Pair conditioning
   - Rectified flows

Outline

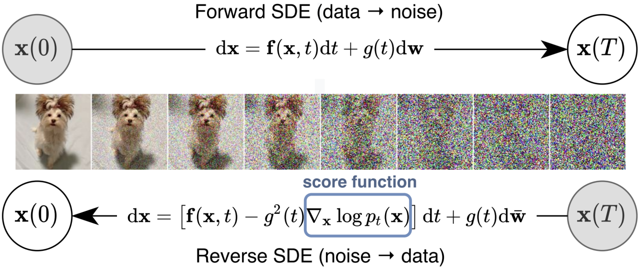
Score-based generative models through SDEs

Discrete-in-time objective

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

Continuous-in-time objective

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



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

Score-based generative models through SDEs

Continuous-in-time objective

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

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

Theorem

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

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

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

Let prove the first one.

Särkkä S., Solin A. Applied stochastic differential equations, 2019

Score-based generative models through SDEs

Theorem

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

Proof

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

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

Examples

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

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

Särkkä S., Solin A. Applied stochastic differential equations, 2019

Score-based generative models through SDEs

Training

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

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

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

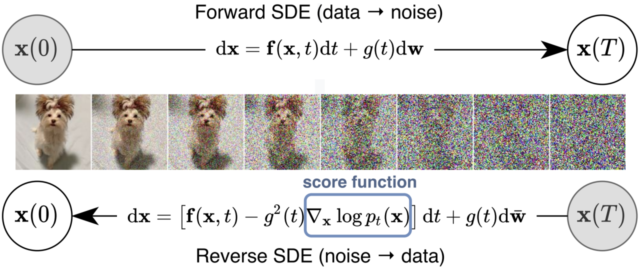
$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\left(\mathbf{x}(0)e^{-\frac{1}{2}\int_0^t \beta(s)ds}, \left(1 - e^{-\int_0^t \beta(s)ds}\right) \cdot \mathbf{I}\right)$$

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

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.

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

Outline

1. Score-based generative models through SDEs

2. Flow Matching
   - Endpoint conditioning
   - Pair conditioning
   - Rectified flows

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)

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

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Continuous-in-time NF

KFP theorem (continuity equation)

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

- 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

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

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

Flow Matching

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

- 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.

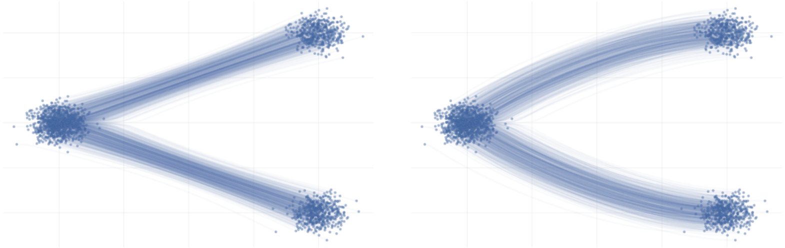


image credit: https://mlg.eng.cam.ac.uk/blog/2024/01/20/flow-matching.html

Flow Matching

Latent variable model

Let 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

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

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 $\mathbf{f}(\mathbf{x}, \mathbf{z}, t)$?

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

Flow Matching

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

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

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

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

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

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Flow Matching

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.

Proof

It is proved similarly with the denoising score matching theorem.

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

Flow Matching

Conditional Flow Matching (CFM)

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

- 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 parametrize $p_t(\mathbf{x}|\mathbf{z})$ instead of $p_t(\mathbf{x})$.

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:

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

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Flow Matching

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

$$\mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{z}) + \boldsymbol{\sigma}_t(\mathbf{z}) \odot \mathbf{x}_0 \quad \Rightarrow \quad \mathbf{x}_0 = \frac{1}{\boldsymbol{\sigma}_t(\mathbf{z})} \odot (\mathbf{x}_t - \boldsymbol{\mu}_t(\mathbf{z}))$$

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

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

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Flow Matching

Conditional Flow Matching

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

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:

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

Gaussian conditional probability path

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

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

Flow Matching

Gaussian conditional probability path

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

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

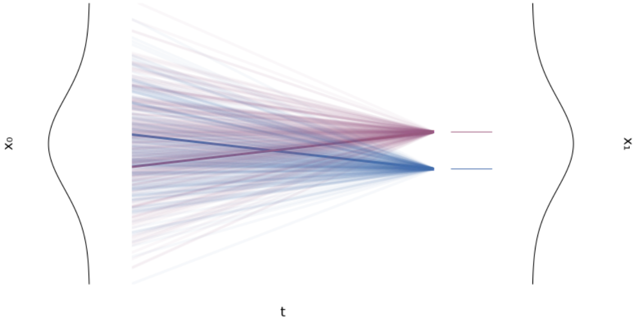

image credit: https://mlg.eng.cam.ac.uk/blog/2024/01/20/flow-matching.html

Flow Matching

$$\begin{cases} p_0(\mathbf{x}|\mathbf{x}_1) = p_0(\mathbf{x}); \\ p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \end{cases} \quad \Rightarrow \quad \begin{cases} \boldsymbol{\mu}_0(\mathbf{x}_1) = 0, \quad \boldsymbol{\sigma}_0(\mathbf{x}_1) = 1; \\ \boldsymbol{\mu}_1(\mathbf{x}_1) = \mathbf{x}_1, \quad \boldsymbol{\sigma}_1(\mathbf{x}_1) = 0. \end{cases}$$

Let consider straight conditional paths

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

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

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{z}, t); \quad \mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) = \frac{\mathbf{x}_1 - \mathbf{x}}{1-t}; \quad \frac{d\mathbf{x}}{dt} = \mathbf{x}_1 - \mathbf{x}_0.$$

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

Flow Matching

Conditional Flow Matching

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

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

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

Flow Matching

- The conditional probability path $p_t(\mathbf{x}|\mathbf{z})$ is an optimal transport path from $p_0(\mathbf{x}|\mathbf{z})$ to $p_1(\mathbf{x}|\mathbf{z})$.
- 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

Flow Matching

Flow matching probability path

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

Variance Exploding SDE probability path

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

Variance Preserving SDE probability path

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

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

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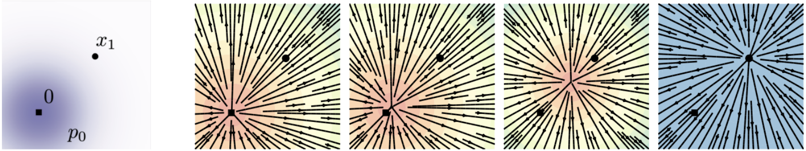
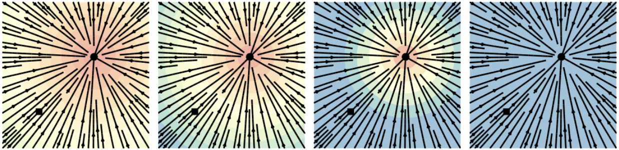
Flow Matching

Diffusion vector field



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

Flow matching vector field



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

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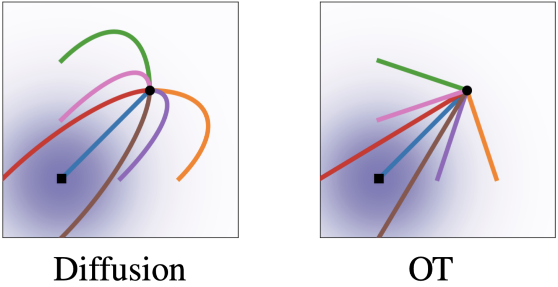
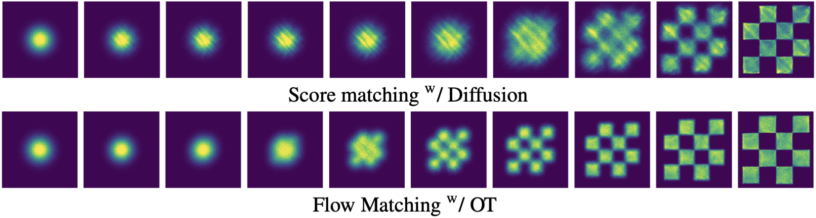
Flow Matching





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Outline

1. Score-based generative models through SDEs

2. Flow Matching
   - Endpoint conditioning
   - Pair conditioning
   - Rectified flows

Flow Matching

Conditional Flow Matching

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

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

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

We need to ensure boundary conditions:

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

Gaussian conditional probability path

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

Flow Matching

$$\begin{cases} p_0(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_0); \\ p_1(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \end{cases} \quad \Rightarrow \quad \begin{cases} \boldsymbol{\mu}_0(\mathbf{x}_0, \mathbf{x}_1) = \mathbf{x}_0, \quad \boldsymbol{\sigma}_0(\mathbf{x}_0, \mathbf{x}_1) = 0 \\ \boldsymbol{\mu}_1(\mathbf{x}_0, \mathbf{x}_1) = \mathbf{x}_1, \quad \boldsymbol{\sigma}_1(\mathbf{x}_0, \mathbf{x}_1) = 0 \end{cases}$$

Let consider straight conditional paths

$$\begin{cases} \boldsymbol{\mu}_t(\mathbf{x}_0, \mathbf{x}_1) = t\mathbf{x}_1 + (1-t)\mathbf{x}_0; \\ \boldsymbol{\sigma}_t(\mathbf{x}_0, \mathbf{x}_1) = 0. \end{cases} \quad \Rightarrow \begin{cases} p_t(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \mathcal{N}\left(t\mathbf{x}_1 + (1-t)\mathbf{x}_0\right. \\ \mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0. \end{cases}$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{x}_1 - \mathbf{x}_0.$$

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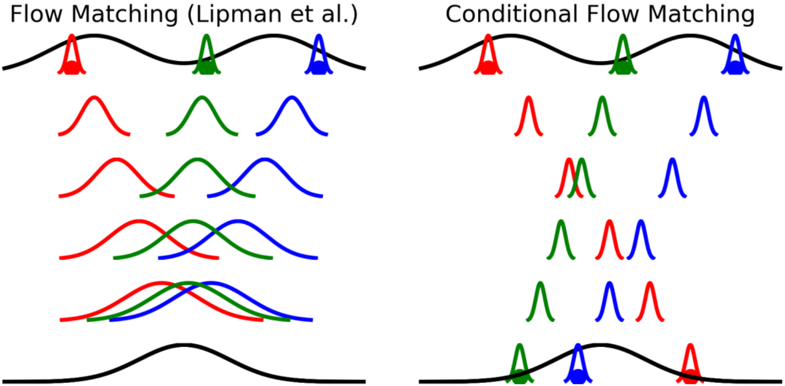
Flow Matching



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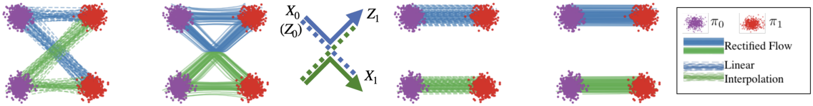
Outline

Flow Matching

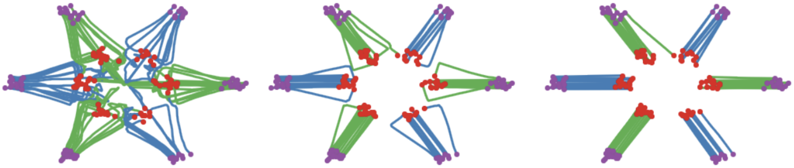


(a) Linear interpolation $X_t = tX_1 + (1-t)X_0$

(b) Rectified flow Z_t induced by (X_0, X_1)

(c) Linear interpolation $Z_t = tZ_1 + (1-t)Z_0$

(d) Rectified flow Z'_t induced by (Z_0, Z_1)



(a)The 1st rectified flow $\boldsymbol{Z}^1$

$\boldsymbol{Z}^1 = \texttt{RectFlow}((X_0, X_1))$

(b) Reflow $\boldsymbol{Z}^2$

$\boldsymbol{Z}^2 = \texttt{RectFlow}((Z_0^1, Z_1^1))$

(c) Reflow $\boldsymbol{Z}^3$

$\boldsymbol{Z}^3 = \texttt{RectFlow}((Z_0^2, Z_1^2))$

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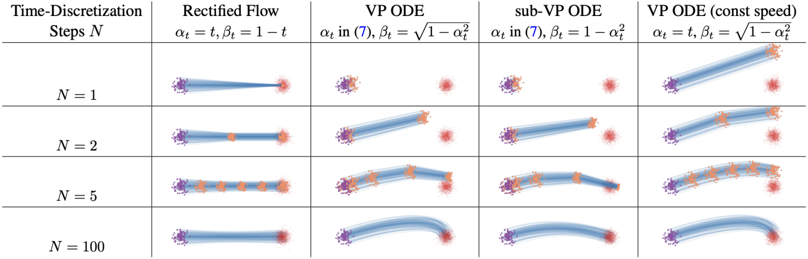
Flow Matching



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Stable Diffusion 3

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Summary

- It is possible to train the continuous-in-time score-based generative models through forward and reverse SDEs.

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