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

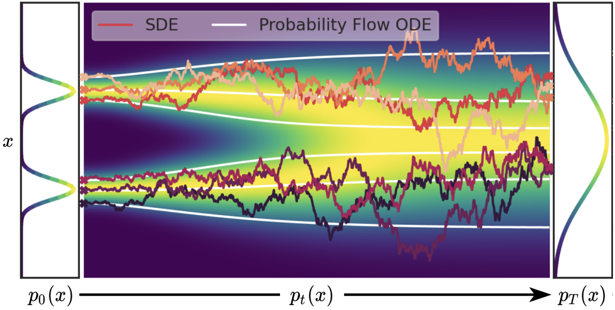
Recap of previous lecture

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

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

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

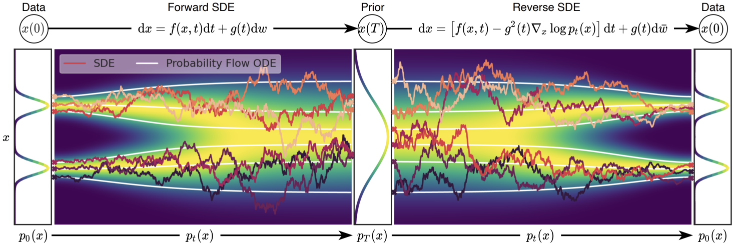
Recap of previous lecture

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

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

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

- 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. Score-based generative models through SDEs

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

Outline

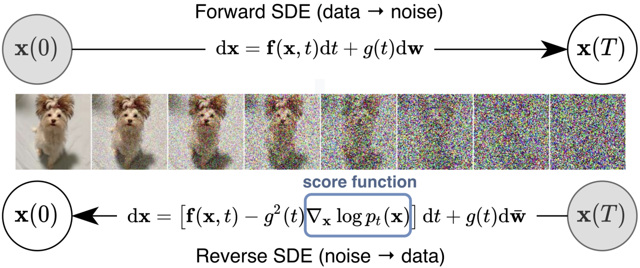
Score-based generative models through SDEs

Discrete-in-time objective

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

Continuous-in-time objective

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



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

Score-based generative models through SDEs

Continuous-in-time objective

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

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

Theorem

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

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

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

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

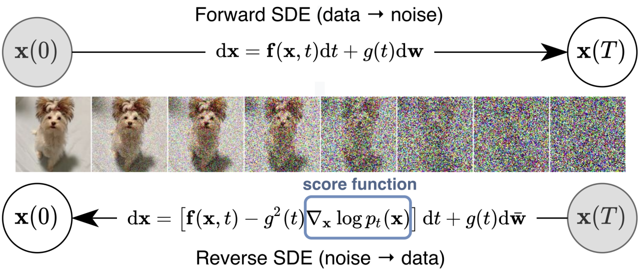
$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\left(\mathbf{x}(0)e^{-\frac{1}{2}\int_0^t \beta(s)ds}, \left(1 - e^{-\int_0^t \beta(s)ds}\right) \cdot \mathbf{I}\right)$$

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

Flow Matching

Continuous-in-time NF

$$\frac{d\mathbf{z}(t)}{dt} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}(t), t); \quad \text{with initial condition } \mathbf{z}(0) = \mathbf{z}_0.$$

Theorem (Kolmogorov-Fokker-Planck: special case)

If $\mathbf{f}$ is uniformly Lipschitz continuous in $\mathbf{z}$ and continuous in t, then

$$\frac{d \log p_t(\mathbf{z}(t))}{dt} = -\mathrm{tr}\left(\frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)}\right).$$

$$\log p_1(\mathbf{z}(1)) = \log p_0(\mathbf{z}(0)) - \int_0^1 \mathrm{tr}\left(\frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)}\right) dt.$$

- Solving KFP using adjoint method is comlicated and unstable process.
- Flow matching generalizes these models and gives the alternative way to solve the continuous dynamics.

Flow Matching

Let consider ODE dynamic $\mathbf{x}_t = \mathbf{x}(t)$ 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 difference with the diffusion models (and CNF) in the opposite time direction.

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

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

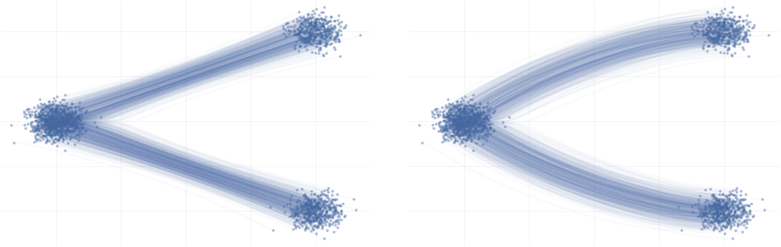
Lipman Y., et al. Flow Matching for Generative Modeling, 2022

Flow Matching

Flow Matching

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

- There exists infinite number of possible $\mathbf{u}(\mathbf{x}, t)$ between $\pi(\mathbf{x})$ and $p(\mathbf{x})$.
- The true vector field $\mathbf{u}(\mathbf{x}, t)$ is **unknown**.



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Flow Matching

Latent variable model

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

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

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

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

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

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

Flow Matching

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

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

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

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

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

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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Flow Matching

Gaussian conditional probability path

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

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

$$\mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{z}) + \boldsymbol{\sigma}_t(\mathbf{z}) \odot \mathbf{x}_0$$

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Flow Matching

Theorem

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

Proof

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

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

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

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

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:

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

Gaussian conditional probability path

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

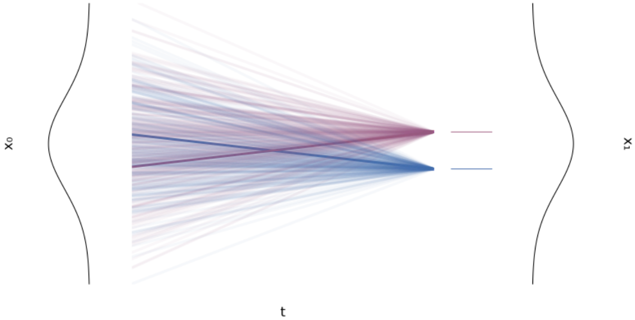
Lipman Y., et al. Flow Matching for Generative Modeling, 2022

Flow Matching

Gaussian conditional probability path

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

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



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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

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

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

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

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

Flow Matching

Conditional Flow Matching

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

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

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 $p_1(\mathbf{x})$.

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Flow Matching

Flow matching probability path

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

Variance Exploding SDE probability path

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

Variance Preserving SDE probability path

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

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

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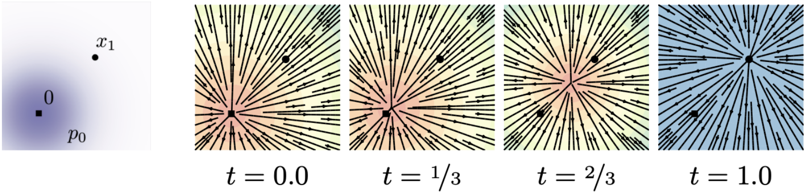
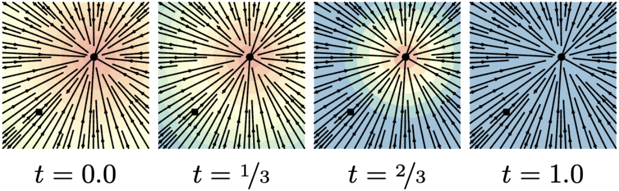
Flow Matching

Diffusion vector field



Flow matching vector field



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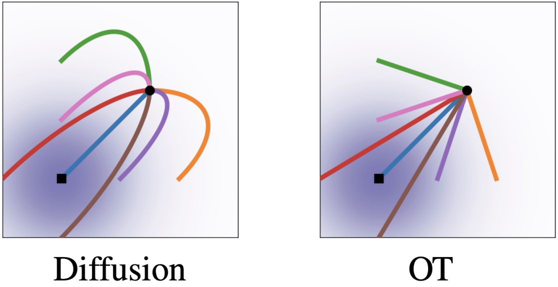
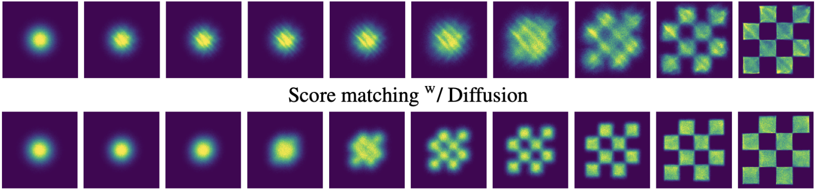
Flow Matching





Score matching w/ Diffusion

Flow Matching w/ OT

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Outline

Flow Matching

Conditional Flow Matching

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

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

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

Let consider straight conditional paths

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

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

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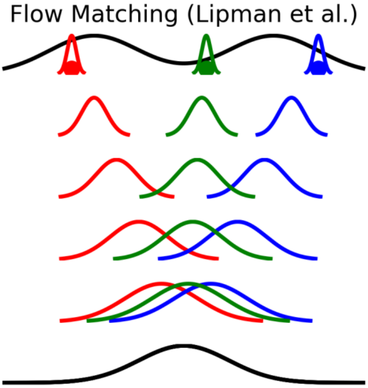
Flow Matching



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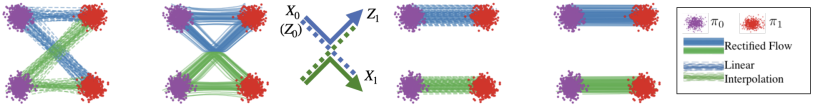
Outline

Flow Matching

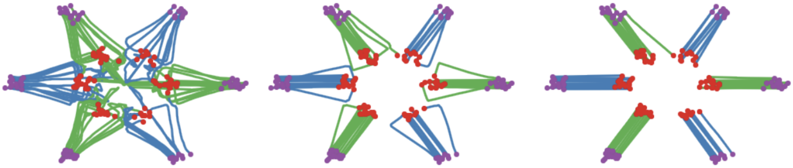


(a) Linear interpolation $X_t = tX_1 + (1-t)X_0$

(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)



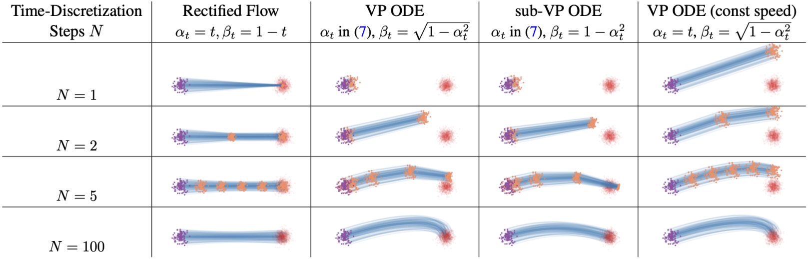
(a)The 1st rectified flow $\boldsymbol{Z}^1$ $\boldsymbol{Z}^1 = \texttt{RectFlow}((X_0, X_1))$

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

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

Liu X., et al. Flow Straight and Fast: Learning to Generate and Transfer Data with Rectified Flow, 2022

Flow Matching



Liu X., et al. Flow Straight and Fast: Learning to Generate and Transfer Data with Rectified Flow, 2022

Stable Diffusion 3

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

Summary

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