Deep Generative Models

Lecture 12

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Recap of Previous Lecture

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t); \quad \text{with initial condition } \mathbf{x}(t_0) = \mathbf{x}_0$$

Theorem (Continuity Equation)

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

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

Solution of the Continuity Equation

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

- This solution gives us the density along the trajectory (not the total probability path).
- However, it's difficult to efficiently estimate the last term.

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

Recap of Previous Lecture

SDE Basics

Let's define a 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):

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

Discretization of SDE (Euler Method) - `SDESolve`

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

- At each time 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)

The evolution of the distribution $p_t(\mathbf{x})$ is given by:

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

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 come from $p(\mathbf{x}|\boldsymbol{\theta})$ under mild regularity conditions for a 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

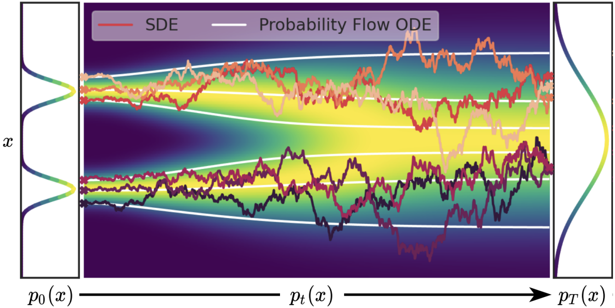
Recap of Previous Lecture

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

Probability Flow ODE

There exists an ODE with the identical 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's a reverse SDE for $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ in 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 the initial SDE to the probability flow ODE.
- Reverse the probability flow ODE.
- Convert the reverse probability flow ODE to the reverse SDE.

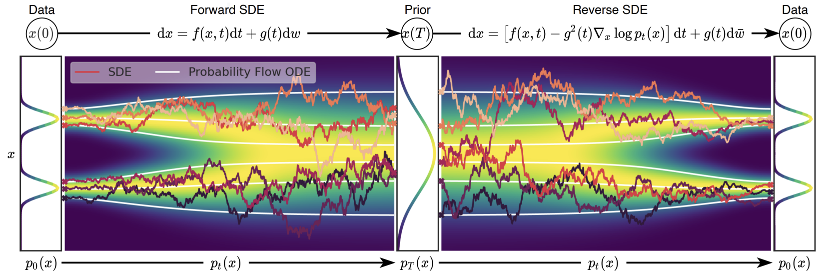
Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Recap of Previous Lecture

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

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

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



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

Outline

1. Diffusion and Score Matching SDEs

2. Score-Based Generative Models Through SDEs

3. Flow Matching

4. Conditional Flow Matching

Outline

Score Matching SDE

Denoising Score Matching

$$\mathbf{x}_t = \mathbf{x} + \sigma_t \cdot \boldsymbol{\epsilon}_t, \qquad q(\mathbf{x}_t|\mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma_t^2 \cdot \mathbf{I})$$

$$\mathbf{x}_{t-1} = \mathbf{x} + \sigma_{t-1} \cdot \boldsymbol{\epsilon}_{t-1}, \qquad q(\mathbf{x}_{t-1}|\mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma_{t-1}^2 \cdot \mathbf{I})$$

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

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$$\mathbf{x}_t = \mathbf{x}_{t-1} + \sqrt{\sigma_t^2 - \sigma_{t-1}^2} \cdot \boldsymbol{\epsilon}, \quad q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_{t-1}, (\sigma_t^2 - \sigma_{t-1}^2) \cdot \mathbf{I})$$

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$$\mathbf{x}_t = \mathbf{x}_{t-1} + \sqrt{\sigma_t^2 - \sigma_{t-1}^2} \cdot \boldsymbol{\epsilon}, \quad q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_{t-1}, (\sigma_t^2 - \sigma_{t-1}^2) \cdot \mathbf{I})$$

Let's transform this Markov chain into the continuous stochastic process $\mathbf{x}(t)$ by letting $T \to \infty$:

$$\mathbf{x}(t) = \mathbf{x}(t - dt) + \sqrt{\sigma^2(t) - \sigma^2(t - dt)} \cdot \boldsymbol{\epsilon}$$

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

Score Matching SDE

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$$\begin{aligned} \mathbf{x}(t) &= \mathbf{x}(t - dt) + \sqrt{\sigma^2(t) - \sigma^2(t - dt)} \cdot \boldsymbol{\epsilon} \\ &= \mathbf{x}(t - dt) + \sqrt{\frac{\sigma^2(t) - \sigma^2(t - dt)}{dt} dt} \cdot \boldsymbol{\epsilon} \end{aligned}$$

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Score Matching SDE

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$$\mathbf{x}_t = \mathbf{x} + \sigma_t \cdot \boldsymbol{\epsilon}_t, \qquad q(\mathbf{x}_t|\mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma_t^2 \cdot \mathbf{I})$$
$$\mathbf{x}_{t-1} = \mathbf{x} + \sigma_{t-1} \cdot \boldsymbol{\epsilon}_{t-1}, \qquad q(\mathbf{x}_{t-1}|\mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma_{t-1}^2 \cdot \mathbf{I})$$

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

Score Matching SDE

$$\mathbf{x}(t) = \mathbf{x}(t - dt) + \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

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

Score Matching SDE

$$\mathbf{x}(t) = \mathbf{x}(t - dt) + \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

Variance Exploding SDE

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

$\sigma(t)$ is a monotonically increasing function.

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

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$\sigma(t)$ is a monotonically increasing function.

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}, \quad \mathbf{f}(\mathbf{x}, t) = 0, \quad g(t) = \sqrt{\frac{d[\sigma^2(t)]}{dt}}$$

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

Score Matching SDE

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$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}, \quad \mathbf{f}(\mathbf{x}, t) = 0, \quad g(t) = \sqrt{\frac{d[\sigma^2(t)]}{dt}}$$

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

$$d\mathbf{x} = \left(-\frac{d[\sigma^2(t)]}{dt}\frac{\partial}{\partial \mathbf{x}}\log p_t(\mathbf{x})\right) dt + \sqrt{\frac{d[\sigma^2(t)]}{dt}} d\mathbf{w} \text{ (reverse SDE)}$$

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Diffusion SDE

Denoising Diffusion

$$\mathbf{x}_t = \sqrt{1-\beta_t}\cdot\mathbf{x}_{t-1} + \sqrt{\beta_t}\cdot\boldsymbol{\epsilon}, \quad q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t}\cdot\mathbf{x}_{t-1}, \beta_t\cdot\mathbf{I})$$

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Let's turn this Markov chain into a continuous stochastic process by letting $T \to \infty$ and setting $\beta_t = \beta(\frac{t}{T}) \cdot \frac{1}{T}$ (where $dt = \frac{1}{T}$):

$$\mathbf{x}(t) = \sqrt{1-\beta(t)dt}\cdot\mathbf{x}(t-dt) + \sqrt{\beta(t)dt}\cdot\boldsymbol{\epsilon}$$

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$$\begin{aligned}\mathbf{x}(t) &= \sqrt{1-\beta(t)dt}\cdot\mathbf{x}(t-dt) + \sqrt{\beta(t)dt}\cdot\boldsymbol{\epsilon} \approx \\ &\approx (1-\frac{1}{2}\beta(t)dt)\cdot\mathbf{x}(t-dt) + \sqrt{\beta(t)dt}\cdot\boldsymbol{\epsilon}\end{aligned}$$

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

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\approx (1 - \frac{1}{2}\beta(t)dt) \cdot \mathbf{x}(t - dt) + \sqrt{\beta(t)dt} \cdot \epsilon = \\
= \mathbf{x}(t - dt) - \frac{1}{2}\beta(t)\mathbf{x}(t - dt)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}
\end{aligned}$$

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Variance Preserving SDE

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}$$

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

Diffusion SDE

Variance Preserving SDE

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}$$

$$\mathbf{f}(\mathbf{x}, t) = -\frac{1}{2}\beta(t)\mathbf{x}(t), \quad g(t) = \sqrt{\beta(t)}$$

Variance is preserved as long as $\mathbf{x}(0)$ has unit variance.

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

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

$$d\mathbf{x} = \left(-\frac{1}{2}\beta(t)\mathbf{x}(t) - \beta(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right) dt + \sqrt{\beta(t)}d\mathbf{w} \quad \text{(reverse SDE)}$$

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Diffusion SDE

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

Lu C. et al. Dpm-solver: A fast ode solver for diffusion probabilistic model sampling in around 10 steps, 2022

Diffusion SDE

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

Variance Exploding SDE (NCSN)

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

Variance Preserving SDE (DDPM)

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}$$

Lu C. et al. Dpm-solver: A fast ode solver for diffusion probabilistic model sampling in around 10 steps, 2022

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Variance Preserving SDE (DDPM)

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Efficient Solvers

- Converting SDEs to PF-ODEs yields more efficient inference.
- We can apply any `ODESolve` procedure to reduce the number of inference steps.
- In practice, this reduces the number of steps from 100–1000 to 20–50.

Lu C. et al. Dpm-solver: A fast ode solver for diffusion probabilistic model sampling in around 10 steps, 2022

Outline

Score-Based Generative Models Through SDEs

Discrete-Time Objective

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

Is it possible to train score-based diffusion models in continuous time?

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

Score-Based Generative Models Through SDEs

Discrete-Time Objective

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

Is it possible to train score-based diffusion models in continuous time?

Continuous-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

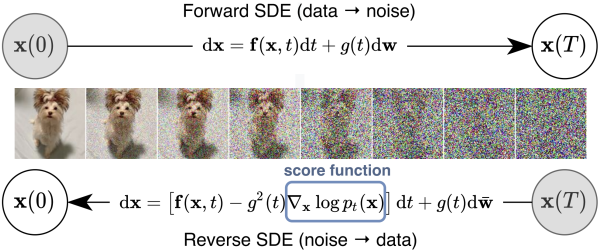
Discrete-Time Objective

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

Is it possible to train score-based diffusion models in continuous time?

Continuous-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-Time Objective

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

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

Score-Based Generative Models Through SDEs

Continuous-Time Objective

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

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

$$\nabla_{\mathbf{x}(t)} \log q(\mathbf{x}(t)|\mathbf{x}(0)) = -\frac{1}{\boldsymbol{\sigma}} \odot (\mathbf{x}(t) - \boldsymbol{\mu})$$

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

Score-Based Generative Models Through SDEs

Continuous-Time Objective

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

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

$$\nabla_{\mathbf{x}(t)} \log q(\mathbf{x}(t)|\mathbf{x}(0)) = -\frac{1}{\boldsymbol{\sigma}} \odot (\mathbf{x}(t) - \boldsymbol{\mu})$$

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w} \quad \text{(Variance Exploding SDE)}$$

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w} \quad \text{(Variance Preserving SDE)}$$

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

Score-Based Generative Models Through SDEs

Continuous-Time Objective

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

$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\Big(\boldsymbol{\mu}(\mathbf{x}(t),\mathbf{x}(0)), \boldsymbol{\sigma}^2(\mathbf{x}(t),\mathbf{x}(0))\cdot\mathbf{I}\Big)$$

$$\nabla_{\mathbf{x}(t)}\log q(\mathbf{x}(t)|\mathbf{x}(0)) = -\frac{1}{\boldsymbol{\sigma}}\odot(\mathbf{x}(t)-\boldsymbol{\mu})$$

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}}\cdot d\mathbf{w} \quad \text{(Variance Exploding SDE)}$$

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)}\cdot d\mathbf{w} \quad \text{(Variance Preserving SDE)}$$

Is it possible to explicitly derive $\boldsymbol{\mu}(\mathbf{x}(t),\mathbf{x}(0))$ and $\boldsymbol{\Sigma}(\mathbf{x}(t),\mathbf{x}(0))$ for VE-SDE and VP-SDE?

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

Score-Based Generative Models Through SDEs

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

Theorem

The moments of the SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ satisfy:

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

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

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

Score-Based Generative Models Through SDEs

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

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The moments of the SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ satisfy:

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Proof

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

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

Score-Based Generative Models Through SDEs

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Proof

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

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

Score-Based Generative Models Through SDEs

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\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}$$

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

Score-Based Generative Models Through SDEs

Theorem

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

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 (Continued)

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

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

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

Proof (Continued)

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

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

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Examples

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

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 (Continued)

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

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

Examples

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

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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 (Continued)

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

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

Examples

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

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$$\boldsymbol{\mu} = \mathbf{x}(0) \exp\left(-\frac{1}{2}\int_0^t \beta(s) ds\right)$$

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

Score-Based Generative Models Through SDEs

Training

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

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

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

Score-Based Generative Models Through SDEs

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NCSN

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

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

Score-Based Generative Models Through SDEs

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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

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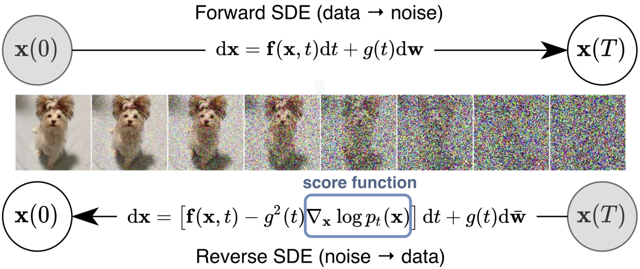
Here we omit the derivations of the variance.

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

Score-Based Generative Models Through SDEs

Sampling

Solve the reverse SDE using numerical solvers (`SDESolve`).



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

Score-Based Generative Models Through SDEs

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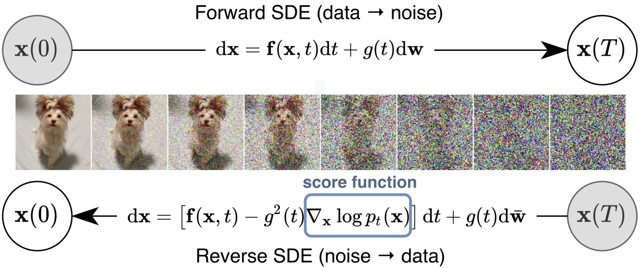

- Discretizing the reverse SDE provides ancestral sampling.
- Discretizing the probability flow ODE yields deterministic sampling.

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

Outline

Continuous-Time Normalizing Flows

Let's return to ODE dynamics $\mathbf{x}(t)$ in the 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 (e.g., $\mathcal{N}(0, \mathbf{I})$), and $\pi(\mathbf{x})$ is the true data distribution.

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

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

Continuous-Time Normalizing Flows

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

KFP Theorem (Continuity Equation)

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

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- It's hard to solve the continuity equation directly due to the trace term.
- There's a method (the adjoint method) that solves this equation directly, but it's unstable and unscalable.

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

Continuous-Time Normalizing Flows

KFP Theorem (Continuity Equation)

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

- Knowing the vector field $\mathbf{f}(\mathbf{x}, t)$, the KFP (or continuity) equation allows us to compute the density $p_t(\mathbf{x})$.
- Flow matching provides an alternative approach to Neural ODEs.

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

Continuous-Time Normalizing Flows

KFP Theorem (Continuity Equation)

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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

Continuous-Time Normalizing Flows

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- Knowing the vector field $\mathbf{f}(\mathbf{x}, t)$, the KFP (or continuity) equation allows us to compute the density $p_t(\mathbf{x})$.
- Flow matching provides an alternative approach to Neural ODEs.

Flow Matching

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

- Approximate the true vector field $\mathbf{f}(\mathbf{x}, t)$ using $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t)$.
- Use $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t)$ for deterministic sampling from the ODE.

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 are infinitely many 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 make the objective tractable.

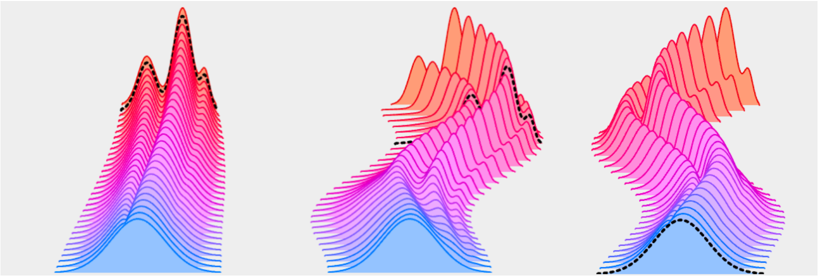

image credit: A Visual Dive into Conditional Flow Matching

Outline

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**.

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

Flow Matching

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

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

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

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Flow Matching

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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's 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

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

Theorem

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

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

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

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

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Flow Matching

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

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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)

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

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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 the FM objective equals the optimal value of the CFM objective.

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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 the FM objective equals the optimal value of the CFM objective.

Proof

This can be proved in a similar way as in the denoising score matching theorem.

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Conditional Flow Matching

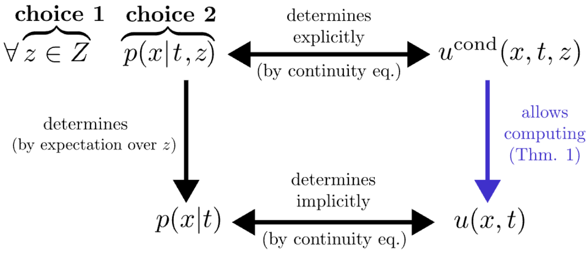

image credit: A Visual Dive into Conditional Flow Matching

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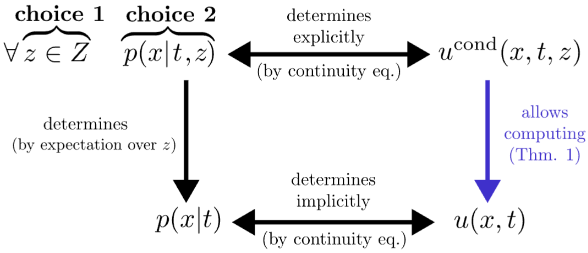

- We don't want to directly model $p_t(\mathbf{x})$, since it's complex.
- We've shown it's possible to solve the CFM task instead of the FM task.
- Let's choose a convenient conditioning latent variable $\mathbf{z}$.
- We'll parametrize $p_t(\mathbf{x}|\mathbf{z})$ instead of $p_t(\mathbf{x})$. It should satisfy the following constraints:

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

image credit: A Visual Dive into Conditional Flow Matching

Summary

- Score matching (NCSN) and diffusion models (DDPM) are discretizations of SDEs (variance exploding and variance preserving).
- It's possible to train continuous-in-time score-based generative models using forward and reverse SDEs.
- Discretizing the reverse SDE yields ancestral sampling of the DDPM.
- Flow matching suggests fitting the vector field directly.
- Conditional flow matching introduces the latent variable $\mathbf{z}$, reformulating the initial task in terms of conditional dynamics.