Deep Generative Models

Lecture 12

Roman Isachenko

Moscow Institute of Physics and Technology
Yandex School of Data Analysis

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Recap of previous lecture

Continuous-in-time dynamics

Consider Ordinary Differential Equation (ODE)

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

$$\mathbf{x}(1) = \int_0^1 \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t) dt + \mathbf{x}_0$$

Here $\mathbf{f}_{\boldsymbol{\theta}} : \mathbb{R}^m \times [0, 1] \to \mathbb{R}^m$ is a vector field.

Euler update step

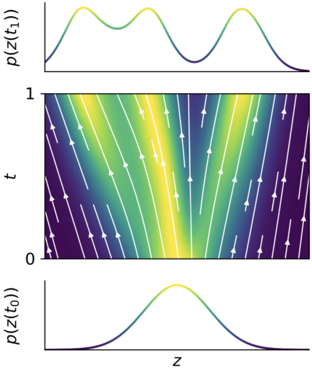
$$\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \Delta t \cdot \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)$$

- Euler method is the simplest version of the ODESolve that is unstable in practice.
- It is possible to use more sophisticated numerical methods instead if Euler (e.x. Runge-Kutta methods).

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

Recap of previous lecture

- $\mathbf{x}(0) \sim p(\mathbf{x}(0))$.
- $\mathbf{x}(1) \sim p(\mathbf{x}(1))$.
- $p_t(\mathbf{x}) = p(\mathbf{x}, t)$ is the **probability path** between $p_0(\mathbf{x})$ and $p_1(\mathbf{x})$.
- $p_0(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$ is the base distribution and $p_1(\mathbf{x}) = \pi(\mathbf{x})$ is the data distribution.



Theorem (Picard)

If $\mathbf{f}$ is uniformly Lipschitz continuous in $\mathbf{x}$ and continuous in t, then the ODE has a **unique** solution.

$$\mathbf{x}(1) = \mathbf{x}(0) + \int_0^1 \mathbf{f}_\theta(\mathbf{x}(t), t)dt; \quad \mathbf{x}(0) = \mathbf{x}(1) + \int_1^0 \mathbf{f}_\theta(\mathbf{x}(t), t)dt$$

Grathwohl W. et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models, 2018

Recap of previous lecture

Theorem (continuity equation)

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

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

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

- **Discrete-in-time NF**: evaluation of determinant of the Jacobian costs $O(m^3)$ (we need invertible $\mathbf{f}$).
- **Continuous-in-time NF**: getting the trace of the Jacobian costs $O(m^2)$ (we need smooth $\mathbf{f}$).

Hutchinson's trace estimator

$$\log p_1(\mathbf{x}(1)) = \log p_0(\mathbf{x}(0)) - \mathbb{E}_{p(\boldsymbol{\epsilon})} \int_0^1 \left[\boldsymbol{\epsilon}^T \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \boldsymbol{\epsilon}\right] dt.$$

Grathwohl W. et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models, 2018

Recap of previous lecture

Forward pass (Loss function)

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

Adjoint functions

$$\mathbf{a}_{\mathbf{x}}(t) = \frac{\partial L}{\partial \mathbf{x}(t)}; \quad \mathbf{a}_{\boldsymbol{\theta}}(t) = \frac{\partial L}{\partial \boldsymbol{\theta}(t)}.$$

Theorem (Pontryagin)

$$\frac{d\mathbf{a}_{\mathbf{x}}(t)}{dt} = -\mathbf{a}_{\mathbf{x}}(t)^T \cdot \frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)}{\partial \mathbf{x}}; \quad \frac{d\mathbf{a}_{\boldsymbol{\theta}}(t)}{dt} = -\mathbf{a}_{\mathbf{x}}(t)^T \cdot \frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)}{\partial \boldsymbol{\theta}}.$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}(0)} = \mathbf{a}_{\boldsymbol{\theta}}(0) = -\int_1^0 \mathbf{a}_{\mathbf{x}}(t)^T \frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)}{\partial \boldsymbol{\theta}(t)} dt + 0$$

$$\frac{\partial L}{\partial \mathbf{x}(0)} = \mathbf{a}_{\mathbf{x}}(0) = -\int_1^0 \mathbf{a}_{\mathbf{x}}(t)^T \frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)}{\partial \mathbf{x}(t)} dt + \frac{\partial L}{\partial \mathbf{x}(1)}$$

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

Recap of previous lecture

Forward pass

$$\mathbf{x}(1) = \mathbf{x}(0) + \int_0^1 \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)dt \quad \Rightarrow \quad \text{ODE Solver}$$

Backward pass

$$\left.\begin{aligned}
\frac{\partial L}{\partial \boldsymbol{\theta}(0)} &= \mathbf{a}_{\boldsymbol{\theta}}(0) = -\int_1^0 \mathbf{a}_{\mathbf{x}}(t)^T \frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)}{\partial \boldsymbol{\theta}(t)} dt + 0 \\
\frac{\partial L}{\partial \mathbf{x}(0)} &= \mathbf{a}_{\mathbf{x}}(0) = -\int_1^0 \mathbf{a}_{\mathbf{x}}(t)^T \frac{\partial \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)}{\partial \mathbf{x}(t)} dt + \frac{\partial L}{\partial \mathbf{x}(1)} \\
\mathbf{x}(0) &= -\int_0^1 \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)dt + \mathbf{x}(1).
\end{aligned}\right\} \Rightarrow \text{ODE Solver}$$

Note: These scary formulas are the standard backprop in the discrete case.

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

Outline

Outline

1. SDE basics
2. Probability flow ODE
3. Reverse SDE
4. Diffusion and Score matching SDEs
5. Score-based generative models through SDEs

Stochastic differential equation (SDE)

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

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

- $\mathbf{f}(\mathbf{x}, t) : \mathbb{R}^m \times [0, 1] \to \mathbb{R}^m$ is the **drift** function of $\mathbf{x}(t)$.
- $g(t) : \mathbb{R} \to \mathbb{R}$ is the **diffusion** function of $\mathbf{x}(t)$.
- $\mathbf{w}(t)$ is the standard Wiener process (Brownian motion):
  1. $\mathbf{w}(0) = 0$ (almost surely);
  2. $\mathbf{w}(t)$ has independent increments;
  3. $\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, (t - s)\mathbf{I})$, for $t > s$.
- $d\mathbf{w} = \mathbf{w}(t + dt) - \mathbf{w}(t) = \mathcal{N}(0, \mathbf{I} \cdot dt) = \boldsymbol{\epsilon} \cdot \sqrt{dt}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
- If $g(t) = 0$ we get standard ODE.

Stochastic differential equation (SDE)

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

- In contrast to ODE, initial condition $\mathbf{x}(0)$ does not uniquely determine the process trajectory.
- We have two sources of randomness: initial distribution $p_0(\mathbf{x})$ and Wiener process $\mathbf{w}(t)$.

Discretization of SDE (Euler method)

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

If $dt = 1$, then

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \mathbf{f}(\mathbf{x}_t, t) + g(t) \cdot \boldsymbol{\epsilon}$$

- 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 $p_1(\mathbf{x})$.
- How to get the distribution path $p_t(\mathbf{x})$ for $\mathbf{x}(t)$?

Stochastic differential equation (SDE)

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}, \quad d\mathbf{w} = \boldsymbol{\epsilon} \cdot \sqrt{dt}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

Theorem (Kolmogorov-Fokker-Planck)

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

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

Here

$$\mathrm{div}(\mathbf{v}) = \sum_{i=1}^{m} \frac{\partial v_i(\mathbf{x})}{\partial x_i} = \mathrm{tr}\left(\frac{\partial \mathbf{v}(\mathbf{x})}{\partial \mathbf{x}}\right)$$

$$\Delta_{\mathbf{x}}p_t(\mathbf{x}) = \sum_{i=1}^{m} \frac{\partial^2 p_t(\mathbf{x})}{\partial x_i^2} = \mathrm{tr}\left(\frac{\partial^2 p_t(\mathbf{x})}{\partial \mathbf{x}^2}\right)$$

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\mathbf{f}(\mathbf{x}, t)p_t(\mathbf{x})\right] + \frac{1}{2}g^2(t)\frac{\partial^2 p_t(\mathbf{x})}{\partial \mathbf{x}^2}\right)$$

Stochastic differential equation (SDE)

Theorem (Kolmogorov-Fokker-Planck)

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\big[\mathbf{f}(\mathbf{x}, t) p_t(\mathbf{x})\big] + \frac{1}{2} g^2(t) \frac{\partial^2 p_t(\mathbf{x})}{\partial \mathbf{x}^2}\right)$$

- KFP theorem does not define the SDE uniquely in general case.
- This is the generalization of KFP theorem that we used in continuous-in-time NF:

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

Langevin SDE (special case)

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

Let apply KFP theorem to this SDE.

Langevin SDE (special case)

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

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[p_t(\mathbf{x})\frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right] + \frac{1}{2}\frac{\partial^2 p_t(\mathbf{x})}{\partial \mathbf{x}^2}\right) =$$

$$= \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\frac{1}{2}\frac{\partial}{\partial \mathbf{x}} p_t(\mathbf{x})\right] + \frac{1}{2}\frac{\partial^2 p_t(\mathbf{x})}{\partial \mathbf{x}^2}\right) = 0$$

The density $p_t(\mathbf{x}) = \mathrm{const}(t)$!
If $\mathbf{x}(0) \sim p_0(\mathbf{x})$, then $\mathbf{x}(t) \sim p_0(\mathbf{x})$.

Discretized Langevin SDE

$$\mathbf{x}_{t+1} - \mathbf{x}_t = \frac{\eta}{2} \cdot \frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x}) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \eta \approx dt.$$

Langevin dynamic

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

Outline

1. SDE basics
2. Probability flow ODE
3. Reverse SDE
4. Diffusion and Score matching SDEs
5. Score-based generative models through SDEs

Probability flow ODE

ODE and continuity equation

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

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

The only source of stochasticity is the distibution $p_0(\mathbf{x})$.

SDE and KFP equation

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

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

We have two sources of randomness: initial distribution $p_0(\mathbf{x})$ and Wiener process $\mathbf{w}(t)$.

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

Probability flow ODE

Theorem

Assume SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ induces the probability path $p_t(\mathbf{x})$. Then there exists ODE with identical probability path $p_t(\mathbf{x})$ of the form

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

Proof

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = \operatorname{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\mathbf{f}(\mathbf{x}, t)p_t(\mathbf{x})\right] + \frac{1}{2}g^2(t)\frac{\partial^2 p_t(\mathbf{x})}{\partial \mathbf{x}^2}\right) =$$

$$= \operatorname{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\mathbf{f}(\mathbf{x}, t)p_t(\mathbf{x}) - \frac{1}{2}g^2(t)\frac{\partial p_t(\mathbf{x})}{\partial \mathbf{x}}\right]\right) =$$

$$= \operatorname{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\mathbf{f}(\mathbf{x}, t)p_t(\mathbf{x}) - \frac{1}{2}g^2(t)p_t(\mathbf{x})\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right]\right) =$$

$$= \operatorname{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\left(\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right) p_t(\mathbf{x})\right]\right)$$

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

Probability flow ODE

Theorem

Assume SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ induces the probability path $p_t(\mathbf{x})$. Then there exists ODE with identical probabilities distribution $p_t(\mathbf{x})$ of the form

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

Proof (continued)

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\left(\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right) p_t(\mathbf{x})\right]\right) =$$

$$= \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\tilde{\mathbf{f}}(\mathbf{x}, t)p_t(\mathbf{x})\right]\right)$$

$$d\mathbf{x} = \tilde{\mathbf{f}}(\mathbf{x}, t)dt + 0 \cdot d\mathbf{w} = \left(\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right) dt$$

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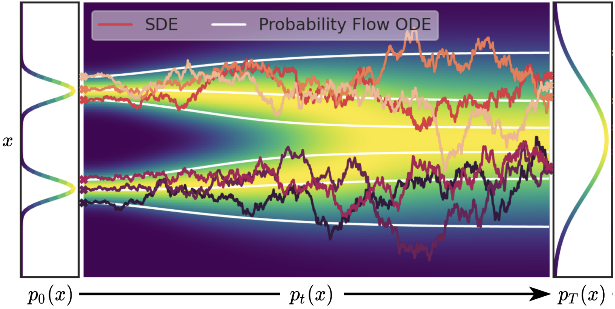
Probability flow ODE

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

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

- The term $\mathbf{s}(\mathbf{x}, t) = \frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})$ is a score function for continuous time.
- ODE has more stable trajectories.



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

Outline

Reverse SDE

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

Here dt could be > 0 or < 0.

Reverse ODE

Let $\tau = 1 - t$ $(d\tau = -dt)$.

$$d\mathbf{x} = -\mathbf{f}(\mathbf{x}, 1 - \tau)d\tau$$

- How to revert SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$?
- Wiener process gives the randomness that we have to revert.

Theorem

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

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

with $dt < 0$.

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

Reverse SDE

Theorem

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

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

with $dt < 0$.

Note: Here we also see the score function $\mathbf{s}(\mathbf{x}, t) = \frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})$.

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

Reverse SDE

Proof

- Convert initial SDE to probability flow ODE

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

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

- Revert probability flow ODE

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

$$d\mathbf{x} = \left(-\mathbf{f}(\mathbf{x}, 1-\tau) + \frac{1}{2}g^2(1-\tau)\frac{\partial}{\partial \mathbf{x}}\log p_{1-\tau}(\mathbf{x})\right)d\tau$$

- Convert reverse probability flow ODE to reverse SDE

$$d\mathbf{x} = \left(-\mathbf{f}(\mathbf{x}, 1-\tau) + \frac{1}{2}g^2(1-\tau)\frac{\partial}{\partial \mathbf{x}}\log p_{1-\tau}(\mathbf{x})\right)d\tau$$

$$d\mathbf{x} = \left(-\mathbf{f}(\mathbf{x}, 1-\tau) + g^2(1-\tau)\frac{\partial}{\partial \mathbf{x}}\log p_{1-\tau}(\mathbf{x})\right)d\tau + g(1-\tau)d\mathbf{w}$$

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

Reverse SDE

Theorem

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

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

with $dt < 0$.

Proof (continued)

$$d\mathbf{x} = \left(-\mathbf{f}(\mathbf{x}, 1 - \tau) + g^2(1 - \tau)\frac{\partial}{\partial \mathbf{x}} \log p_{1-\tau}(\mathbf{x})\right) d\tau + g(1 - \tau)d\mathbf{w}$$

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

Here $d\tau > 0$ and $dt < 0$.

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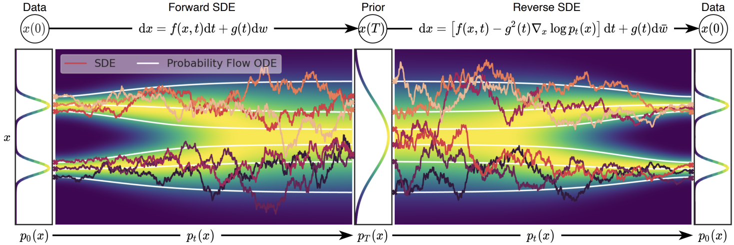
Reverse SDE

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

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

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

- 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.



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Outline

Score matching SDE

Denoising score matching

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

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

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

Let turn this Markov chain to the continuous stochastic process $\mathbf{x}(t)$ taking $T \to \infty$:

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

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.

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

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

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

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

Diffusion SDE

Denoising Diffusion

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

Let turn this Markov chain to the continuous stochastic process taking $T \to \infty$ and taking $\beta(\frac{t}{T}) = \beta_t \cdot T$

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

Variance Preserving SDE

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

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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 if $\mathbf{x}(0)$ has a unit variance.

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

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

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Diffusion SDE

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

Variance Exploding SDE (NCSN)

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

Variance Preserving SDE (DDPM)

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

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

Is it possible to train score-based generative model (DDPM or NCSN) in continuous time?

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Outline

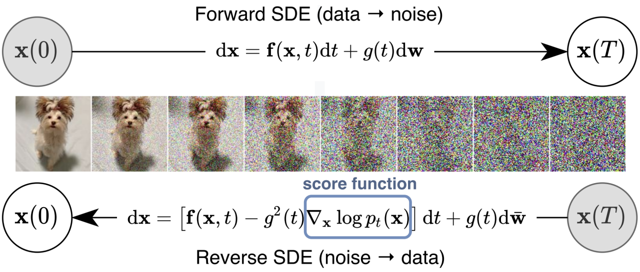
Score-based generative models through SDEs

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

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



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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.

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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

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

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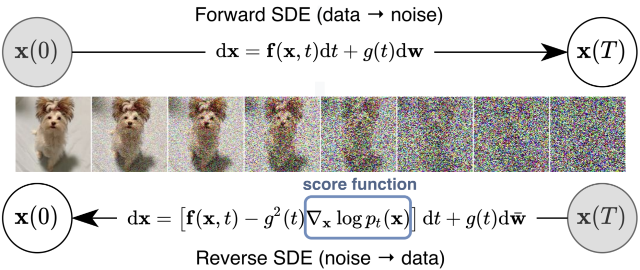
Score-based generative models through SDEs

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.

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Summary

- SDE defines a stochastic process with drift and diffusion terms. ODEs are the special case of SDEs.
- KFP equation defines the dynamic of the probability function for the SDE.
- Langevin SDE has constant probability path.
- There exists special probability flow ODE for each SDE that gives the same probability path.
- It is possible to revert SDE using the score function.
- Score matching (NCSN) and diffusion models (DDPM) are the discretizations of the SDEs (variance exploding and variance preserving).
- It is possible to train the continuous-in-time score-based generative models through forward and reverse SDEs.