

Deep Generative Models

Lecture 12

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2024, Autumn

Recap of previous lecture

Theorem (Kolmogorov-Fokker-Planck: special case)

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

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

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

- ▶ **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

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

Recap of previous lecture

Forward pass (Loss function)

$$\mathbf{z} = \mathbf{x} + \int_1^0 \mathbf{f}_{\theta}(\mathbf{z}(t), t) dt, \quad L(\mathbf{z}) = -\log p(\mathbf{x}|\theta)$$

$$L(\mathbf{z}) = -\log p(\mathbf{z}) + \int_0^1 \text{tr} \left(\frac{\partial \mathbf{f}_{\theta}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)} \right) dt$$

Adjoint functions

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

These functions show how the gradient of the loss depends on the hidden state $\mathbf{z}(t)$ and parameters θ .

Theorem (Pontryagin)

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

Recap of previous lecture

Forward pass

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

Backward pass

$$\left. \begin{aligned} \frac{\partial L}{\partial \theta(t_1)} &= \mathbf{a}_{\theta}(1) = - \int_0^1 \mathbf{a}_{\mathbf{z}}(t)^T \frac{\partial \mathbf{f}_{\theta}(\mathbf{z}(t), t)}{\partial \theta(t)} dt + 0 \\ \frac{\partial L}{\partial \mathbf{z}(1)} &= \mathbf{a}_{\mathbf{z}}(1) = - \int_0^1 \mathbf{a}_{\mathbf{z}}(t)^T \frac{\partial \mathbf{f}_{\theta}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)} dt + \frac{\partial L}{\partial \mathbf{z}(0)} \\ \mathbf{z}(1) &= - \int_1^0 \mathbf{f}_{\theta}(\mathbf{z}(t), t) dt + \mathbf{z}_0. \end{aligned} \right\} \Rightarrow \text{ODE Solver}$$

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

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)

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

Discretization of SDE (Euler method)

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

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

Recap of previous lecture

Theorem (Kolmogorov-Fokker-Planck)

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

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

Langevin SDE (special case)

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

The density $p(\mathbf{x}|\boldsymbol{\theta})$ 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 small enough η .

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

Outline

1. Probability flow ODE
2. Reverse SDE
3. Diffusion and Score matching SDEs

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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

$$\begin{aligned} \frac{\partial p_t(\mathbf{x})}{\partial t} &= \text{tr} \left(-\frac{\partial}{\partial \mathbf{x}} [\mathbf{f}(\mathbf{x}, t)p_t(\mathbf{x})] + \frac{1}{2}g^2(t)\frac{\partial^2 p_t(\mathbf{x})}{\partial \mathbf{x}^2} \right) = \\ &= \text{tr} \left(-\frac{\partial}{\partial \mathbf{x}} \left[\mathbf{f}(\mathbf{x}, t)p_t(\mathbf{x}) - \frac{1}{2}g^2(t)\frac{\partial p_t(\mathbf{x})}{\partial \mathbf{x}} \right] \right) = \\ &= \text{tr} \left(-\frac{\partial}{\partial \mathbf{x}} \left[\mathbf{f}(\mathbf{x}, t)p_t(\mathbf{x}) - \frac{1}{2}g^2(t)p_t(\mathbf{x})\frac{\partial \log p_t(\mathbf{x})}{\partial \mathbf{x}} \right] \right) = \\ &= \text{tr} \left(-\frac{\partial}{\partial \mathbf{x}} \left[\left(\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial \log p_t(\mathbf{x})}{\partial \mathbf{x}} \right) p_t(\mathbf{x}) \right] \right) \end{aligned}$$

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)

$$\begin{aligned} \frac{\partial p_t(\mathbf{x})}{\partial t} &= \text{tr} \left(-\frac{\partial}{\partial \mathbf{x}} \left[\left(\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial \log p_t(\mathbf{x})}{\partial \mathbf{x}} \right) p_t(\mathbf{x}) \right] \right) = \\ &= \text{tr} \left(-\frac{\partial}{\partial \mathbf{x}} \left[\tilde{\mathbf{f}}(\mathbf{x}, t)p_t(\mathbf{x}) \right] \right) \end{aligned}$$

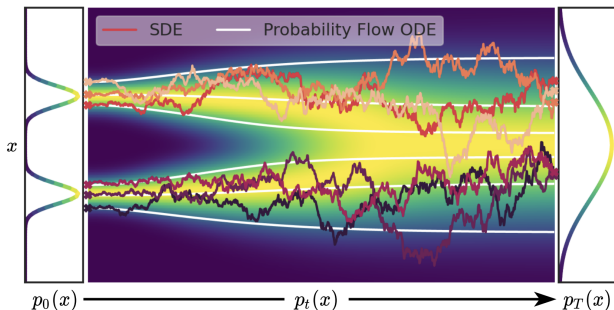
$$d\mathbf{x} = \tilde{\mathbf{f}}(\mathbf{x}, t)dt + 0 \cdot d\mathbf{w} = \left[\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x}) \right] dt$$

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.



Outline

1. Probability flow ODE
2. Reverse SDE
3. Diffusion and Score matching SDEs

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

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

with $dt < 0$.

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

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

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.

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

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

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

- Convert reverse probability flow ODE to reverse SDE

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

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

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

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

with $dt < 0$.

Proof (continued)

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

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

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

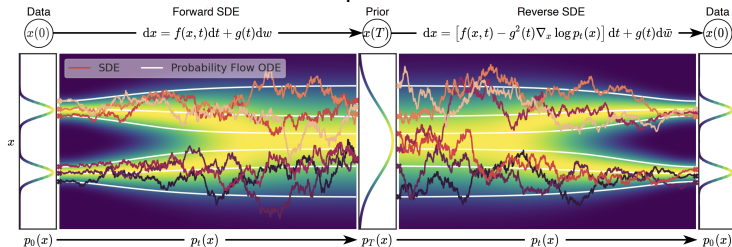
Reverse SDE

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

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

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

- ▶ 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.



Outline

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Score matching SDE

Denosing score matching

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

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

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

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

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

Variance Exploding SDE

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

Diffusion SDE

Denoising Diffusion

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

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

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

Variance Preserving SDE

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

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 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.

Summary

- ▶ There exists special probability flow ODE for each SDE that gives the same probability path.
- ▶ It is possible to revert SDE using score function.
- ▶ Score matching (NCSN) and diffusion models (DDPM) are the discretizations of the SDEs (variance exploding and variance preserving).