Deep Generative Models

Lecture 12

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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

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

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

- **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

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

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

Recap of previous lecture

Forward pass (Loss function)

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

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

Adjoint functions

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

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

Theorem (Pontryagin)

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

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

Recap of previous lecture

Forward pass

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

Backward pass

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

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

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

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)

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

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

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.

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

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

Outline

1. Probability flow ODE

2. Reverse SDE

3. Diffusion and Score matching SDEs

Outline

1. Probability flow ODE

2. Reverse SDE

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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

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

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

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

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

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)

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

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

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

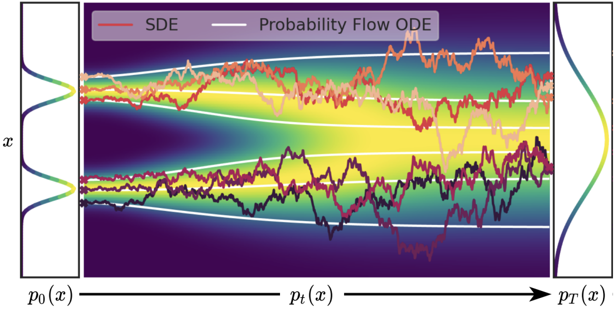
Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

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

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 $dt < 0$.

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

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

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.

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

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

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

- Convert reverse probability flow ODE to reverse SDE

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

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

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

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

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 $dt < 0$.

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

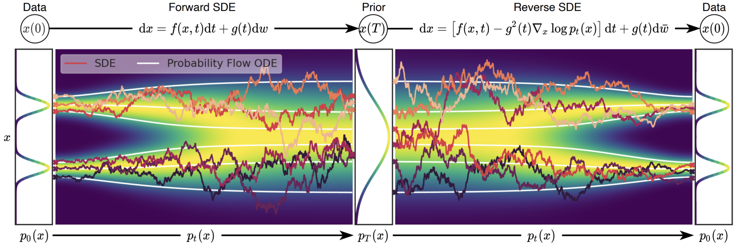
Reverse SDE

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

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

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

- 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.



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

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Score matching SDE

Denoising score matching

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

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

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

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

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

Variance Exploding SDE

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

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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 $T \to \infty$ and taking $\beta(\frac{t}{T}) = \beta_t \cdot T$

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

Variance Preserving SDE

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

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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 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

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).