

Deep Generative Models

Lecture 11

Roman Isachenko

Moscow Institute of Physics and Technology
Yandex School of Data Analysis

2024, Autumn

Recap of previous lecture

Training of DDPM

1. Get the sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Sample timestamp $t \sim U\{1, T\}$ and the noise $\epsilon \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \epsilon$.
4. Compute loss $\mathcal{L}_{\text{simple}} = \|\epsilon - \epsilon_{\theta,t}(\mathbf{x}_t)\|^2$.

Sampling of DDPM

1. Sample $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$.
2. Compute mean of $p(\mathbf{x}_{t-1}|\mathbf{x}_t, \theta) = \mathcal{N}(\mu_{\theta,t}(\mathbf{x}_t), \sigma_t^2 \cdot \mathbf{I})$:

$$\mu_{\theta,t}(\mathbf{x}_t) = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \epsilon_{\theta,t}(\mathbf{x}_t)$$

3. Get denoised image $\mathbf{x}_{t-1} = \mu_{\theta,t}(\mathbf{x}_t) + \sigma_t \cdot \epsilon$, where $\epsilon \sim \mathcal{N}(0, \mathbf{I})$.

Recap of previous lecture

DDPM objective

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

In practice the coefficient is omitted.

NCSN objective

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

Note: The objective of DDPM and NCSN is almost identical. But the difference in sampling scheme:

- ▶ NCSN uses annealed Langevin dynamics;
- ▶ DDPM uses ancestral sampling.

$$\mathbf{s}_{\theta, t}(\mathbf{x}_t) = -\frac{\epsilon_{\theta, t}(\mathbf{x}_t)}{\sqrt{1 - \bar{\alpha}_t}} = \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \theta)$$

Recap of previous lecture

Unconditional generation

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t + \frac{1 - \alpha_t}{\sqrt{\alpha_t}} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \boldsymbol{\theta}) + \sigma_t \cdot \epsilon$$

Conditional generation

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t + \frac{1 - \alpha_t}{\sqrt{\alpha_t}} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{y}, \boldsymbol{\theta}) + \sigma_t \cdot \epsilon$$

Conditional distribution

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{y}, \boldsymbol{\theta}) = \nabla_{\mathbf{x}_t} \log p(\mathbf{y} | \mathbf{x}_t) - \frac{\epsilon_{\boldsymbol{\theta},t}(\mathbf{x}_t)}{\sqrt{1 - \bar{\alpha}_t}}$$

Here $p(\mathbf{y} | \mathbf{x}_t)$ – classifier on noisy samples (we have to learn it separately).

Classifier-corrected noise prediction

$$\epsilon_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y}) = \epsilon_{\boldsymbol{\theta},t}(\mathbf{x}_t) - \sqrt{1 - \bar{\alpha}_t} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y} | \mathbf{x}_t)$$

Recap of previous lecture

Guidance scale

$$\epsilon_{\theta,t}(\mathbf{x}_t, \mathbf{y}) = \epsilon_{\theta,t}(\mathbf{x}_t) - \gamma \cdot \sqrt{1 - \bar{\alpha}_t} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

$$\nabla_{\mathbf{x}_t}^{\gamma} \log p(\mathbf{x}_t|\mathbf{y}, \theta) = \nabla_{\mathbf{x}_t} \log \left(\frac{p(\mathbf{y}|\mathbf{x}_t)^{\gamma} p(\mathbf{x}_t|\theta)}{Z} \right)$$

Note: Guidance scale γ tries to sharpen the distribution $p(\mathbf{y}|\mathbf{x}_t)$.

Guided sampling

$$\epsilon_{\theta,t}(\mathbf{x}_t, \mathbf{y}) = \epsilon_{\theta,t}(\mathbf{x}_t) - \gamma \cdot \sqrt{1 - \bar{\alpha}_t} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

$$\mu_{\theta,t}(\mathbf{x}_t, \mathbf{y}) = \frac{1}{\sqrt{\alpha_t}} \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \epsilon_{\theta,t}(\mathbf{x}_t, \mathbf{y})$$

$$\mathbf{x}_{t-1} = \mu_{\theta,t}(\mathbf{x}_t, \mathbf{y}) + \sigma_t \cdot \epsilon, \quad \epsilon \sim \mathcal{N}(0, \mathbf{I})$$

Recap of previous lecture

- ▶ Previous method requires training the additional classifier model $p(\mathbf{y}|\mathbf{x}_t)$ on the noisy data.
- ▶ Let try to avoid this requirement.

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) = \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) - \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta})$$

$$\begin{aligned}\nabla_{\mathbf{x}_t}^\gamma \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) &= \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \gamma \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) = \\ &= (1 - \gamma) \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \gamma \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta})\end{aligned}$$

Classifier-free-corrected noise prediction

$$\hat{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y}) = \gamma \cdot \epsilon_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y}) + (1 - \gamma) \cdot \epsilon_{\boldsymbol{\theta},t}(\mathbf{x}_t)$$

- ▶ Train the single model $\epsilon_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y})$ on **supervised** data alternating with real conditioning \mathbf{y} and empty conditioning $\mathbf{y} = \emptyset$.
- ▶ Apply the model twice during inference.

Recap of previous lecture

Continuous-in-time dynamic (neural ODE)

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

$$\mathbf{z}(t_1) = \int_0^1 \mathbf{f}_{\theta}(\mathbf{z}(t), t) dt + \mathbf{z}_0 \approx \text{ODESolve}(\mathbf{z}(0), \mathbf{f}_{\theta}, t_0 = 0, t_1 = 1).$$

Euler update step

$$\frac{\mathbf{z}(t + \Delta t) - \mathbf{z}(t)}{\Delta t} = \mathbf{f}_{\theta}(\mathbf{z}(t), t) \Rightarrow \mathbf{z}(t + \Delta t) = \mathbf{z}(t) + \Delta t \cdot \mathbf{f}_{\theta}(\mathbf{z}(t), t)$$

Theorem (Picard)

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

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

$$\mathbf{z} = \mathbf{z}(0) = \mathbf{z}(1) + \int_1^0 \mathbf{f}_{\theta}(\mathbf{z}(t), t) dt$$

Outline

1. Kolmogorov-Fokker-Planck equation for NF log-likelihood
2. FFJORD (Hutchinson's trace estimator)
3. Adjoint method for continuous-in-time NF
4. SDE basics

Outline

1. Kolmogorov-Fokker-Planck equation for NF log-likelihood
2. FFJORD (Hutchinson's trace estimator)
3. Adjoint method for continuous-in-time NF
4. SDE basics

Continuous-in-time Normalizing Flows

What do we need?

- ▶ We need the way to compute $p_t(\mathbf{z})$ at any moment t .
- ▶ We need the way to find the optimal parameters θ of the dynamic \mathbf{f}_θ .

Theorem (Kolmogorov-Fokker-Planck: special case)

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

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

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

It means that if we have the value $\mathbf{z}_0 = \mathbf{z}(0)$ then the solution of the ODE will give us the density at the moment $t = 1$.

Continuous-in-time Normalizing Flows

Forward transform + log-density

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

Here $p(\mathbf{x}|\theta) = p_1(\mathbf{z})$, $p(\mathbf{z}) = p_0(\mathbf{z})$.

- ▶ **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}).

Why $O(m^2)$?

$\text{tr} \left(\frac{\partial \mathbf{f}_\theta(\mathbf{z}(t))}{\partial \mathbf{z}(t)} \right)$ costs $O(m^2)$ (m evaluations of \mathbf{f}), since we have to compute a derivative for each diagonal element. It is possible to reduce cost from $O(m^2)$ to $O(m)$!

Outline

1. Kolmogorov-Fokker-Planck equation for NF log-likelihood
2. FFJORD (Hutchinson's trace estimator)
3. Adjoint method for continuous-in-time NF
4. SDE basics

Continuous-in-time Normalizing Flows

Hutchinson's trace estimator

If $\epsilon \in \mathbb{R}^m$ is a random variable with $\mathbb{E}[\epsilon] = 0$ and $\text{cov}(\epsilon) = \mathbf{I}$, then

$$\begin{aligned}\text{tr}(\mathbf{A}) &= \text{tr}(\mathbf{A} \cdot \mathbf{I}) = \text{tr}\left(\mathbf{A} \cdot \mathbb{E}_{p(\epsilon)}\left[\epsilon\epsilon^T\right]\right) = \\ &= \mathbb{E}_{p(\epsilon)}\left[\text{tr}\left(\mathbf{A}\epsilon\epsilon^T\right)\right] = \mathbb{E}_{p(\epsilon)}\left[\epsilon^T \mathbf{A} \epsilon\right]\end{aligned}$$

Jacobian vector products $\mathbf{v}^T \frac{\partial \mathbf{f}}{\partial \mathbf{z}}$ can be computed for approximately the same cost as evaluating \mathbf{f} (`torch.autograd.functional.jvp`).

FFJORD density estimation

$$\begin{aligned}\log p_1(\mathbf{z}(1)) &= \log p_0(\mathbf{z}(0)) - \int_0^1 \text{tr}\left(\frac{\partial \mathbf{f}_\theta(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)}\right) dt = \\ &= \log p_0(\mathbf{z}(0)) - \mathbb{E}_{p(\epsilon)} \int_0^1 \left[\epsilon^T \frac{\partial \mathbf{f}}{\partial \mathbf{z}} \epsilon\right] dt.\end{aligned}$$

Outline

1. Kolmogorov-Fokker-Planck equation for NF log-likelihood
2. FFJORD (Hutchinson's trace estimator)
3. Adjoint method for continuous-in-time NF
4. SDE basics

Neural ODE

Continuous-in-time NF

$$\begin{aligned}\frac{d\mathbf{z}(t)}{dt} &= \mathbf{f}_{\theta}(\mathbf{z}(t), t) & \frac{d \log p_t(\mathbf{z}(t))}{dt} &= -\text{tr} \left(\frac{\partial \mathbf{f}_{\theta}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)} \right) \\ \mathbf{x} &= \mathbf{z} + \int_0^1 \mathbf{f}_{\theta}(\mathbf{z}(t), t) dt & \log p(\mathbf{x}|\theta) &= \log p(\mathbf{z}) - \int_0^1 \text{tr} \left(\frac{\partial \mathbf{f}_{\theta}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)} \right) dt\end{aligned}$$

How to get optimal parameters of θ ?

For fitting parameters we need gradients. We need the analogue of the backpropagation.

Forward pass (Loss function)

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

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

Neural ODE

Adjoint functions

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

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

Theorem (Pontryagin)

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

Solution for adjoint function

$$\begin{aligned} \frac{\partial L}{\partial \theta(1)} &= \mathbf{a}_\theta(1) = - \int_0^1 \mathbf{a}_z(t)^T \frac{\partial \mathbf{f}_\theta(\mathbf{z}(t), t)}{\partial \theta(t)} dt + 0 \\ \frac{\partial L}{\partial \mathbf{z}(1)} &= \mathbf{a}_z(1) = - \int_0^1 \mathbf{a}_z(t)^T \frac{\partial \mathbf{f}_\theta(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)} dt + \frac{\partial L}{\partial \mathbf{z}(0)} \end{aligned}$$

Note: These equations are solved in reverse time direction.

Adjoint method

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

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

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

Outline

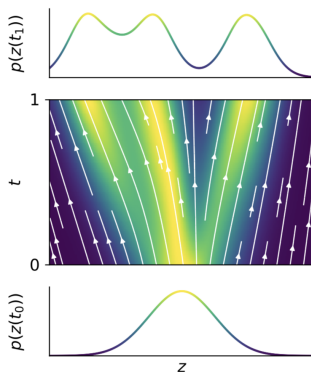
1. Kolmogorov-Fokker-Planck equation for NF log-likelihood
2. FFJORD (Hutchinson's trace estimator)
3. Adjoint method for continuous-in-time NF
4. SDE basics

Ordinary differential equation (ODE)

Neural ODE

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

- ▶ $\mathbf{z}(t_0)$ is a random variable with the density function $p(\mathbf{z}(t_0))$.
- ▶ $\mathbf{z}(t_1)$ is a random variable with the density function $p(\mathbf{z}(t_1))$.
- ▶ $p_t(\mathbf{z}) = p(\mathbf{z}, t)$ is the joint density function (probability path).
What is the difference between $p_t(\mathbf{z}(t))$ and $p_t(\mathbf{z})$?
- ▶ Let consider time interval $[t_0, t_1] = [0, 1]$ without loss of generality.



Ordinary differential equation (ODE)

$$d\mathbf{z} = \mathbf{f}_{\theta}(\mathbf{z}, t) \cdot dt$$

Discretization of ODE (Euler method)

$$\mathbf{z}(t + dt) = \mathbf{z}(t) + \mathbf{f}_{\theta}(\mathbf{z}(t), t) \cdot dt$$

Theorem (Kolmogorov-Fokker-Planck: special case)

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

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

It means that if we have the value $\mathbf{z}_0 = \mathbf{z}(0)$ then the solution of the ODE will give us the density at the moment $t = 1$.

Stochastic differential equation (SDE)

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

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

- ▶ $\mathbf{f}(\mathbf{x}, t) : \mathbb{R}^m \times [0, 1] \rightarrow \mathbb{R}^m$ is the **drift** function of $\mathbf{x}(t)$.
- ▶ $g(t) : \mathbb{R} \rightarrow \mathbb{R}$ 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 $t > s$.
- ▶ $d\mathbf{w} = \mathbf{w}(t + dt) - \mathbf{w}(t) = \mathcal{N}(0, \mathbf{I} \cdot dt) = \epsilon \cdot \sqrt{dt}$, where $\epsilon \sim \mathcal{N}(0, \mathbf{I})$.
- ▶ 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)

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

If $dt = 1$, then

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

- ▶ 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 $p_1(\mathbf{x})$.
- ▶ 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:

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

Here

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

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

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

Stochastic differential equation (SDE)

Theorem (Kolmogorov-Fokker-Planck)

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

- ▶ 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:

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

Langevin SDE (special case)

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

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

Let apply KFP theorem to this SDE.

Langevin SDE (special case)

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

$$\begin{aligned} \frac{\partial p_t(\mathbf{x})}{\partial t} &= \text{tr} \left(-\frac{\partial}{\partial \mathbf{x}} \left[p_t(\mathbf{x}) \frac{1}{2} \frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x}) \right] + \frac{1}{2} \frac{\partial^2 p_t(\mathbf{x})}{\partial \mathbf{x}^2} \right) = \\ &= \text{tr} \left(-\frac{\partial}{\partial \mathbf{x}} \left[\frac{1}{2} \frac{\partial}{\partial \mathbf{x}} p_t(\mathbf{x}) \right] + \frac{1}{2} \frac{\partial^2 p_t(\mathbf{x})}{\partial \mathbf{x}^2} \right) = 0 \end{aligned}$$

The density $p_t(\mathbf{x}) = \text{const}(t)$!

If $\mathbf{x}(0) \sim p_0(\mathbf{x})$, then $\mathbf{x}(t) \sim p_0(\mathbf{x})$.

Discretized Langevin SDE

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

Langevin dynamic

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

Summary

- ▶ Kolmogorov-Fokker-Planck theorem allows to calculate $\log p(\mathbf{z}, t)$ at arbitrary moment t .
- ▶ FFJORD model makes such kind of NF scalable.
- ▶ SDE defines 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.