

A sample method for overdamped Langevin Equation

Zhang Jinrui*
jerryzhang40@gmail.com

20250714

Abstract

In this article, I tried to get the solution distribution of the overdamped Langevin Equation.

1 recite of the problem

The overdamped Langevin Equation use the following version from wikipedia [2, LangevinDynamics]

$$d\mathbf{X} = -\frac{1}{\gamma} \nabla U(\mathbf{X}) dt + \frac{\sqrt{2}\sigma}{\gamma} d\mathbf{W}(t)$$

I choose to solve this one for some simplisity.

$$d\mathbf{X} = \nabla U(\mathbf{X}) dt + d\mathbf{W}(t)$$

or this one.

$$\dot{\mathbf{X}} = \nabla U(\mathbf{X}) + \boldsymbol{\eta}(t)$$

where $\boldsymbol{\eta} = \dot{\mathbf{W}}$

$$\langle \eta_i(t) \rangle = 0, \quad \langle \eta_i(t) \eta_j(t') \rangle = \delta_{ij} \delta(t - t')$$

2 roadmap

The main idea to solve this equation is to use the pinn [1] to fitting the solution distribution $p(x, t)$ where for every t we have $\int_{-\infty}^{\infty} p(x, t) dx = 1$

We need a differential equation about this $p(x, t)$ to make the pinn work.

First we need to find a differential relation only involves $p(x, t)$. Then we can use pinn to get the solution distribution $p(x, t)$.

*alternative email: zhangjr1022@mails.jlu.edu.cn

2.1 definite equation

To simplify the original equation

$$\dot{\mathbf{X}} = \nabla U(\mathbf{X}) + \boldsymbol{\eta}(t)$$

We first remove the wienier term, as following.

$$\dot{\mathbf{X}} = \nabla U(\mathbf{X}) = u$$

For a short period of time increment dt the problem involves two distribution $p(x, t)$ and $p(x, t + dt)$ and we choose a initial point at t denote as x_t and the solution point at time $t + dt$ is x_{t+dt}

So the Lagrangian derivative is as follow

$$\begin{aligned} \frac{Dp}{Dt} &= \frac{\partial p}{\partial t} + u \cdot \nabla p \\ \frac{Dp}{Dt} &= \frac{p(x_{t+dt}, t + dt) - p(x_t, t)}{dt} \end{aligned}$$

and Consider the probabilistic mass around the point x_{t+dt} and x_t we can get a following relation

$$p(x_{t+dt}, t + dt)(dx)(e^{vdt}) = p(x_t, t)(dx)$$

, where

$$v = \nabla \cdot u$$

which is the same as follow

$$p(x_{t+dt}, t + dt) = p(x_t, t)(e^{-vdt})$$

as the dt is infinitesimal so $e^{-vdt} = 1 - vdt$ so we can get

$$p(x_{t+dt}, t + dt) - p(x_t, t) = -vdt$$

which is

$$\frac{Dp}{Dt} = -v = -\nabla \cdot u = -\Delta U = \frac{\partial p}{\partial t} + u \cdot \nabla p$$

then we get a formula only involves $p(x, t)$

$$\frac{\partial p}{\partial t} + u \cdot \nabla p + \nabla \cdot u = 0$$

the initial distribution may take any thing, but for one case we can chose the dirac function

$$p(x, 0) = \delta(x - x_0)$$

in this case this model is just a plain ODE. but in a distribution case.

2.2 sochastic equation

Add back the wenier term the equation backs to

$$\dot{\mathbf{X}} = \nabla U(\mathbf{X}) + \boldsymbol{\eta}(t)$$

For the same period of time increment dt the problem involves two distribution $p(x, t)$ and $p(x, t + dt)$ and we choose a initial point at t denote as x_t and the solution point at time $t + dt$ is x_{t+dt}

then for the point relations by the solution of the equation, x_t gose to x_{t+dt} we denote this as $x_{t+dt} = F(x_t)$ and $x_t = B(x_{t+dt})$

For a certain point x at time $t + dt$ we want $p(x, t + dt)$ this involves a convolution process.

$$p(x, t + dt) = \int_{-\infty}^{\infty} g(y)p(B(x), t)e^{-vdt} dy$$

where $g(y)$ is the probabilistic density function of normal distribution

$$\mathcal{N}(0, dt)$$

If we can some how transform this equation to a differential equation only involves $p(x, t)$, then we can solve this by pinn as the definite model. But this process is way too hard to deal.

2.3 sochastic equation:sampling

I suppose to sample the

$$\boldsymbol{\eta}(t)$$

According to the time discrete size when we use pinn. when we have sample a specific sample of

$$\boldsymbol{\eta}_k(t)$$

we can then rewrite

$$\dot{\mathbf{X}} = u_t = \nabla U(\mathbf{X}) + \boldsymbol{\eta}_k(t)$$

$$\frac{\partial p}{\partial t} + u_t \cdot \nabla p + \nabla \cdot u_t = 0$$

sove this equaiton we can get a sample solution

$$p_k(x, t)$$

to sample a lot

$$\boldsymbol{\eta}_k(t)$$

we can average all the p_k to get the estimated distribution function $p \sim \frac{\sum_{k=1}^N p_k}{N}$

References

- [1] Maziar Raissi, Paris Perdikaris, and George Em Karniadakis. Physics informed deep learning (part i): Data-driven solutions of nonlinear partial differential equations. *arXiv preprint arXiv:1711.10561*, 2017.
- [2] wikipedia. Langevindynamics. https://en.m.wikipedia.org/wiki/Langevin_dynamics. Accessed: 2025-07-14.