LangevinDynamics Experiments Report

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Abstract

In this article, I tried to do some experiments of the overdamped Langevin Equation. Basically, I compared three equations solution using both PDE and Euler-Maruyama method.

1 recite of the problem

The overdamped Langevin Equation use the following version from wikipedia [3, LangevinDynamics]

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

I choose to solve this one for some simplisity.

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

or this one.

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

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

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

2 PDE and Euler-Maruyama:roadmap

the current roadmap contains three separate comparison. basically I want to do same comparison over three equations.

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

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and

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

These three equations can be written in their PDE form according to [2, Fokker-Planck Equation] as follow.

$$\frac{\partial p}{\partial t} = \frac{\epsilon^2}{2}\Delta p - \nabla \cdot (p\nabla U)$$

$$\frac{\partial p}{\partial t} = \frac{\epsilon^2}{2}\Delta p$$

and

$$\frac{\partial p}{\partial t} = -\nabla \cdot (p\nabla U)$$

For each equation, I'll use both PDE solver to get the $p(x,t)$.and the Euler-Maruyama method to sample paths and get the distribution

3 PDE and Euler-Maruyama:experiments

3.1 simulation of the heat equation

3.1.1 PDE part

The equation will have a form of the following, if we only care about the wenier term.

$$\dot{\mathbf{X}} = \epsilon \boldsymbol{\eta}(t)$$

if we consider the probabilistic distribution function over time. We have.

$$\frac{\partial p}{\partial t} = \frac{\epsilon^2}{2}\Delta p$$

This is a heat equaiton.

To make this one feasible for computer to deal with I constrain the space interver just in $X = (0, 0.1)$, and time period in $T = (0, 1)$.

So I need to add a boundary condition. For a heat equation, which from a brownian motion I think choose the derivative free condition is fit this case which is,

$$\frac{\partial p}{\partial x}(x,t) = 0, x \in \partial X, t \in T$$

and a initial distribution I choose the following function,

$$p(x,0) = \frac{-1}{1 + e^{-100*(x-0.9)}} + \frac{1}{(1 + e^{-100*(x-0.1)})}$$

Although this is not a normalized distribution, but it's okay for the simulation i think.

3.1.2 Euler-Maruyama part

We have a second method which is the Euler-Maruyama method which we sample the initial value through distribution $p(x, 0)$ and do the Euler-Maruyama method to get a lot solution $x_k(t)$ then the distribution of $x_k(t)$ should be equation to $p(x, t)$

the iteration relation as following

$$x_{n+1} = x_n + \sqrt{\Delta t}\,\xi_n, \xi_n \sim \mathcal{N}(0, 1)$$

3.1.3 code & results

the computational code are in [1]. the results are shown by the following pictrues which generated by the code. I have done some normalization to make the scale of the PDE solution same as the Euler-Maruyama solution.

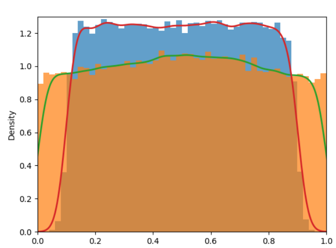

Figure 1: Euler-Maruyama method

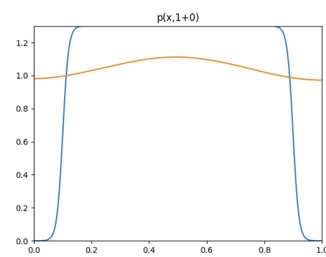

Figure 2: PDE method

3.2 simulation of definite equation

3.2.1 PDE part

undergoing.

3.2.2 Euler-Maruyama part

undergoing.

3.3 simulation of the combined equation

3.3.1 PDE part

undergoing.

3.3.2 Euler-Maruyama part

undergoing.

4 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 $p(x,t)$.

4.1 definite equation

To simplify the original equation

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

We first remove the wenier 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

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

$$\frac{Dp}{Dt} = \frac{p(x_{t+dt}, t+dt) - p(x_t, t)}{dt}$$

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.

4.2 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.

4.3 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. Fokker-planck. `https://www.wikiwand.com/en/articles/Fokker%E2%80%93Planck_equation`. Accessed: 2025-01-19.

[3] wikipedia. Langevindynamics. `https://en.m.wikipedia.org/wiki/Langevin_dynamics`. Accessed: 2025-07-14.