Langevin Dynamics and Deep Neural Network

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Outline

1. Sampling via Langevin Dynamics.
2. Sampling and Non-convex Optimization.
3. Langevin Dynamics and DNN.

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Overview of Langevin Dynamics

In physics, Langevin dynamics is an approach to the mathematical modeling of the dynamics of molecular systems. It was originally developed by French physicist **Paul Langevin**.The approach is characterized by the use of simplified models while accounting for omitted degrees of freedom by the use of stochastic differential equations. (from *Wikipedia*)

Overview of Langevin Dynamics

Consider the following Stochastic Differential Equation:

$$d\mathbf{X}_t = -\nabla f(\mathbf{X}_t)dt + \sqrt{2}d\mathbf{W}_t \tag{1}$$

where $\{\mathbf{X}_t\}_t \in \mathbb{R}^p$ is a stochastic process, $\{\mathbf{W}_t\}_t$ is a standard Wiener process, and f is any smooth function. Then the stationary distribution of X_t when $t \to \infty$ is

$$p(\mathbf{x}) \propto e^{-f(\mathbf{x})}$$

Overview of Langevin Dynamics

The reason behind this is the **Fokker-Planck** equation. Consider the general stochastic differential equation in this form:

$$d\mathbf{X}_t = \mu(\mathbf{X}_t, t)dt + \sigma(\mathbf{X}_t, t)d\mathbf{W}_t \tag{2}$$

where the drift term is $\mu(\mathbf{X}_t, t)$, diffusion coefficient is $D(\mathbf{X}_t, t) = \sigma^2(\mathbf{X}_t, t)/2$.

Overview of Langevin Dynamics

For 1-D case, the **Fokker-Planck** equation for the probability density $p(\mathbf{x}, t)$ of the random variable $\mathbf{X}_t$ is:

$$\frac{\partial}{\partial t} p(\mathbf{x}, t) = -\frac{\partial}{\partial x}[\mu(\mathbf{X}_t, t) p(\mathbf{x}, t)] + \frac{\partial^2}{\partial x^2}[D(\mathbf{X}_t, t) p(\mathbf{x}, t)] \tag{3}$$

Simple Proof

See the whiteboard for details.

Sampling and Langevin Dynamics

Problem: given a high dimensional density $p(\mathbf{x})$, we want to generate a series of points $\{\mathbf{x}_i\}$ such that

$$\lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \delta(\mathbf{x} - \mathbf{x}_i) = p(\mathbf{x})$$

Sampling and Langevin Dynamics

We can solve the following SDE

$$d\mathbf{X}_t = -\nabla f(\mathbf{X}_t)dt + \sqrt{2}d\mathbf{W}_t \tag{4}$$

by using the Euler discretization method:

$$\mathbf{X}_{t+1} - \mathbf{X}_t = -\nabla f(\mathbf{X}_t)h + \sqrt{2h}\xi_t \tag{5}$$

where ξ_t is a series of Gaussian vector and h is the step-size (learning rate).

Sampling and Langevin Dynamics

We can simultaneously solve N SDEs at the same time to get N points. Then when $t \to \infty$ and $N \to \infty$, we have:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \delta(\mathbf{x} - \mathbf{x}_i) = p(\mathbf{x}) \tag{6}$$

Compare with Stein's Variational Importance Sampling

- **Langevin Dynamics**: solve the SDE by discretization and get $\mathbf{x}$. (Just get one point, get N points by solving N SDEs simultaneously)
- **Stein's variational Importance Sampling**: generate a series of data points from distribution q, after enough iterations, the empirical distribution of these points will converge to target distribution p. (See white board for details)

ULA and MALA

- **ULA (Unadjusted Langevin Algorithm)**: directly solve the SDE without any adjustment.
- **MALA (Metropolis-adjusted Langevin Algorithm)**: induce the reject and accept process. (See the whiteboard for details)

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Non-convex Optimization

- In DNN, the most fundamental thing is to minimize the cost function or maximize the utility function.
- For convex optimization, it is easy.
- However, in many cases, we have to face the non-convex optimization problem.

Non-convex Optimization

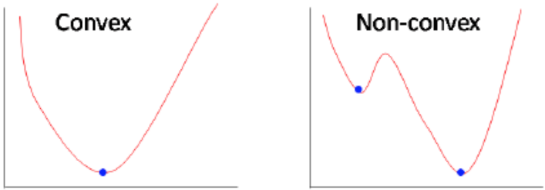

Figure: convex optimization v.s. non-convex optimization

Existing Method

- Gradient Descent?
- Often be trapped by the saddle points or local minima.(See https://arxiv.org/abs/1906.02613)
- Very sensitive to the choice of initial point.

Improvement

Simulated Annealing (SA): a probabilistic technique for approximating the global optimum of a given function. Specifically, it is a metaheuristic to approximate global optimization in a large search space for an optimization problem. (from *Wikipedia*)

Details about Simulated Annealing

See the whiteboard for details.

Sampling and Optimization

- If we try to use gradient descent, then the choice of initial point is very important.
- If the objective function that we are trying to minimize is $f(x)$, then what would be the properties of $p(x) \propto e^{-f(x)}$?

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Literature

- Langevin Dynamics with Continuous Tempering for Training Deep Neural Networks. *Nanyang Ye, Zhanxi Zhu and Rafal K.Mantiuk*
- Preconditioned Stochastic Gradient Langevin Dynamics for Deep Neural Networks. Chuanyuan Li, Changyou Chen, David Carlson and Lawrence Carin

Two Phases for Training Neural Network

- Sampling enough points to capture the modes before running the optimization algorithm.
- Pick up a point near the the top mode as the initialization.

Two Phases for Training Neural Network

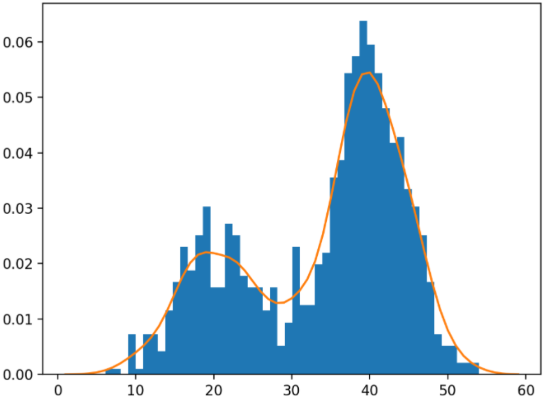

Figure: 1D case capture the modes

Combining SA and Langevin

Langevin Dynamics and SA:

$$d\mathbf{X}_t = -\nabla f(\mathbf{X}_t)dt + \sqrt{2\beta^{-1}(t)}d\mathbf{W}_t \tag{7}$$

where $\beta^{-1}(t) = k_B T(t)$ decays as $T(t) = c/\log(2+t)$. The idea is very similar to MALA.

Insight

We can create a reversible Markov chain by adding the reject-accept process. This is just a very superficial part of Langevin Dynamics and sampling. (Overdamped Langevin) I will introduce more about *Underdamped* Langevin Dynamics in the note.

Thank you!