SDE笔记

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目录

1 Motivation

In this section, we first illustrate the motivation of studying SDE from a machine learning perspective.

1.1 Approximating SGD

First, we look at the SGD process:

$$x^{n+1} = x^n - \eta_k \nabla \mathcal{L}(x^n; \xi^n), \tag{ SGD}$$

where the white noise ξ^n characterize the randomness of the surrogate gradient in SGD method. Denote $\Sigma(x) := \mathbb{E}_\xi \left[(\nabla \mathcal{L}(x;\xi) - \nabla \mathcal{L}(x)) \left(\nabla \mathcal{L}(x;\xi) - \nabla \mathcal{L}(x) \right)^T \right]$ and SGD writes:

$$x^{n+1} = x^n - \eta_k \nabla \mathcal{L}(x^n) + \sqrt{\eta \Sigma} \sqrt{\eta} \mathcal{Z}^n, \mathcal{Z}^n \sim N(0, I_d).$$

If we take the limit $\eta \to 0$ and regard $\sqrt{\eta}\mathcal{Z}^n = \mathrm{d}W_t$, the SDE form of SGD is:

$$\mathrm{d}X(t) = -\nabla \mathcal{L}(X(t))\mathrm{d}t + \sqrt{\eta \Sigma}\mathrm{d}W_t. \tag{ SDE-1}$$

Q:

- Is SDE-1 a good approximation of SGD?
- Good in what sense?
- Is there a better one?

A:

- SDE-1 is a first-order weak approximation of SGD.
- Good in sense of testing: $\forall\, |g(x)| < K(1+|x|)^K, |\mathbb{E}g(X(n\eta)) - g(X^n)| < C\eta^\alpha$
- There are higher order approximations!

For example, the second-order approximation of SGD writes:

$$\mathrm{d}X(t) = -\nabla \left(\mathcal{L}(X(t)) + \frac{\eta}{4} \left\| \nabla \mathcal{L}(X(t)) \right\|^2 \right) \mathrm{d}t + \sqrt{\eta \Sigma}\mathrm{d}W_t. \tag{ SDE-2}$$

And another formulation (1-d Xiang) writes:

$$\mathrm{d}X(t) = \frac{\log(1 - \eta \mathcal{L}''(x))}{\eta \mathcal{L}''(x)} \mathcal{L}'(x)\mathrm{d}t + \sqrt{\frac{2\Sigma \cdot \log(1 - \mathcal{L}''(x)\eta)}{\mathcal{L}''(x)(\mathcal{L}''(x)\eta - 2)}}\mathrm{d}W_t. \tag{ SDE-Xiang-1-dim}$$

The d-dimensional Xiang-Formulation is still under developing. Another class of questions is follows:

Q:

- How are these more advanced flows derived?
- Why would the SDE approximation be useful?

, which will be answered in the following.

1.2 Langevin Dynamics

Our goal of Langevin Dynamics is sampling from a Gibbs measure $\frac{e^{-\frac{\mathcal{L}(x)}{\sigma}}}{\mathcal{Z}_{\mathcal{L},\sigma}}$, where $\mathcal{Z}_{\mathcal{L},\sigma}$ is the normalizing constant. The Langevin dynamics writes:

$$\mathrm{d}X(t) = -\nabla\mathcal{L}(X(t))\mathrm{d}t + \sqrt{2\sigma}\mathrm{d}W_t. \tag{LD}$$

Q:

- Why is this approach correct? I.e. why does LD have the correct equilibrium?
- How fast is the convergence?

The discrete-time version of LD writes:

$$X^{k+1} = X^k - \eta\nabla\mathcal{L}(X^k) + \sqrt{2\sigma}\sqrt{\eta}\mathcal{Z}^k, \mathcal{Z}^n \sim N(0, I_d). \tag{LD-discrete}$$

Q:

- What is the convergence property?
- Can we accelerate the convergence?

2 Ordinary Differential Equations

To better understand the behavior of SDE, we can first take a look at its non-random counterpart, i.e., ODEs (Ordinary Differential Equations).

$$\mathrm{d}X(t) = f(t, X(t))\mathrm{d}t, X(0) = X_0 \tag{ODE}$$

Example: Linear ODE, i.e., $f(t, X(t)) = LX(t)$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}e^{-tL}X(t) &= -e^{-tL}LX(t) + e^{-tL}\frac{\mathrm{d}}{\mathrm{d}t}X(t)\\ &= e^{-tL}\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t) - LX(t)\right) = 0\\ &\Rightarrow e^{-tL}X(t) = e^{-tL}X(t)|_{t=0} = X_0\\ &\Rightarrow X(t) = e^{tL}X_0\end{aligned} \tag{1}$$

Next we look at the conception of Principle Flow proposed in Rosca et al. (2023), consider minimizing the quadratic objective $f(x) = \frac{1}{2}x^T Hx$, assuming that H is positive definite.

Consider the Gradient Descent Dynamic here:

$$X^{n+1} = X^n - \eta\nabla\mathcal{L}(x) = X^n - \eta HX^n = (1 - \eta H)X^n$$

Therefore $X^n = (1 - \eta H)^n X_0$, if we want to have $X^n = X(n\eta)$ for all n, we should have:

$$(1 - \eta H)^n = e^{n\eta L} \Rightarrow L = \frac{\log(1 - \eta H)}{\eta}$$

We obtain $\mathrm{d}X(t) = \frac{\log(1-\eta H)}{\eta}X(t)\mathrm{d}t$, which is the Principle Flow in the quadratic case. This can be generalized to the non-linear case:

$$\mathrm{d}X(t) = \sum_{i=1}^{d}\frac{\log(1 - \eta\lambda_i)}{\eta\lambda_i}\nabla\mathcal{L}(X(t))^T u_i \cdot u_i,$$

where $\nabla^2\mathcal{L}(X(t)) = \sum_{i=1}^{d}\lambda_i u_i u_i^T$ is the SVD of $\nabla^2\mathcal{L}(X(t))$. This generalization is derived in the sense of "backwards error analysis":

$$\begin{cases}\dot{\theta} = -\nabla\mathcal{L}(\theta) + \eta f_1(\theta) + \cdots + \eta^n f_n(\theta),\\ \theta^{n+1} = \theta^n - \eta\nabla\mathcal{L}(\theta^n),\end{cases} \tag{2}$$

We want to have $\theta^{n+1} = \theta(n\eta + \eta)$ and $\theta^n = \theta(n\eta)$

2.1 Numerical Solvers for ODE

Write the ODE in the integral form:

$$X(t+\Delta t) = X(t) + \int_t^{t+\Delta t} f(X(\tau),\tau)\,\mathrm{d}\tau$$

Explicit Euler method:

$$\overline{X}(t+\Delta t) = X(t) + \int_t^{t+\Delta t} f(X(t),t)\,\mathrm{d}\tau$$

Implicit Euler method:

$$X(t+\Delta t) = X(t) + \int_t^{t+\Delta t} f(X(t+\Delta t),t+\Delta t)\,\mathrm{d}\tau$$

Heun method:

$$X(t+\Delta t) = X(t) + \frac{1}{2}\int_t^{t+\Delta t} f(X(t),t) + f(\overline{X}(t+\Delta t),t+\Delta t)\,\mathrm{d}\tau$$

Fourth order Runge-Kutta method:

$$\begin{aligned}
\Delta X_k^1 &= f(\widehat{X}(t_k),t_k)\Delta t \\
\Delta X_k^2 &= f(\widehat{X}(t_k)+\Delta X_k^1/2, t_k+\Delta t/2)\Delta t \\
\Delta X_k^3 &= f(\widehat{X}(t_k)+\Delta X_k^2/2, t_k+\Delta t/2)\Delta t \\
\Delta X_k^4 &= f(\widehat{X}(t_k)+\Delta X_k^3, t_k+\Delta t)\Delta t \\
\widehat{X}(t_{k+1}) &= \widehat{X}(t_k) + \frac{1}{6}(\Delta X_k^1 + 2\Delta X_k^2 + 2\Delta X_k^3 + \Delta X_k^4)
\end{aligned}$$

Order of approximation: $\left|\widehat{X}(t_M) - X(t_M) \le k\Delta t^P\right|, M = \frac{1}{\Delta t}$

2.2 Existence and Uniqueness of the solution to the ODE

Picard iteration: start from the initial guess $\varphi_0(t) = X_0$, recursively compute

$$\varphi_{n+1}(t) = X_0 + \int_{t_0}^{t} f(\varphi_n(\tau),\tau)\,\mathrm{d}\tau.$$

If f is continuous in both x and t and Lipschitz continuous in x, then:

$$\lim_{n\to\infty}\varphi_n(t) = X(t)$$

3 Heuristic Derivation of SDE

3.1 Linear SDE

For SDE, we assume $\mathrm{d}W_t \sim N(0, \mathrm{d}t)$ and SDE writes:

$$\mathrm{d}X_t = FX_t\mathrm{d}t + \sqrt{\widehat{\Sigma}}\mathrm{d}W_t$$

Then,

$$\begin{aligned}
&\mathrm{d}\exp(-Ft)X_t \\
=& -F \cdot \exp(-Ft)X_t\mathrm{d}t + \exp(-Ft)\mathrm{d}X_t \\
=& \exp(-Ft)\sqrt{\widehat{\Sigma}}\mathrm{d}W_t \\
\Rightarrow& \exp(-Ft)X_t = X_0 + \int_0^t \exp(-F\tau)\sqrt{\widehat{\Sigma}}\,\mathrm{d}W_\tau \\
\Rightarrow& X_t = \exp(Ft)X_0 + \exp(F(t-\tau))\sqrt{\widehat{\Sigma}}\,\mathrm{d}W_\tau
\end{aligned}$$

So we know that X_t remains Gaussian given $X_0 \sim N(m_0, P_0)$.

$$\begin{aligned}
m_t =& \mathbb{E}X_t = \exp(F_t)m_0 \\
P_t =& \mathbb{E}\left[(X_t - m_t)(X_t - m_t)^T\right] \\
=& \exp(Ft)P_0\exp(Ft)^T + \int_0^t \exp(F(t-\tau))\widehat{\Sigma}\exp(F(t-\tau))^T\,d\tau
\end{aligned}$$

, which reveals the property of OU process.

3.2 Informal derivation of Xiang's approach

Consider the stochastic dynamics ($d = 1$):

$$X^{n+1} = X^n - \eta\left(HX^n + \sqrt{\Sigma}Z^n\right), Z^n \sim N(0, I)$$

so, X^n remains Gaussian.

$$\begin{aligned}
&X^{n+1} = (1-\eta H)X^n - \eta\sqrt{\Sigma}Z^n \\
\Rightarrow& \frac{X^{n+1}}{(1-\eta H)^{n+1}} = \frac{X^n}{(1-\eta H)^n} - \frac{\eta\sqrt{\Sigma}Z^n}{(1-\eta H)^{n+1}} \\
\Rightarrow& \frac{X^n}{(1-\eta H)^n} = X^0 - \eta\sqrt{\Sigma}\sum_{i=1}^n \frac{Z^i}{(1-\eta H)^i} \\
\Rightarrow& X^n = (1-\eta H)^n X^0 - \eta\sqrt{\Sigma}\sum_{i=1}^n (1-\eta H)^{n-i} Z^i
\end{aligned}$$

We can further calculate its mean and variance:

$$m^n = \mathbb{E}X^n = (1-\eta H)^n \mathbb{E}X^0$$

$$\begin{aligned}
\mathbb{E}\left[(x^n - m^n)(x^n - m^n)^T\right] =& \eta^2 \Sigma \sum_{i=1}^{n} (1-\eta H)^{2(n-i)} \\
=& \eta^2 \Sigma \sum_{i=0}^{n-1} (1-\eta H)^{2i} \\
=& \eta^2 \Sigma \frac{1-(1-\eta H)^{2n}}{1-(1-\eta H)^2}
\end{aligned}$$

Following the idea of principle flow, first we let the mean of two meet:

$$\begin{aligned}
(1-\eta H)^n &= \exp(Fn\eta) \\
\Rightarrow F &= \log(1-\eta H)/\eta
\end{aligned}$$

then look at the variance:

$$\int_0^t \exp(F(t-\tau))\widehat{\Sigma}\exp(F(t-\tau))^T \, d\tau = \eta^2 \Sigma \frac{1-(1-\eta H)^{2n}}{2\eta H - (\eta H)^2}$$

For the left side, we have:

$$\begin{aligned}
\int_0^t \exp(F(t-\tau))\widehat{\Sigma}\exp(F(t-\tau))^T \, d\tau &= \frac{1}{2F}\exp(2F\tau) \mid_0^t \widehat{\Sigma} \\
&= \frac{1}{2F}\widehat{\Sigma} \cdot (\exp(2Fn\eta) - 1) \\
&= \frac{(1-\eta H)^{2n} - 1}{2F} \cdot \widehat{\Sigma}
\end{aligned}$$

So,

$$\begin{aligned}
\frac{(1-\eta H)^{2n} - 1}{2F} \cdot \widehat{\Sigma} &= \eta^2 \Sigma \frac{1-(1-\eta H)^{2n}}{2\eta H - (\eta H)^2} \\
\Rightarrow \widehat{\Sigma} &= -\frac{2F \cdot \eta^2 \cdot \Sigma}{2\eta H - \eta^2 H^2} = \frac{2\Sigma \log(1-\eta H)}{H(H\eta - 2)}
\end{aligned}$$

4 ItoCalculus and SDE

4.1 Stochastic Integral

SDE should be understood as a shorthand of the stochastic integrated equation:

$$X(t) = X(0) + \int_0^t f(\tau, X(\tau))\mathrm{d}\tau + \int_0^t L(\tau, X(\tau))\mathrm{d}W_\tau$$

where the integral w.r.t. the Brownian motion should be understood as the limit:

$$\int_{t_0}^t L(\tau, X(\tau))\mathrm{d}W(\tau) = \lim_{n\to\infty} \sum_k L(t_k, X(t_k)) \left[W(tk+1) - W(t_k)\right]$$

where $t_0 < t_1 < \cdots < t_n = t$ is a partition of $[0, t]$ and $\min t_{i+1} - t_i \to 0$ as $n \to \infty$. We would not make this definition rigorous in this overview. This would be the main objective of this course.

4.2 Ito's formula

We directly assume the Ito's formula to be true. For SDE: $\mathrm{d}X_t = -(t, X_t)\mathrm{d}t + L(t, X(t))\mathrm{d}W_t$

定理 4.1. *(Itoformula). Assume that $X(t)$ is an Itoprocess, and consider an arbitrary (scalar) function $\phi(X(t), t)$ of the process. Then the Itodifferential of ϕ, that is, the ItoSDE for ϕ is given as*

$$\begin{aligned} \mathrm{d}\phi &= \frac{\partial\phi}{\partial t} + \sum_i \frac{\partial\phi}{\partial x_i}\mathrm{d}x_i + \frac{1}{2}\sum_{i,j}\left(\frac{\partial^2\phi}{\partial x_i\partial x_j}\right)\mathrm{d}x_i\mathrm{d}x_j \\ &= \frac{\partial\phi}{\partial t}\mathrm{d}t + (\nabla\phi)^T\mathrm{d}x + \frac{1}{2}\nabla^2\phi : LL^T\mathrm{d}t \end{aligned}$$

where $A : B = tr(A^TB)$

As a sanity check, consider $X(t) = W(t)$ (i.e. $f \equiv 0, L = I$) and $\phi(x) = \frac{1}{2}x^2$, then

$$\mathrm{d}\phi(X(t)) = X(t)\cdot\mathrm{d}W(t) + \frac{1}{2}\mathrm{d}t = W(t)\mathrm{d}W(t) + \frac{1}{2}\mathrm{d}t$$

4.3 Uniqueness and existence

If both f and L grow at most linearly w.r.t. x and are Lipschitz continuous w.r.t. x, the solution is unique.

5 Evolution of the Distribution

5.1 Forward and Backward Kolmogorov's equation

Fokker-Planck equation: Let $p(x,t)$ be the density of $X(t)$, where $X(0) \sim p(x,0)$ and

$$\mathrm{d}X(t) = f(t, X(t))\mathrm{d}t + \sqrt{2\Sigma(t, X(t))}\mathrm{d}W_t$$

We have:

$$\frac{\partial}{\partial t}p + \nabla \cdot (pf) = \nabla \cdot (\nabla \cdot \Sigma p)$$

where for a matrix field, $\nabla\cdot$ is applied row-wisely.

证明. Consider a twice differentiable function ϕ.

$$\mathbb{E}[\phi(X_t)] = \int \phi(x)p(t,x)\mathrm{d}x$$

Using Ito's Lemma, we have:

$$\mathrm{d}\phi(X_t) = (\nabla\phi \cdot f + \nabla^2\phi : \Sigma)\mathrm{d}t + \nabla\phi \cdot \sqrt{2\Sigma}\mathrm{d}W_t$$

$$\begin{aligned}
\mathbb{E}\left[\phi(X_t)\right] =& \mathbb{E}\left[\phi(X_0) + \int_0^t (\nabla\phi \cdot f + \nabla^2\phi : \Sigma)\mathrm{d}\tau + \int_0^t \nabla\phi \cdot \sqrt{2\Sigma}\mathrm{d}W_\tau\right] \\
=& \mathbb{E}\left[\phi(X_0)\right] + \int_0^t \mathbb{E}(\nabla\phi \cdot f + \nabla^2\phi : \Sigma)\mathrm{d}\tau \\
\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}\left[\phi(X_t)\right] =& \mathbb{E}_{x\sim p(t,x)}\left[\nabla\phi(x) \cdot f(t,x) + \nabla^2\phi(x) : \Sigma(t,x)\right] \\
=& \int \nabla\phi(x) \cdot f(t,x) \cdot (t,x) + \nabla^2\phi(x) : \Sigma(t,x) \cdot (t,x)\,\mathrm{d}x \\
=& \int -\nabla \cdot (p \cdot f) \cdot \phi + \phi \cdot \nabla \cdot (\nabla \cdot \Sigma p)\,\mathrm{d}x \\
=& \int \phi(x) \cdot \frac{\partial}{\partial t}p(t,x)\mathrm{d}x
\end{aligned}$$

Since ϕ is chosen arbitrarily, we have

$$\frac{\partial}{\partial t}p + \nabla \cdot (pf) = \nabla \cdot (\nabla \cdot \Sigma p)$$

□

5.2 Deriving Xiang's approach rigorously

5.3 Convergence analysis of Langevin dynamics.

参考文献

Rosca, M.; Wu, Y.; Qin, C.; and Dherin, B. 2023. On a continuous time model of gradient descent dynamics and instability in deep learning. *Transactions on Machine Learning Research.*