

WEEK 1

DAVID LI

Exercise 1. Derive the Fokker-Planck operator \mathcal{L} for the OU process.

The Ornstein-Uhlenbeck SDE is the equation,

$$dX = -\gamma X dt + \sigma dW. \quad (1)$$

The corresponding Fokker-Planck equation is,

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}(\gamma x \rho) + \frac{1}{2} \frac{\partial^2}{\partial x^2}(\sigma^2 \rho). \quad (2)$$

Therefore, the Fokker-Planck operator for the OU process is

$$\mathcal{L}^\dagger \rho = \frac{\partial}{\partial x}(\gamma x \rho) + \frac{1}{2} \frac{\partial^2}{\partial x^2}(\sigma^2 \rho). \quad (3)$$

Exercise 2. Show that $\llbracket OABA \rrbracket$ and $\llbracket BAOAB \rrbracket$ are conjugates, i.e., show that

$$\left(\mathcal{U}_h^{\llbracket OABA \rrbracket}\right)^{n+1} = \mathcal{U}_{h/2}^A \circ \mathcal{U}_{h/2}^B \circ \left(\mathcal{U}_h^{\llbracket BAOAB \rrbracket}\right)^n \circ \mathcal{U}_{h/2}^B \circ \mathcal{U}_{h/2}^A \circ \mathcal{U}_h^O \quad (4)$$

It's not obvious how these two operations are conjugate pairs.

Exercise 3. Explain why Stochastic Position Verlet (SPV) is unsuitable for large choices of γ .

As $\gamma \rightarrow \infty$, $\eta \rightarrow 0$ diminishes the force evaluation term.

Exercise 4. With the Hamiltonian of a one-dimensional harmonic oscillator with spring potential $U(q) = \Omega^2 q^2/2$,

$$H(q, p) = \frac{p^2}{2m} + \frac{\Omega^2 q^2}{2}, \quad (5)$$

where $(q, p) \in \mathbb{R}^2$, show that $\langle q \rangle = \langle p \rangle = 0$, $\langle \Omega^2 q^2 \rangle = \langle p^2/m \rangle = k_B T$, and $\langle qp \rangle = 0$.

We first solve for the distribution,

$$\rho_\beta = \frac{1}{Z} \exp(-\beta H),$$

where the partition function is

$$Z = \iint d\omega \exp(-\beta H).$$

Separating integrands for q and p yields

$$Z = \int_{-\infty}^{\infty} dq \exp(-\beta \Omega^2 q^2/2) \int_{-\infty}^{\infty} dp \exp(-\beta p^2/2m).$$

We know

$$\int_{-\infty}^{\infty} dx \exp(-x^2) = \sqrt{\pi}. \quad (6)$$

Let $x^2 = \beta \Omega^2 q^2/2$, then $x = q\sqrt{\beta \Omega^2/2}$ and $dx = \sqrt{\beta \Omega^2/2} dq$, so that

$$\int_{-\infty}^{\infty} dq \exp(-\beta \Omega^2 q^2/2) = \frac{1}{\sqrt{\beta \Omega^2/2}} \int_{-\infty}^{\infty} dx \exp(-x^2) = \frac{1}{\Omega} \sqrt{\frac{2\pi}{\beta}}. \quad (7)$$

Next, we solve for the p integrand factor. Let $y^2 = \beta p^2/2m$, then $y = p\sqrt{\beta/2m}$ and $dy = dp\sqrt{\beta/2m}$. Therefore,

$$\int_{-\infty}^{\infty} dp \exp(-\beta p^2/2m) = \sqrt{2m/\beta} \int_{-\infty}^{\infty} dy \exp(-y^2) = \sqrt{\frac{2\pi m}{\beta}} \quad (8)$$

Substituting (??) and (??) into Z gives our partition function,

$$Z = \frac{1}{\Omega} \frac{2\pi}{\beta} \sqrt{\frac{2\pi m}{\beta}} = \frac{2\pi\sqrt{m}}{\Omega\beta} \quad (9)$$

This solves the probability density function,

$$\rho_\beta = \frac{\Omega\beta}{2\pi\sqrt{m}} \exp(-\beta p^2/2m) \exp(-\beta\Omega^2 q^2/2). \quad (10)$$

We find $\langle q \rangle$:

$$\begin{aligned} \langle q \rangle &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int d\omega \exp(-\beta p^2/2m) q \exp(-\beta\Omega^2 q^2/2) \\ &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int_{-\infty}^{\infty} dp [\exp(-\beta p^2/2m)] \int_{-\infty}^{\infty} dq [q \exp(-\beta\Omega^2 q^2/2)], \end{aligned}$$

but $q \exp(-\beta\Omega^2 q^2/2)$ is an odd, integrable function, so $\int_{-\infty}^{\infty} dq [q \exp(-\beta\Omega^2 q^2/2)] = 0$, and $\langle q \rangle = 0$. Similarly, $\langle p \rangle = 0$.

Next, we find $\langle \Omega^2 q^2 \rangle$:

$$\begin{aligned} \langle \Omega^2 q^2 \rangle &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int d\omega \exp(-\beta p^2/2m) \Omega^2 q^2 \exp(-\beta\Omega^2 q^2/2) \\ &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int_{-\infty}^{\infty} dp [\exp(-\beta p^2/2m)] \int_{-\infty}^{\infty} dq [\Omega^2 q^2 \exp(-\beta\Omega^2 q^2/2)] \\ &= \frac{\Omega\beta}{2\pi\sqrt{m}} \frac{\sqrt{2\pi m}}{\sqrt{\beta}} \int_{-\infty}^{\infty} dq [\Omega^2 q^2 \exp(-\beta\Omega^2 q^2/2)]. \end{aligned}$$

Let $x^2 = \beta\Omega^2 q^2/2$, then $x = q\sqrt{\beta\Omega^2/2}$ and $dx = \sqrt{\beta\Omega^2/2} dq$, and

$$\int_{-\infty}^{\infty} dq [\Omega^2 q^2 \exp(-\beta\Omega^2 q^2/2)] = \frac{1}{\sqrt{\beta^3\Omega^2/2}} \int_{-\infty}^{\infty} dx [2x^2 \exp(-x^2)] = \sqrt{\frac{\pi}{\beta^3\Omega^2/2}}.$$

Then,

$$\langle \Omega^2 q^2 \rangle = \frac{1}{\beta} = k_B T. \quad (11)$$

By similar methods, we also find $\langle p^2/m \rangle = k_B T$.

Finally, we find $\langle qp \rangle$:

$$\begin{aligned} \langle qp \rangle &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int d\omega p \exp(-\beta p^2/2m) q \exp(-\beta\Omega^2 q^2/2) \\ &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int_{-\infty}^{\infty} dp [p \exp(-\beta p^2/2m)] \int_{-\infty}^{\infty} dq [q \exp(-\beta\Omega^2 q^2/2)]. \end{aligned}$$

Since each integral equals zero by symmetry, $\langle qp \rangle = 0$.

Exercise 5. Show that the expectations of Equation (7.12) are $\langle q \rangle_h^{[ABO]} = \langle p \rangle_h^{[ABO]} = 0$.

Taking the expectations of (7.12), we have

$$\begin{aligned} \langle q \rangle &= \langle q \rangle + h \langle p \rangle / m \\ \langle p \rangle &= -\Omega^2 h e^{-h\gamma} \langle q \rangle + (1 - \Omega^2 h^2 / m) e^{-h\gamma} \langle p \rangle. \end{aligned}$$

From the first equation, $\langle p \rangle = 0$. Substituting into the second equation gives $\langle q \rangle = 0$.

Exercise 6. Show from example (7.2) that $\mathbb{E}(\mu_{n,1}q_n) = \mathbb{E}(\mu_{n,2}q_n) = 0$, $\mathbb{E}(\mu_{n,1}p_n) = \kappa_1\kappa_3$, $\mathbb{E}(\mu_{n,1}\mu_{n,2}) = \kappa_1\kappa_2$, and $\mathbb{E}(\mu_{n,2}^2) = \kappa_2^2 + \kappa_3^2$.

Proof. The proof is straightforward. We find $\mathbb{E}(\mu_{n,2}^2)$ as an example:

$$\mathbb{E}(\mu_{n,2}^2) = \mathbb{E}((\kappa_2 R_n + \kappa_3 R_{n+1})^2) = \kappa_2^2 + \kappa_3^2.$$

□

Exercise 7. Let $H(q, p) = p^2/2 + q^2/2 + \epsilon q^4/4$. Find $\langle q^2 \rangle$ and $\langle p^2 \rangle$.

We find the partition function Z :

$$Z = \int d\omega \exp(-\beta H) = \sqrt{\frac{2\pi}{\beta}} \int_{-\infty}^{\infty} dq \exp(-\beta(q^2/2 + \epsilon q^4/4)),$$

since $\int_{-\infty}^{\infty} dp \exp(-\beta p^2/2) = \sqrt{2\pi/\beta}$. However, solving

$$\int_{-\infty}^{\infty} dq \exp(-\beta(q^2/2 + \epsilon q^4/4))$$

is problematic.