OU process notes

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1 Brownian Motion

We begin with the standard Brownian motion problem. This will lead to useful results for understanding the Ornstein-Uhlenbeck process. The equation of motion is

$$m\frac{du}{dt} = -\gamma u + A'(t) \tag{1}$$

where m is the mass of the particle, u is the velocity, γ is the drag coefficient of the particle in the fluid, and $A'(t)$ is the random force from collisions with surrounding particles. For a homogeneous spherical particle, $\gamma = 6\pi\eta r$ where r is the radius of the sphere and η is the viscosity of the fluid.

Dividing both sides by m and rearranging leads to the first-order linear ordinary differential equation

$$\frac{du}{dt} + \beta u = A(t) \tag{2}$$

for $\beta = \gamma/m$ and $A(t) = A'(t)/m$. The method of integrating factors for indicates we should multiply both sides of 2 by $e^{\beta t}$ to get

$$e^{\beta t}\frac{du}{dt} + e^{\beta t}\beta u = A(t)e^{\beta t} \tag{3}$$

$$\frac{d}{dt}\left(ue^{\beta t}\right) = A(t)e^{\beta t}. \tag{4}$$

Integrating over time on both sides of 4 leads to the solution

$$ue^{\beta t} - u_0 = \int_0^t A(\xi)e^{\beta\xi}\ d\xi \tag{5}$$

where u_0 is the initial velocity and ξ is a dummy variable for integration. Rearranging 5 yields

$$u = u_0e^{-\beta t} + e^{-\beta t}\int_0^t A(\xi)e^{\beta\xi}\ d\xi. \tag{6}$$

Consider $U = u - u_0 e^{-\beta t}$ and 6 becomes

$$U = e^{-\beta t} \int_0^t A(\xi) e^{\beta \xi} \, d\xi. \tag{7}$$

This is a random process since $A(t)$ is a random fluctuation force. It makes sense to consider the distribution of u given a function $A(t$, rather than any exact value. We make the assumption that $\langle A(t) \rangle = 0$ and $A(t)$ is not time correlated, which means

$$\langle A(t_1) A(t_2) \rangle = \left\{ \begin{array}{cc} \tau & \text{if } t_1 = t_2 \\ 0 & \text{otherwise} \end{array} \right\} = \tau \delta(t_1 - t_2). \tag{8}$$

Since u has a distribution, let's look at its moments. The first moment is $\langle u \rangle = 0$ since the expected value is taken over all possible functions $A(t)$; this space is uniform and $\langle A(t) \rangle = 0$. The second moment is

$$\langle U^2 \rangle = \left(e^{-\beta t} \int_0^t A(\xi) e^{\beta \xi} \, d\xi \right)^2 =$$

$$\langle e^{-2\beta t} \int_0^t \int_0^t e^(\beta(t_1 + t_2) A(t_1) A(t_2) \, dt_1 \, dt_2 \rangle =$$

$$e^{-2\beta t} \int_0^t \int_0^t e^{\beta(t_1 + t_2)} \langle A(t_1) A(t_2) \rangle \, dt_1 \, dt_2$$

Making the substitutions $x = t_1 + t_2$, $y = t_1 - t_2$, and $\phi(y) = \langle A(t_1) A(t_2) \rangle$

$$\langle U^2 \rangle = \frac{1}{2} e^{-2\beta t} \int_0^{2t} e^{\beta x} \, dx \int \phi(y) \, dy = \frac{\tau}{2\beta} \left(1 - e^{-2\beta t} \right) \tag{9}$$

From the equipartition theorem, the long term average velocity of the particle should be $\frac{k_B T}{m}$. From 9, $\lim_{t \to \infty} \langle U^2 \rangle = \frac{\tau}{2\beta} = \frac{k_B T}{m}$ so

$$\tau = \frac{2\beta k_B T}{m} \tag{10}$$

It can be shown (according to MacQuarrie) that U follows a normal distribution - this can be confirmed by calculating the further moments and comparing them to those of a normal distribution. Let's now consider times where $\beta t \gg 1$. The initial velocity term becomes negligible, that is $u \approx U$. In this limit, the distribution of u is also normal with expected value 0 and variance $\frac{k_B T}{m}$, in agreement with the equipartition theorem.

2 Ornstein-Uhlenbeck Process

As in the Brownian motion section, we begin with defining the equation of motion.

$$\frac{du}{dt} = -\gamma u + A'(t) + \frac{kx}{m} \tag{11}$$

The only difference between equations 11 and 2 is the additional term accounting for restoring force due to the optical trap. We can simplify the problem by looking at time steps from t to $t + \Delta t$ where the initial velocity no longer has an impact, but short enough such that the acceleration caused by the trap is negligible - both $\beta \Delta t \gg 1$ and $\Delta t \ll 1$. We show in the next section this assumption is valid. Integrating 11 over this period yields

$$\Delta u = \beta \Delta x = \int_t^{t+\Delta t} A(\xi)\ d\xi + \frac{kx}{m}\Delta t \tag{12}$$

In this time limit, the initial velocity can be ignored as determined in the previous section, so

$$\Delta x = \frac{kx}{m\beta}\Delta t = \frac{kx}{\gamma}\Delta t \tag{13}$$

and

$$\langle(\Delta x)^2\rangle = \left(\frac{kx}{m\beta}\Delta t\right)^2 + 2\frac{kx}{m\beta^2}\Delta t \int_t^{t+\Delta t} A(\xi)\ d\xi + \frac{1}{\beta^2}\left(\int_t^{t+\Delta t} A(\xi)\ d\xi\right)^2$$

The first term goes to zero due to the factor of $(\Delta t)^2$, the second term equals zero due to the integral, and the last term goes to

$$\langle(\Delta x)^2\rangle = \frac{1}{\beta^2}\tau = \frac{2k_BT}{m\beta} = \frac{2k_BT}{\gamma} \tag{14}$$

Given the moments from 13 and 14, we can set up the following Langevin equation for the motion of the particle:

$$\frac{dx}{dt} = -\frac{k}{\gamma}x + \sqrt{\frac{2k_BT}{\gamma}}\eta(t) \tag{15}$$

where $\eta(t)$ represents a standard normal random variable. This equation can be solved in the method as 2 leading to

$$\langle x^2\rangle = \frac{k_BT}{k}\left(1 - e^{-2kt/\gamma}\right) \approx \frac{k_BT}{k} \tag{16}$$

in the limit where $\frac{k}{\gamma}t \gg 1$. Equation 16 means that the trap stiffness is given by

$$k = \frac{k_BT}{\langle x^2\rangle} \tag{17}$$

and this relation serves as the basis for the equipartition method of calibrating the trap stiffness.

3 Applying OU to bead simulation

Using following approximate values:

$$
\begin{aligned}
r &= 3 \cdot 10^{-6} \text{ m} \\
\eta &= 10^{-3} \ \frac{\text{N} \cdot \text{s}}{\text{m}^2} \\
k &= 5 \cdot 10^{-4} \ \frac{\text{N}}{\text{m}}
\end{aligned}
$$

we can calculate the following parameters:

$$
\begin{aligned}
\gamma = 6\pi\eta r &\approx 5.655 \cdot 10^{-8} \ \frac{\text{N} \cdot \text{s}}{\text{m}} \\
\beta = \frac{\gamma}{m} = \frac{3\gamma}{4\rho\pi r^3} &\approx 4.6 \cdot 10^{5} \ \frac{\text{N} \cdot \text{s}}{\text{m} \cdot \text{kg}} \\
\theta = \frac{k}{\gamma} &\approx 10^4 \ \text{s}^{-1} \\
\sigma = \sqrt{\frac{2k_B T}{\gamma}} &\approx 4 \cdot 10^{-7} \ \text{m} \cdot \text{s}^{-1/2}
\end{aligned}
$$

With these parameter values, it is reasonable to believe that all of our assumptions in the above sections hold, namely that there exists a Δt such that $\Delta t \ll 1$ and $\beta \Delta t \gg 1$ and that $1 - e^{-2\theta} \approx 1$ for any reasonable time between frames of a video recording. We conclude that we can simulate the positions of a bead following the OU process simply by drawing normal random variables from $N(0, \sqrt{\frac{2k_B T}{\gamma}})$. Further, the stiffness of the trap can be directly calculated by equation 17.