3.1 Langevin equation

Consider a particle moving in an aqueous environment and subject to some external force \( F \). Collisions with fluid molecules have two distinct effects: they induce the diffusive motion of the particle, and an effective frictional force that opposes motion induced by the external force. In the case of microscopic particles, water acts as a highly viscous medium (low Reynolds number) so that any particle quickly approaches terminal velocity and inertial effects can be ignored.

If we ignore the effects of diffusion, then we have the deterministic equation

\[
\frac{dx}{dt} = \frac{F(x)}{\gamma} \equiv A(x),
\]

(3.1)

where \( \gamma^{-1} \) is known as a friction coefficient. In order to incorporate the effects of diffusion, we rewrite the ODE as a difference equation, and add a Wiener process for finite \( \Delta t \) as follows:

\[
\Delta X(t) = X(t + \Delta t) - X(t) = A(X(t)) \Delta t + \sqrt{2D} \Delta W(t),
\]

(3.2)

where \( \Delta W(t) \) is a Gaussian random variable with

\[
\langle \Delta W(t) \rangle = 0, \quad \langle \Delta W(t)^2 \rangle = \Delta t.
\]

(3.3)

The Langevin equation can be solved numerically using a forward Euler scheme with \( \Delta W(t) \) at each time step generated from the Gaussian distribution.

3.2 Ornstein-Uhlenbeck process

One of the simplest, non-trivial examples of a continuous stochastic process is the Ornstein-Uhlenbeck (OU) process. This evolves according to the Langevin equation

\[
X(t + \Delta t) = X(t) - kX(t) \Delta t + \sqrt{2D} \Delta W(t),
\]

(3.4)

Taking expectations of both sides, we have

\[
\langle X(t + \Delta t) \rangle = \langle X(t) \rangle - k\langle X(t) \rangle \Delta t + \sqrt{2D}\langle \Delta W(t) \rangle.
\]

Since \( \Delta W(t) \) has zero mean, we have

\[
\langle X(t + \Delta t) \rangle - \langle X(t) \rangle = -k\langle X(t) \rangle \Delta t.
\]

Dividing both sides by \( \Delta t \) and taking the limit \( \Delta t \to 0 \) then gives the first moment equation

\[
\frac{dX}{dt} = -kX(t),
\]

(3.5)
where $\bar{X}(t) = \langle X(t) \rangle$. This can be integrated to give

$$\bar{X}(t) = X_0 e^{-kt}.$$ 

Now consider the variance

$$\Sigma(t) = \langle X(t)X(t) \rangle - \langle X(t) \rangle \langle X(t) \rangle.$$ 

We have

$$\langle X(t + \Delta t)X(t + \Delta t) \rangle = \left( \langle X(t) - kX(t)\Delta t + \sqrt{2D}\Delta W(t) \rangle \right)^2$$

$$= \langle X(t)^2 \rangle - 2k\langle X(t)^2 \rangle \Delta t + 2D\langle \Delta W(t)\Delta W(t) \rangle + O(\Delta t^2)$$

and

$$\langle X(t + \Delta t) \rangle^2 = \langle X(t) \rangle^2(1 - 2k\Delta t) + O(\Delta t^2).$$

Subtracting these two equations and using the fact that

$$\langle \Delta W(t)\Delta W(t) \rangle = \Delta t,$$

we obtain the result

$$\Sigma(t + \Delta t) = \Sigma(t) - 2k\Sigma(t)\Delta t + 2D\Delta t.$$ 

Rearranging, dividing by $\Delta t$ and taking the limit $\Delta t \to 0$ finally yields

$$\frac{d\Sigma(t)}{dt} = -2k\Sigma(t) + 2D \quad (3.6)$$

This has the solution, assuming $\Sigma(0) = 0$,

$$\Sigma(t) = 2D \int_0^t e^{-2k(t-s)} ds = \frac{D}{k}(1 - e^{-2kt}). \quad (3.7)$$

Note that in the limit $k \to 0$ for fixed $t$, we recover the mean-square displacement of 1D Brownian motion, since $1 - e^{-2kt} \approx 1 - [1 - 2kt + (2kt)^2/2 \ldots] \approx 2kt$.

3.3 Power spectrum

An important concept in stochastic processes is stationarity: a stochastic process $X(t)$ is stationary if all correlations are invariant under a global time shift. This means that $\langle X(t) \rangle$ is independent of time $t$,

$$C_2(t_1, t_2) = \langle X(t_1)X(t_2) \rangle = C(t_1 - t_2), \quad C_3(t_1, t_2, t_3) = \langle X(t_1)X(t_2)X(t_3) \rangle = C(t_2 - t_1, t_3 - t_1)$$

etc.

A very useful quantity for investigating stationary stochastic process $X(t)$ is the power spectrum, which is defined as the Fourier transform of the autocorrelation function $C_X(\tau)$,

$$S_X(\omega) = \int_{-\infty}^{\infty} e^{i\omega \tau} C_X(\tau) d\tau, \quad C_X(\tau) = \langle X(t)X(t + \tau) \rangle. \quad (3.8)$$
Wiener-Khinchin theorem: Consider the covariance of two frequency components of \( X(t) \):

\[
\langle \tilde{X}(\omega) \tilde{X}(\omega') \rangle = \left\langle \int_{-\infty}^{\infty} e^{i\omega t} X(t)dt \int_{-\infty}^{\infty} e^{i\omega' t'} X(t')dt' \right\rangle
\]

\[
= \int_{-\infty}^{\infty} e^{i\omega t} \int_{-\infty}^{\infty} e^{i\omega' t'} \langle X(t)X(t') \rangle dt' dt
\]

\[
= \int_{-\infty}^{\infty} e^{i\omega t} \int_{-\infty}^{\infty} e^{i\omega' t'} \left[ \int_{-\infty}^{\infty} e^{-\Omega(t-t')} S_X(\Omega) \frac{d\Omega}{2\pi} \right] dt' dt
\]

\[
= \int_{-\infty}^{\infty} S_X(\Omega) \left[ \int_{-\infty}^{\infty} e^{i(\omega-\Omega)t} dt \right] \left[ \int_{-\infty}^{\infty} e^{i(\omega'+\Omega)t'} dt' \right] \frac{d\Omega}{2\pi},
\]

assuming that it is possible to rearrange the order of integration. Using the Fourier representation of the Dirac delta function, \( \int_{-\infty}^{\infty} e^{i\omega t} dt = 2\pi \delta(\omega) \), we have

\[
\langle \tilde{X}(\omega) \tilde{X}(\omega') \rangle = \int_{-\infty}^{\infty} S_X(\Omega) \cdot 2\pi \delta(\omega - \Omega) \cdot 2\pi \delta(\omega' + \Omega) \frac{d\Omega}{2\pi},
\]

which establishes the Wiener-Khinchin theorem:

\[
\langle \tilde{X}(\omega) \tilde{X}(\omega') \rangle = 2\pi S_X(\omega) \delta(\omega + \omega')
\]

(3.9)

The Fourier transform of a real-valued variable satisfies \( \tilde{X}(-\omega) = \tilde{X}^*(\omega) \) so

\[
\langle \tilde{X}(\omega) \tilde{X}^*(\omega') \rangle = 2\pi S_X(\omega) \delta(\omega - \omega').
\]

(3.10)

In the case of linear SDEs, it is possible to calculate the spectrum explicitly by formally setting \( dW(t) = \xi(t)dt \) with \( \xi(t) \) a white noise process:

\[
\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = \delta(t - t').
\]

For example, consider the Ornstein-Uhlenbeck process

\[
dX(t) = -kX(t)dt + \sqrt{2D}dW(t).
\]

In order to have a stationary OU process, we take the initial time to be at \( t = -\infty \). The solution can be expressed formally in terms of the integral solution

\[
X(t) = \sqrt{2D} \int_{-\infty}^{t} G(\tau) \xi(t - \tau)d\tau,
\]

(3.11)

where \( G(\tau) \) is known as the causal Green’s function or linear response function with the important property that \( G(\tau) = 0 \) for \( \tau < 0 \). In the case of the OU process

\[
G(\tau) = e^{-\tau k} H(\tau),
\]

where \( H(t) \) is the Heaviside function. The main point to emphasize is that although \( \xi(t) \) is not a mathematically well-defined object, one still obtains correct answers when taking expectations.
For example, it is clear that in the stationary state $\langle X(t) \rangle = 0$ and (for $s > 0$)

$$\langle X(t)X(t + s) \rangle = 2D \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(\tau)G(\tau')\langle \xi(t - \tau)\xi(t + s - \tau') \rangle d\tau d\tau'$$

$$= 2D \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(\tau)G(\tau')\delta(s + \tau - \tau') d\tau d\tau' = \int_{-\infty}^{\infty} G(\tau)G(\tau + s) d\tau$$

$$= \int_{0}^{\infty} e^{-\kappa(2\tau + s)} d\tau = \frac{D}{k} e^{-ks}.$$

This is the expected result for the autocorrelation function of the OU process.

One of the useful features of formally expressing a solution to a linear SDE in the form (3.11) is that one can view the dynamical system as acting as a filter of the white noise process. Applying the Wiener-Khinchin theorem to the white noise autocorrelation function, we see that the spectrum is given by the Fourier transform of a Dirac delta function, which is unity. However, once the noise has been passed through a filter with linear response function $G(t)$, the spectrum is no longer flat. This follows from applying the convolution theorem of Fourier transforms to equation (3.11):

$$\tilde{X}(\omega) = \sqrt{2DG(\omega)}\tilde{\xi}(\omega),$$

so

$$2\pi S_X(\omega)\delta(\omega - \omega') = 2D\tilde{G}(\omega)\tilde{\xi}(\omega)\tilde{\xi}^*(\omega').$$

Evaluating the various Fourier transforms, we have

$$\tilde{G}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}G(t) dt = \int_{0}^{\infty} e^{i\omega t}e^{-kt} dt = \frac{1}{k - i\omega},$$

and

$$\langle \tilde{\xi}(\omega)\tilde{\xi}^*(\omega') \rangle = \int_{-\infty}^{\infty} e^{i\omega t} \int_{-\infty}^{\infty} e^{-i\omega' t'} \langle \xi(t)\xi(t') \rangle dt' dr = 2\pi \cdot \delta(\omega - \omega').$$

Hence,

$$S_X(\omega) = \frac{2D}{k^2 + \omega^2}.$$  \hspace{1cm} (3.12)

The spectrum can be used to recover the variance by noting that

$$\langle X(t)^2 \rangle = \int_{-\infty}^{\infty} S_X(\omega) \frac{d\omega}{2\pi}.$$ 

Substituting for $S_X(\omega)$ and using the identity

$$\int_{-\infty}^{\infty} \frac{d\omega}{\omega^2 + k^2} = \frac{\pi}{k},$$

we see that

$$\langle X(t)^2 \rangle = \frac{D}{k}.$$