5.1 Langevin equation

Now suppose we have 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

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

(5.1)

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:

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

(5.2)

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

\[
\langle \Delta W(m \Delta t) \rangle = 0, \quad \langle \Delta W(m \Delta t) \Delta W(n \Delta t) \rangle = \delta_{n,m} \Delta t.
\]

(5.3)

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. It is possible to make sense of the Langevin equation in the limit \( \Delta t \to 0 \) using an area of mathematics known as stochastic calculus. The corresponding SDE is written as

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

5.2 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

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

(5.4)

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

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

(5.5)
where $\overline{X}(t) = \langle X(t) \rangle$. This can be integrated to give

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

Now consider the variance

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

We have

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

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

and

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

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

$$
\frac{d\Sigma(t)}{dt} = -2k\Sigma(t) + 2D \tag{5.6}
$$

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

$$
\Sigma(t) = 2D \int_0^t e^{-2k(t-s)} ds = \frac{D}{k} (1 - e^{-2kt}). \tag{5.7}
$$

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

### 5.3 Higher dimensions

It is straightforward to generalize the Langevin equation (5.2) to higher dimensions ($d > 1$). Assuming, for simplicity, isotropic diffusion and friction, equation (5.2) becomes

$$
\Delta X_i = \frac{F_i(X)}{\gamma} \Delta t + \sqrt{2D}\Delta W_i(t), \quad i = 1, \ldots, d \tag{5.8}
$$

with $X = (X_1, X_2, \ldots, X_d)$, and

$$
\langle \Delta W_i(m\Delta t) \rangle = 0, \quad \langle \Delta W_i(m\Delta t)\Delta W_j(n\Delta t) \rangle = \delta_{i,j}\delta_{n,m}\Delta t. \tag{5.9}
$$
As an example, the multivariate version of the OU process is given by
\[ \Delta X_i = \sum_{j=1}^{d} M_{ij} X_j \Delta t + \sum_{j=1}^{d} B_{ij} \Delta W_j(t). \] (5.10)

This equation can be used to derive the following moment equations in the limit \( \Delta t \to 0 \):
\[ \frac{d\langle X_i \rangle}{dt} = \sum_{j=1}^{d} M_{ij} \langle X_j(t) \rangle, \] (5.11)

and
\[ \frac{d\Sigma(t)}{dt} = M \Sigma(t) + \Sigma(t) M^\top + D, \] (5.12)

where \( M^\top \) indicates the matrix transpose of \( M \), that is, \( M^\top_{ij} = M_{ji} \), and
\[ D_{ij} = \sum_l B_{il} B_{jl}, \quad \Sigma_{ij}(t) = \langle X_i(t) X_j(t) \rangle - \langle X_i(t) \rangle \langle X_j(t) \rangle. \]

### 5.4 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 \( t \),
\[ C_2(t_1, t_2) = \langle X(t_1) X(t_2) \rangle = C(t_1 - t_2), \quad C_3(t_1, t_2, t_3) = \langle X(t_1) X(t_2) X(t_3) \rangle = C(t_2 - t_1, t_3 - t_1) \]
e tc.

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 \( C_X(\tau) \),
\[ S_X(\omega) = \int_{-\infty}^{\infty} e^{i\omega \tau} C_X(\tau) d\tau, \quad C_X(\tau) = \langle X(t) X(t + \tau) \rangle. \] (5.13)

In the case of linear Langevin equations one can explicitly calculate the spectrum of each component of a Langevin equation using Fourier transforms and linear response theory explicitly.

Consider a deterministic linear differential equation of the form
\[ \frac{dX_i}{dt} = \sum_{j=1}^{d} M_{ij} X_j(t) + I_j(t), \] (5.14)

where \( I_i(t) \) is some external input. Fourier transforming this equation with
\[ \tilde{X}_i(\omega) = \int_{-\infty}^{\infty} e^{i\omega \tau} X(\tau) d\tau \]
e tc., gives
\[ i\omega \tilde{X}_i(\omega) = \sum_{j=1}^{d} M_{ij} \tilde{X}_j(\omega) + \tilde{I}_i(\omega). \] (5.15)
This can be rearranged to show that
\[
\tilde{X}_i(\omega) = \sum_{j=1}^{d} \Phi_{ij}^{-1}(\omega) \tilde{I}_j(\omega),
\]  
(5.16)
where
\[
\Phi_{ij}(\omega) = -i\omega \delta_{ij} + M_{ij}
\]
is known as the transfer matrix. It follows that
\[
\tilde{X}_i(\omega) \tilde{X}_i(\omega') = \sum_{j=1}^{d} \sum_{j'=1}^{d} \Phi_{ij}^{-1}(\omega) \Phi_{ij'}^{-1}(\omega') \tilde{I}_j(\omega) \tilde{I}_{j'}(\omega').
\]

Now suppose that we replace the ODE by the linear Langevin equation
\[
dX_i(t) = \sum_{j=1}^{d} M_{ij} X_j(t) dt + \sum_{j=1}^{d} B_{ij} dW_j(t),
\]  
(5.17)
that is, \(I_i(t)dt\) becomes \(\sum_{j=1}^{d} B_{ij} dW_j(t)\). Using properties of the Wiener process, it can be shown that
\[
\langle \tilde{X}_i(\omega) \tilde{X}_i(\omega') \rangle = \delta(\omega + \omega') \sum_{j=1}^{d} \sum_{j'=1}^{d} \Phi_{ij}^{-1}(\omega) \Phi_{ij'}^{-1}(\omega) D_{jj'},
\]
It then follows from the Wiener-Khinchine theorem that the spectrum is
\[
S_X(\omega) = \sum_{j=1}^{d} \sum_{j'=1}^{d} \Phi_{ij}^{-1}(\omega) \Phi_{ij'}^{-1}(-\omega) D_{jj'}.
\]

In the case of the 1D OU equation
\[
\Delta X = -kX \Delta t + \sqrt{2D} \Delta W(t),
\]
we have
\[
S_X(\omega) = 2D \Phi^{-1}(\omega) \Phi^{-1}(-\omega) = 2D \frac{1}{-i\omega + k} \frac{1}{i\omega + k} = \frac{2D}{k^2 + \omega^2}.
\]  
(5.18)
It follows from the definition of the power spectrum that
\[
C(\tau) = \langle X(t) X(t + \tau) \rangle = 2D \int_{0}^{2\pi} \frac{e^{-i\omega\tau} \, dk}{k^2 + \omega^2}.
\]
In particular, evaluating the integral when \(\tau = 0\) recovers the stationary variance \(C(0) = D/k\).

The power spectrum of a continuous stochastic process has a wide range of applications, including the analysis of noise-induced oscillations in biochemical and genetic networks and the propagation of noise in signaling cascades.
The Wiener-Khinchine theorem states that

\[ \langle \tilde{X}(\omega) \tilde{X}(\omega') \rangle = 2\pi S_X(\omega)\delta(\omega + \omega'), \quad (5.19) \]

where \( \delta(\omega) \) is the Dirac delta function. Since the Fourier transform of a real-valued variable satisfies \( \tilde{X}(-\omega) = \tilde{X}^*(\omega) \), we can also write

\[ \langle \tilde{X}(\omega) \tilde{X}^*(\omega') \rangle = 2\pi S_X(\omega)\delta(\omega - \omega'). \quad (5.20) \]

### 5.5 Fokker-Planck equation

In the absence of a force, the position \( X(t) \) of a Brownian particle evolves according to a Wiener process, and the corresponding distribution of trajectories is determined by the solution to the diffusion equation. Similarly, the position \( X(t) \) of a driven Brownian particle evolves according to the Langevin equation (5.2), and the corresponding distribution of trajectories is determined by the solution to a Fokker-Planck equation. Consider a Brownian particle subject to a force \( F(x) \), and let \( X(t) \) be its position at time \( t \). Define the conditional probability density \( p(x,t|y,\tau) \) according to

\[ p(x,t|y,\tau) \Delta x = \mathbb{P}[x < X(t) < x + \Delta x|X(\tau) = y]. \]

The probability density \( p(x,t) = p(x,t|y,\tau) \) for the position \( x \) of the particle at time \( \tau \), given that it started at position \( y \) at time \( \tau \), satisfies the forward Fokker-Planck (FP) equation

\[ \frac{\partial p(x,t)}{\partial t} = -\frac{\partial [A(x)p(x,t)]}{\partial x} + D \frac{\partial^2 p(x,t)}{\partial x^2} \quad (5.21) \]

where \( A(x) = F(x)/\gamma \).

The 1D FP equation (5.21) can also be rewritten as a probability conservation law according to

\[ \frac{\partial p(x,t)}{\partial t} = - \frac{\partial J(x,t)}{\partial x}, \quad (5.22) \]

where

\[ J(x,t) = \frac{1}{\gamma} F(x)p(x,t) - D \frac{\partial p(x,t)}{\partial x} \quad (5.23) \]

is the probability flux. An equilibrium steady-state solution corresponds to the conditions \( \partial p/\partial t = 0 \) and \( J = 0 \). This leads to the first-order ODE for the equilibrium density \( P(x) \):

\[ D \frac{dP(x)}{dx} - \gamma^{-1} F(x)P(x) = 0, \]

which has the solution

\[ P(x) = \mathcal{N} e^{-U(x)/\gamma D}. \]

Here \( U(x) = -\int^x F(y)dy \) is a potential energy function and \( \mathcal{N} \) is a normalization factor (assuming that it exists).
Einstein relation. Comparison of the equilibrium distribution with the Boltzmann-Gibbs distribution (1.2) yields the Einstein relation

\[ D_\gamma = k_B T, \]  

(5.24)

where \( T \) is the temperature (in degrees Kelvin) and \( k_B \approx 1.4 \times 10^{-23} \text{J} K^{-1} \) is the Boltzmann constant. This formula relates the variance of environmental fluctuations to the strength of dissipative forces and the temperature. In the case of a sphere of radius \( R \) moving in a fluid of viscosity \( \eta \), Stoke’s formula can be used, that is, \( \gamma = 6\pi \eta R \). For water at room temperature, \( \eta \sim 10^{-3} \text{kgm}^{-1} \text{s}^{-1} \) so that a particle of radius \( R = 10^{-9} \text{m} \) has a diffusion coefficient \( D \sim 100 \mu \text{m}^2 \text{s}^{-1} \).

Example 3. The FP equation for the OU process is

\[ \frac{\partial p(x, t)}{\partial t} = \frac{\partial [kxp(x, t)]}{\partial x} + D \frac{\partial^2 p(x, t)}{\partial x^2}. \]  

(5.25)

Given the initial condition \( p(x, 0) = \delta(x - x_0) \), this has the Gaussian solution

\[ p(x, t) = \frac{1}{\sqrt{2\pi D[1 - e^{-2kt}]}} \exp \left( -\frac{(x - x_0e^{-kt})^2}{2D[1 - e^{-2kt}]}/k \right) \]  

(5.26)

Clearly the mean and variance are consistent with the previous calculation. Note that

\[ \lim_{t \to \infty} p(x, t) = p_s(x) = \frac{1}{\sqrt{2\pi D/k}} e^{-kx^2/2D}, \]

which is the stationary probability density.

Similarly, the Fokker-Planck equation corresponding to the multivariate Langevin equation

\[ \Delta X_i = \frac{F_i(X)}{\gamma} \Delta t + \sqrt{2D} \Delta W_i(t), \quad i = 1, \ldots, d, \]  

(5.27)

with \( X = (X_1, X_2, \ldots, X_d) \), is takes the form

\[ \frac{\partial p(x, t)}{\partial t} = -\frac{1}{\gamma} \sum_{i=1}^{d} \frac{\partial}{\partial x_i} [F_i(x)p(x, t)] + D \nabla^2 p(x, t), \quad \nabla^2 p = \sum_{j=1}^{d} \frac{\partial^2 p}{\partial x_i^2}. \]  

(5.28)

The probability flux is given by the vector \( J \) with components

\[ J_i(x, t) = \frac{F_i(x)}{\gamma} p(x, t) - D \frac{\partial}{\partial x_i} p(x, t). \]  

(5.29)

In the case of a multivariate OU process, the FP equation is

\[ \frac{\partial p}{\partial t} = -\sum_{i,j=1}^{K} M_{ij} \frac{\partial}{\partial x_i} p(x, t) + \frac{1}{2} \sum_{i,j=1}^{K} D_{ij} \frac{\partial^2 p(x, t)}{\partial x_i \partial x_j}, \]  

(5.30)

with \( D_{ij} = \sum_k B_{ik} B_{kj} \).