

Lecture 10 summary

Kramers' problem: escape over potential barrier

mean first passage time

$$\Gamma (a \rightarrow x_0 \approx b) \approx 2\pi \alpha \delta \exp \left[\frac{u(b) - u(a)}{\delta} \right]$$

2.3 Langevin equation (SDE)

$$\dot{x} = a(x, t) + b(x, t) \xi(t)$$

Gaussian white noise

$$\langle \xi(t) \rangle = 0$$

$$\langle \xi(t) \xi(t') \rangle = \delta(t - t')$$



Langevin vs. FPE

$$\frac{\partial}{\partial t} p(x, t) = - \frac{\partial}{\partial x} [a(x, t) p(x, t)] + \frac{1}{2} \frac{\partial^2}{\partial x^2} [b(x, t)^2 p(x, t)]$$

drift coeff. $A=a$ $\mathcal{D} = \frac{B}{2} = \frac{b^2}{2}$ diffusion

Examples

(i) Wiener process (no drift)

$$x = \sqrt{2\mathcal{D}} \xi(t) \quad \frac{\partial}{\partial t} p(x, t/x_0, t_0) = \mathcal{D} \frac{\partial^2}{\partial x^2} p(x, t/x_0, t_0)$$

Langevin (SDE) FPE $\mathcal{D} = \frac{B}{2} = \frac{1}{2}$

Using I.C. $p(x, t_0/x_0, t_0) = \delta(x - x_0)$ we can solve FPE with the help of charact. function

$$g_0(s, t) = \int_{-\infty}^{\infty} dx p(x, t/x_0, t_0) e^{isx} \quad (\text{Fourier transform})$$

which satisfies the equation:

$$\frac{\partial g_0}{\partial t} = -\mathcal{D} s^2 g_0, \quad \text{so that} \quad \mathcal{D} \int_{-\infty}^{\infty} dx \left(\frac{\partial^2}{\partial x^2} p \right) e^{isx} \stackrel{\text{integr. by parts}}{=} \mathcal{D} \int dx p \left(\frac{\partial^2}{\partial x^2} e^{isx} \right) = -\mathcal{D} s^2 g_0$$

$$\Rightarrow g_0(s, t) = \exp[-\mathcal{D} s^2 (t - t_0)] g_0(s, t_0)$$

$\stackrel{\text{I.C.}}{=} e^{isx_0}$ (I.C.)

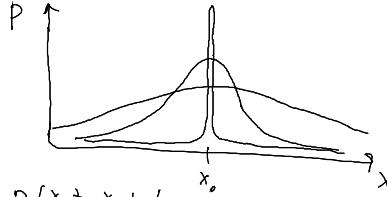
Performing inverse Fourier transform we have the solution:

$$p(x, t/x_0, t_0) = \frac{1}{\sqrt{2\pi 2\mathcal{D}(t-t_0)}} \exp \left[- \frac{(x-x_0)^2}{4\mathcal{D}(t-t_0)} \right]$$

$$\langle x(t) \rangle = x_0$$

$$\langle (\Delta X(t))^2 \rangle = 2D(t-t_0)$$

Initially sharp distribution spreads in time.



ACF

$$\langle X(t_1) X(t_2) \rangle_{x_0, t_0} = \iint dx_1 dx_2 x_1 x_2 p(x_1, t_1, x_2, t_2 / x_0, t_0) \quad t_1 \neq t_2 \geq t_0$$

$$= \iint dx_1 dx_2 x_1 x_2 p(x_1, t_1 / x_2, t_2) p(x_2, t_2 / x_0, t_0) \quad \text{Markov}$$

$$= \int dx_2 \left[\int dx_1 x_1 p(x_1, t_1 / x_2, t_2) \right] x_2 p(x_2, t_2 / x_0, t_0)$$

$$\underbrace{\langle X_1(t_1) \rangle_{x_2, t_2}}_{= x_2 \text{ (mean value remains constant in time, reason } \rightarrow \text{ Markov)}} = \frac{1}{\sqrt{4\pi D(t_1 - t_2)}} \int_{-\infty}^{\infty} dx_1 x_1 e^{-\frac{(x_1 - x_2)^2}{4D(t_1 - t_2)}}$$

$$= \int dx_2 x_2^2 p(x_2, t_2 / x_0, t_0) = \langle X(t_2)^2 \rangle_{x_0, t_0}$$

$$= 2D(t_2 - t_0) + x_0^2 \quad \left(\text{since variance of Gaussian distrib.} \right.$$

$$\left. \langle \Delta X^2 \rangle = \langle X^2 \rangle - x_0^2 = 2D(t - t_0) \right)$$

does not depend on t_1 !

Wiener process is characterized by statistical independence of the increments ΔX (important for stoch. integration)

Without D.C. x_0, t_0 : ACF

$$\langle X(t_1) X(t_2) \rangle = \iint dx_1 dx_2 x_1 x_2 p(x_1, t_1, x_2, t_2)$$

$$= \int dx_2 \left[\int dx_1 x_1 p(x_1, t_1 / x_2, t_2) \right] x_2 p(x_2, t_2)$$

$$\underbrace{\langle X_1(t_1) \rangle_{x_2, t_2}}$$

\Rightarrow ACF for linear Markov processes satisfies the same eq. as the mean values

For example

$$\frac{d}{dt} \langle X(t) \rangle_{x_0, t_0} = -A \langle X(t) \rangle_{x_0, t_0}$$

$$\Rightarrow \frac{d}{dt} \langle X(t) X(t_0) \rangle = -A \langle X(t) X(t_0) \rangle$$

Wiener process is fundamental to study diffusion processes and by means of SDE we can express any diffusion process in terms of Wiener process.

(ii) Ornstein-Uhlenbeck process (if compared to Wiener process, it is a more realistic model of Brownian motion)

$$\text{SDE} \quad \dot{X} = \underbrace{-kX}_{\text{linear drift}} + \sqrt{2D} \xi(t)$$

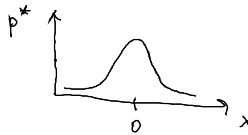
$$\text{FPE} \quad \frac{\partial}{\partial t} p = \frac{\partial}{\partial x} (kx p) + D \frac{\partial^2}{\partial x^2} p \quad p = p(x, t | X_0, t_0)$$

stationary solution on the interval $[a, b]$ with reflecting boundaries ($J(x) = 0$)

$$p^*(x) = \int^x \exp \left[\frac{1}{D} \int_0^x dx' (-kx') \right] = \sqrt{\frac{k}{2\pi D}} \exp \left[-\frac{k}{2D} x^2 \right]$$

$$\langle X(t) \rangle = 0 \quad \text{mean}$$

$$\langle \Delta X^2 \rangle = \frac{D}{k} \quad \text{variance}$$



The time-dependent solution

$$\langle X(t) \rangle_{x_0, t_0} = x_0 e^{-k(t-t_0)}$$

$$\langle \Delta X^2 \rangle_{x_0, t_0} = \frac{D}{k} (1 - e^{-2k(t-t_0)})$$

As $t \rightarrow \infty$, the mean and variance approach

limits 0 and $\frac{D}{k}$, respectively, which gives a limiting

stationary solution. This solution can be obtained directly

by requiring $\partial_t p = 0$, so that p satisfies stationary FPE.

ACF (stationary, $t_0 \rightarrow -\infty$)

$$\begin{aligned} \langle X(t_1) X(t_2) \rangle_{x_0, t_0} &= \iint dx_1 dx_2 x_1 x_2 p(x_1, t_1, x_2, t_2 | x_0, t_0) \quad t_1 \geq t_2 \geq t_0 \\ &= \int dx_2 \left[\int dx_1 x_1 p(x_1, t_1 | x_2, t_2) x_2 p(x_2, t_2 | x_0, t_0) \right] \\ &\quad \langle x_1 \rangle_{x_2, t_2} = x_2 e^{-k(t_1-t_2)} \quad \sqrt{\frac{k}{2\pi D}} \exp \left[-\frac{k}{2D} x_2^2 \right] \\ &\quad t_0 \rightarrow -\infty \\ &= e^{-k(t_1-t_2)} \int dx_2 x_2^2 p^* \\ &\quad \langle x^2 \rangle_* = \underbrace{\langle \Delta X^2 \rangle_*}_{\frac{D}{k}} + \underbrace{\langle x \rangle_*^2}_0 \\ &= \frac{D}{k} e^{-k|t_1-t_2|} \end{aligned}$$

Stationary ACF is typically considered. It is obtained by allowing the system to approach the stationary distribution. It is achieved by putting J.C. in the remote past and $t_0 \rightarrow -\infty$

This result $\langle X(t_1) X(t_2) \rangle_{x_0, t_0} = \frac{D}{k} e^{-k|t_1 - t_2|}$

demonstrates general property of stationary processes: the correlations depend only on time differences.

$$\tau_c = \frac{1}{k} \quad \text{correlation time}$$

$$\text{ACF} \quad G(\tau) = \langle X(t+\tau) X(t) \rangle = \frac{D}{k} e^{-k|\tau|} = D \tau_c e^{-|\tau|/\tau_c}$$

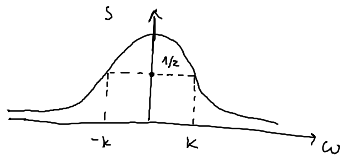
Power spectral density

$$S(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\tau e^{-i\omega\tau} G(\tau)$$

$$S(\omega) = \frac{D}{2\pi k} \int_0^{\infty} d\tau e^{-k\tau} (e^{-i\omega\tau} + e^{i\omega\tau})$$

$$= \frac{D}{2\pi k} \left[\frac{-1}{k+i\omega} e^{-k\tau - i\omega\tau} \Big|_0^{\infty} + \frac{-1}{k-i\omega} e^{-k\tau + i\omega\tau} \Big|_0^{\infty} \right]$$

$$S(\omega) = \frac{D}{2\pi k} \left(\frac{1}{k+i\omega} + \frac{1}{k-i\omega} \right) = \frac{D}{\pi} \frac{1}{\omega^2 + k^2} \quad \text{Lorentzian}$$



Spectral width at half maximum is equal to $2k$

O.-U. process in its stationary state is often used to model a realistic noise signal in which $X(t)$ and $X(t+\tau)$ are only significantly correlated if $\tau \sim \frac{1}{k}$.

These results can be obtained by solving SDE directly

$$\dot{x} = -kx + \sqrt{2D} \zeta(t)$$

$$\text{substitute } y = x e^{kt}$$

$$\dot{y} = (\dot{x} + kx) e^{kt}$$

$$\dot{y} = [-kx + \sqrt{2D} \zeta(t)] e^{kt} + kx e^{kt}$$

$$\dot{y} = \sqrt{2D} e^{kt} \zeta(t)$$

$$y(t) = \sqrt{2D} \int_0^t e^{kt'} \zeta(t') dt' + y(0) \stackrel{= x(0) \text{ J.C.}}{}$$

$$\Rightarrow x(t) = x(0) e^{-kt} + \sqrt{2D} \int_0^t e^{-k(t-t')} \underbrace{\zeta(t') dt'}_{dW'}$$

If J.C. is deterministic or Gaussian distributed then $x(t)$ is Gaussian

$$\langle x(t) \rangle = \langle x(0) \rangle e^{-kt} + \sqrt{2D} \int_0^t e^{-k(t-t')} \underbrace{\langle \dot{x}(t') \rangle}_{=0} dt'$$

ACF can be calculated directly

$$\begin{aligned} & \langle x(t) x(t') \rangle - \langle x(t) \rangle \langle x(t') \rangle \\ &= \left[\langle x(0)^2 \rangle - \langle x(0) \rangle^2 \right] e^{-k(t+t')} + 2D \int_0^t dt'' e^{-k(t-t'')} \int_0^{t'} dt''' e^{-k(t'-t''')} \frac{\langle \dot{x}(t'') \dot{x}(t''') \rangle}{\delta(t''-t''')} \end{aligned}$$

$$= \left[\langle x(0)^2 \rangle - \langle x(0) \rangle^2 \right] e^{-k(t+t')} + \frac{2D}{2k} e^{-k(t+t')} \int_0^{t'} dt'' e^{-2kt''}$$

$\int dt''$ vanishes for $t > t'$,
otherwise $\int dt''$ vanishes

$$= \left[\langle x(0)^2 \rangle - \langle x(0) \rangle^2 - \frac{D}{k} \right] e^{-k(t+t')} + \frac{D}{k} e^{-k|t-t'|}$$

stationary: $t, t' \rightarrow \infty$, $t-t'$ finite

$$= \frac{D}{k} e^{-k|t-t'|} \quad (\text{the same as from FPE!})$$

variance $t = t'$

$$\langle (\Delta x)^2 \rangle = \int \langle \Delta x(0)^2 \rangle - \frac{D}{k} \left] e^{-k(t+t')} + \frac{D}{k} \xrightarrow{t, t' \rightarrow \infty} \frac{D}{k} \quad (\text{the same as from FPE!})$$