Lecture 10 summary

Kramers' problem : escape over potential barrier

mean first passage time

$$T\,(a \to x_0 \approx b) \approx 2\pi \alpha \delta \exp\left[\frac{U(b)-U(a)}{D}\right]$$

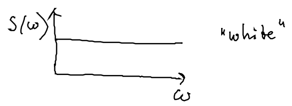
2.3 Langevin equation (SDE)

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

Gaussian white noise

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

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



Langevin vs. FPE

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

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

Examples

(i) Wiener process (no drift)

$\dot{x} = \sqrt{2D}\,\xi(t)$ Langevin (SDE)

$$\frac{\partial}{\partial t} p(x,t/x_0,t_0) = D\frac{\partial^2}{\partial x^2} p(x,t/x_0,t_0)$$ FPE

$D = \frac{B}{2} = \frac{1}{2}$

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

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

which satisfies the equation:

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

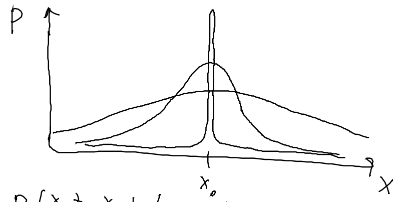
$$\Rightarrow \varphi(s,t) = \exp\left[-D s^2 (t-t_0)\right] \underbrace{\varphi(s,t_0)}_{= e^{isx_0}\ \text{(I.C.)}}$$

Performing inverse Fourier transform we have the solution:

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

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

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



Initially sharp distribution spreads in time.

ACF

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

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

$$= \int dx_2\,\underbrace{\left[\int dx_1\;x_1\;p(x_1,t_1\,/\,x_2,t_2)\right]}_{\langle X_1(t_1)\rangle_{x_2 t_2}}\;x_2\;p(x_2 t_2\,/\,x_0,t_0)$$

$$\langle X_1(t_1)\rangle_{x_2 t_2} = \underbrace{\frac{1}{\sqrt{4\pi\mathcal{D}(t_1-t_2)}}\int_{-\infty}^{\infty} dx_1\,x_1\,e^{-\frac{(x_1-x_2)^2}{4\mathcal{D}(t_1-t_2)}}}_{=x_2}$$

$= x_2$ (mean value remains constant in time, reason $\to$ Markov)

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

$$= 2\mathcal{D}(t_2-t_0) + x_0^2$$

(since variance of Gaussian distrib.

$\langle\Delta X^2\rangle = \langle X^2\rangle - x_0^2 =$

$= 2\mathcal{D}(t-t_0)$)

does not depend on t_1 !

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

Without I.C. x_0, t_0 : ACF

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

$$= \int dx_2\,\underbrace{\left[\int dx_1\,x_1\;p(x_1,t_1\,/\,x_2,t_2)\right]}_{\langle X_1(t_1)\rangle_{x_2,t_2}}\;x_2\;p(x_2,t_2)$$

$\Rightarrow$ 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)

SDE

$$\boxed{\dot{X} = \underbrace{-\kappa x}_{\text{linear drift}} + \sqrt{2\mathcal{D}}\,\xi(t)}$$

FPE

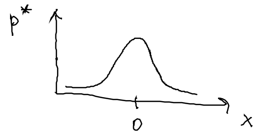
$$\boxed{\frac{\partial}{\partial t} p = \frac{\partial}{\partial x}(\kappa x p) + \mathcal{D}\frac{\partial^2}{\partial x^2} p} \qquad p = p(x,t\,/\,x_0,t_0)$$

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

$$p^*(x) = \mathcal{N}\exp\left[\frac{1}{\mathcal{D}}\int_0^x dx'\,(-\kappa x')\right] = \sqrt{\frac{\kappa}{2\pi\mathcal{D}}}\exp\left[-\frac{\kappa}{2\mathcal{D}}x^2\right]$$

$\langle X(t)\rangle = 0$ mean

$\langle \Delta X^2\rangle = \frac{\mathcal{D}}{\kappa}$ variance



The time-dependent solution

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

$$\langle \Delta X^2\rangle_{x_0 t_0} = \frac{\mathcal{D}}{\kappa}\left(1 - e^{-2\kappa(t-t_0)}\right)$$

As $t\to\infty$, the mean and variance approach limits 0 and $\frac{\mathcal{D}}{\kappa}$, 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, $t_0\to-\infty$)

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

$$= \int dx_2 \Big[\underbrace{\int dx_1\,x_1\,p(x_1,t_1\,/\,x_2,t_2)}_{\langle x_1\rangle_{x_2 t_2} = x_2 e^{-\kappa(t_1-t_2)}}\Big]\, x_2\,\underbrace{p(x_2,t_2\,/\,x_0,t_0)}_{\sqrt{\frac{\kappa}{2\pi\mathcal{D}}}\exp\left[-\frac{\kappa}{2\mathcal{D}}x_2^2\right]\ t_0\to-\infty}$$

$$= e^{-\kappa(t_1-t_2)}\underbrace{\int dx_2\,x_2^2\,p^*}_{\langle X^2\rangle_* = \underbrace{\langle\Delta X^2\rangle_*}_{\frac{\mathcal{D}}{\kappa}} + \underbrace{\langle X\rangle_*^2}_{0}}$$

$$= \frac{\mathcal{D}}{\kappa}e^{-\kappa|t_1-t_2|}$$

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

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.

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

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

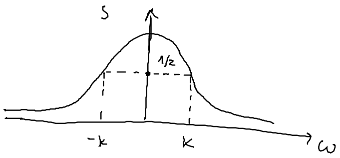
Power spectral density

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

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

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

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

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

substitute $y = x e^{kt}$

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

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

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

$$y(t) = \sqrt{2D} \int_0^t e^{kt'} \xi(t')\, dt' + \underbrace{y(0)}_{= x(0) \text{ I.C.}}$$

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

If I.C. is deterministic or Gaussian distributed then $X(t)$ is Gaussian

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

ACF can be calculated directly

$$\langle x(t)\, x(t')\rangle - \underline{\langle x(t)\rangle\langle x(t')\rangle}$$

$$= [\langle x(0)^2\rangle - \underline{\langle x(0)\rangle^2}]\, e^{-k(t+t')} + 2D\int_0^t dt''\, e^{-k(t-t'')} \int_0^{t'} dt'''\, e^{-k(t'-t''')} \underbrace{\langle \xi(t'')\xi(t''')\rangle}_{\delta(t''-t''')}$$

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

$$= [\langle x(0)^2\rangle - \langle x(0)\rangle^2]\, e^{-k(t+t')} + \frac{2D}{2k} e^{-k(t+t')} e^{2kt'''}\Big|_0^{t'}$$

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

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

$$= \underline{\frac{D}{k} e^{-k|t-t'|}}$$

(the same as from FPE!)

variance $t = t'$

$$\langle (\Delta x)^2\rangle = [\langle \Delta x(0)^2\rangle - \frac{D}{k}]\, e^{-k(t+t')} + \frac{D}{k} \xrightarrow{t,t'\to\infty} \frac{D}{k}$$

(the same as from FPE!)