Lecture 4 summary

Ergodicity: for stationary process

ensemble average = time average

$$\langle x \rangle = \bar{x}(T)$$

$$\bar{x}(T) = \frac{1}{2T} \int_{-T}^{T} dt\, x(t), \quad T \to \infty$$

Autocorrelation function $G(\tau) = \langle x(t)\, x(t+\tau) \rangle$

Power spectrum $S(\omega) = \lim_{T \to \infty} \frac{\pi}{T} |\hat{x}(\omega_j, T)|^2$

Wiener-Khinchin theorem

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

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

relation between ACF and power spectrum of a stoch. process

1.3 Differential Chapman-Kolmogorov equation

(i) $\lim_{\Delta t \to 0} \frac{p(x, t+\Delta t / z, t)}{\Delta t} = W(x / z, t)$ transition probability per unit time $z \to x$ (jump from $z$ to $x$)

(ii) $A_i(z,t)$ drift

(iii) $B_{ij}(z,t)$ diffusion

$$\boxed{\begin{aligned} \frac{\partial}{\partial t} p(z,t/y,t') = &-\sum_i \frac{\partial}{\partial z_i} \left[ A_i(z,t)\, p(z,t/y,t') \right] + \\ &+ \sum_{ij} \frac{1}{2} \frac{\partial^2}{\partial z_i \partial z_j} \left[ B_{ij}(z,t)\, p(z,t/y,t') \right] + \\ &+ \int dx \left[ \underbrace{W}_{\text{prob-ty of trans. per unit time}}(z/x,t)\, p(x,t/y,t') - W(x/z,t)\, p(z,t/y,t') \right] \end{aligned}}$$

differential Chapman-Kolmogorov equation

Each of conditions (i), (ii), (iii) can now be seen to give rise to a distinctive part of the equation, whose interpretation can be provided. We can identify three processes taking place, which are known as jumps, drift and diffusion.

(a) jump processes: $A_i(z,t) = B_{ij}(z,t) = 0$

$$\boxed{\begin{aligned} \frac{\partial}{\partial t} p(z,t/y,t') = \int dx \big[ &W(z/x,t)\, p(x,t/y,t') - \\ &- W(x/z,t)\, p(z,t/y,t') \big] \end{aligned}}$$ Master equation

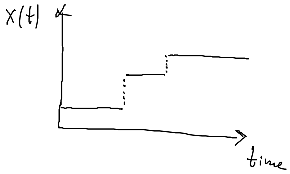
To first order in $\Delta t$ we can solve approx-ly.
We notice that

$p(z,t/y,t) = \delta(y-z)$. Therefore,

$$p(z,t+\Delta t\,/\,y,t) = \delta(y-z)\underline{\left[1-\int dx\, W(x\,/\,y,t)\,\Delta t\right]} + \underline{W(z\,/\,y,t)}\,\Delta t$$

We see that for any $\Delta t$ there is a finite probability given by the coefficient of the $\delta(y-z)$, for the particle to stay at the original position $y$. And the distribution of particles which do not remain at $y$ is given by $W(z\,/\,y,t)$.

$\Rightarrow$ a typical path $x(t)$ will consist of sections of straight lines $x(t)=\text{const}$ combined with discont. jumps whose distribution is given by $W(z\,/\,y,t)$.




(b) diffusion processes (continuous transitions)

$$W(z\,/\,x,t)=0, \quad A_i(z,t)=0$$

$$\frac{\partial}{\partial t}\, p(z,t\,/\,y,t') = \frac{1}{2}\sum_{ij}\frac{\partial^2}{\partial z_i\,\partial z_j}\left[B_{ij}(z,t)\,p(z,t\,/\,y,t')\right]$$

$B_{ij}$ is diffusion matrix

The diffusion matrix $B_{ij}$ is positive semidefinite and symmetric as a result of its definition (see assumption (iii))

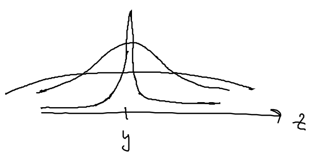
$B_{ij}=B_{ji}$

For one-dim. $\frac{1}{2}B_{ij} = \mathcal{D}$ diffusion constant $\quad \boxed{\frac{\partial}{\partial t}p = \mathcal{D}\,\frac{\partial^2}{\partial z^2}p}$ diffusion equation

Solution for I.C. $p(z,t\,/\,y,t)=\delta(z-y)$ and small $\Delta t$:

$$p(z,t+\Delta t\,/\,y,t) = \frac{1}{\sqrt{2\pi}}\,\frac{1}{\sqrt{2\mathcal{D}\Delta t}}\,\exp\left\{-\frac{(z-y)^2}{4\mathcal{D}\Delta t}\right\}$$

Gaussian (normal) distribution with variance $\sigma^2 = 2\mathcal{D}\Delta t$ and mean $y$.




(c) Drift (contin.)

The first term is non-zero, so we are led to the special case of a Liouville equation:

$$\frac{\partial p(z,t\,/\,y,t')}{\partial t} = -\sum_i \left[A_i(z,t)\,p(z,t\,/\,y,t')\right]$$

which occurs in classical mechanics; $A_i(z,t)$ is a drift vector.

This equation describes a completely deterministic motion, i.e., if $x(y,t)$ is the solution of the ODE:

$$(*) \qquad \frac{dX(t)}{dt} = A[X(t), t] \quad \text{with} \quad X(y,t') = y$$

then the solution of the Liouville eq. with I.C.

$$p(z, t'/y, t') = \delta(z-y)$$

is $p(z,t/y,t') = \delta[z - X(y,t)]$

The proof of this statement is best obtained by direct substitution:

$$-\sum_i \frac{\partial}{\partial z_i}\{A_i(z,t)\,\delta(z-X(y,t))\} =$$

$$= -\sum_i \frac{\partial}{\partial z_i}\{A_i[X(y,t),t]\,\delta[z-X(y,t)]\}$$

$$= -\sum_i \left\{ A_i[X(y,t),t]\frac{\partial}{\partial z_i}\delta[z-X(y,t)]\right\} \quad (**)$$

and $\dfrac{\partial}{\partial t}\delta[z-X(y,t)] = -\sum\limits_i \dfrac{\partial}{\partial z_i}\delta[z-X(y,t)]\dfrac{dX_i(y,t)}{dt} \quad (***)$

and by use of $(*)$ we see that $(**)$ and $(***)$ are equal $\square$.

Thus, if the particle is in a well-defined position (state) $y$ at time $t'$, it stays on the trajectory obtained by solving the ODE $(*)$ (deterministic motion of a particle).

<u>Combination (b) and (c)</u>

We assume that $W(z/x,t)$ is zero. In this case the diff. Chapman-Kolmogorov equation reduces to the Fokker-Planck equation:

$$\frac{\partial p(z,t/y,t')}{\partial t} = -\sum_i \frac{\partial}{\partial z_i}[A_i(z,t)\,p(z,t/y,t')]$$
$$+ \frac{1}{2}\sum_{ij}\frac{\partial^2}{\partial z_i \partial z_j}[B_{ij}(z,t)\,p(z,t/y,t')]$$

Hence, the FPE describes a process in which $X(t)$ has continuous sample paths. Let us consider computing $p(z,t+\Delta t/y,t)$, given $p(z,t/y,t) = \delta(z-y)$ $(\star)$ I.C.

For small $\Delta t$, the solution of the FPE will still be on the whole sharply peaked, and hence derivatives of $A_i(z,t)$ and $B_{ij}(z,t)$ will be negligible compared to those of $p$. Therefore,

$$\frac{\partial p(z,t/y,t')}{\partial t} = -\sum_i A_i(y,t)\frac{\partial p(z,t/y,t')}{\partial z_i} + \sum_{ij}\frac{1}{2}B_{ij}(y,t)\frac{\partial^2 p(z,t/y,t')}{\partial z_i \partial z_j}$$
$$(\star\star)$$

where we have also neglected the time dependence of $A_i$ and $B_{ij}$ for small $t-t'$.
Equation $(\star\star)$ can now be solved, subject to I.C. $(\star)$ and we get:

$$p(z, t+\Delta t / y, t) = (2\pi)^{-\frac{N}{2}} \{ \det [B(y,t)] \}^{\frac{1}{2}} [\Delta t]^{-\frac{1}{2}} \times$$
$$\times \exp \left\{ -\frac{1}{2} \frac{[z-y-A(y,t)\Delta t]^T [B(y,t)]^{-1} [z-y-A(y,t)\Delta t]}{\Delta t} \right\},$$

that is, a Gaussian distribution with variance matrix $B(y,t)$ and mean $y + A(y,t)\Delta t$

We get the picture of a system moving with a systematic drift, whose velocity is $A(y,t)$, on which is superimposed a Gaussian fluctuation with covariance matrix $B(y,t)\Delta t$, that is, we can write

$$\boxed{y(t+\Delta t) = y(t) + A(y(t),t)\Delta t + \eta(t)\Delta t^{1/2}}$$

where $\langle \eta(t) \rangle = 0$

$\langle \eta(t) \eta(t)^T \rangle = B(y,t)$

i) sample paths which are always continuous — for, clearly, as $\Delta t \to 0$, $y(t+\Delta t) \to y(t)$;

ii) sample paths which are nowhere differentiable, because of the $\Delta t^{1/2}$

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2. Classical statistics in non-equilibrium

2.1 Master equation

For Markov processes there is Chapman–Kolmogorov equation

$$p(x, t'' / x', t') = \int dz \, p(x, t'' / z, t) \, p(z, t / x', t') \quad (1)$$
$$t'' \geq t \geq t'$$

For jump processes

$$\underset{\substack{\text{prob-ty of transition} \\ \text{per unit time}}}{W(x/z,t)} = \lim_{\Delta t \to 0} \frac{p(x, t+\Delta t / z, t)}{\Delta t}$$

We assume $\Delta t$ is small

$$p(x, t+\Delta t / z, t) = \delta(x-z) \Big[ 1 - \underbrace{\int dx_2 \, W(x_2 / z, t) \, \Delta t}_{\substack{\text{Prob-ty that no transition} \\ \text{will take place within} \\ \text{interval } [t, t+\Delta t]}} \Big] + W(x / z, t)\Delta t$$

probability of transition per unit time from $z$ to some state $x_2$

prob-ty of transition per unit time $z \to x$