Lecture 2

Continuity in a stochastic process

Is a sample $\vec{X}(t)$ trajectory continuous or not?

E.g., classical gas of hard spheres : $\vec{X}(t)$ is contin.

coordinates

$\vec{V}(t)$ is not, but at a finer scale it is, but

velocity

collision time

the process is no longer Markovian

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So Markov processes are <u>idealizations</u>, which may be characterized by discontinuous paths depending on the system.

<u>Lindeberg condition</u>:

$$(*) \quad \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{|x-z|>\epsilon} d\vec{x}\, p(\vec{x}, t+\Delta t | \vec{z}, t) = 0 \quad , \forall \epsilon > 0$$

(*) is a cond'n for continuous paths

As $\Delta t \to 0$, the prob. to make a finite jump from $\vec{z}$ to $\vec{x} \to 0$ faster than Δt.

1D Brownian motion (Einstein's formulation):

$$p(x, t+\Delta t | z, t) = \frac{e^{-(x-z)^2/4D\Delta t}}{\sqrt{4\pi D \Delta t}}$$

$$(*) \Rightarrow \underset{\substack{\uparrow \\ \text{symm.}}}{2} \int_{z+\epsilon}^{+\infty} dx \frac{e^{-(x-z)^2/4D\Delta t}}{\sqrt{4\pi D\Delta t}} \underset{x'=x-z}{=}$$

$$= 2 \int_{\epsilon}^{+\infty} dx' \frac{e^{-x'^2/4D\Delta t}}{\sqrt{4\pi D \Delta t}} \underset{x''=\frac{x'}{\sqrt{4D\Delta t}}}{=}$$

$$= 4\sqrt{D\Delta t} \int_{\epsilon/\sqrt{4D\Delta t}}^{+\infty} dx'' \frac{e^{-x''^2}}{\sqrt{4\pi D \Delta t}} =$$

$$= \frac{2}{\sqrt{\pi}} \int_{\epsilon/\sqrt{4D\Delta t}}^{+\infty} dx'' e^{-x''^2} =$$

$$= \operatorname{erfc}(\underbrace{\epsilon/\sqrt{4D\Delta t}}_{>0}) \leq e^{-\epsilon^2/(4D\Delta t)}$$

So, $\lim_{\Delta t \to 0} \frac{e^{-\epsilon^2/(4D\Delta t)}}{\Delta t} \to 0$

Brownian motion has <u>continuous</u> sample trajectories.

Ex. → Cauchy process

Differential CK eq'n

Reduce CK eq'n to a differential eq'n

Goal: separate contin. & discontin. motion

$\forall \epsilon > 0$: i) $\lim\limits_{\Delta t \to 0} p(\vec{x}, t+\Delta t | \vec{z}, t)/\Delta t = W(\vec{x}|\vec{z}, t)$
$|\vec{x}-\vec{z}| \geq \epsilon$

ii) $$\lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{|\vec{x}-\vec{z}|<\epsilon} d\vec{x} \, (x_i - z_i) \, p(\vec{x}, t+\Delta t | \vec{z}, t) = A_i(\vec{z}, t) + \theta(\epsilon)$$

iii) $$\lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{|\vec{x}-\vec{z}|<\epsilon} d\vec{x} \, (x_i - z_i)(x_j - z_j) \, p(\vec{x}, t+\Delta t | \vec{z}, t) = B_{ij}(\vec{z}, t) + \theta(\epsilon)$$

If $W(\vec{x}|\vec{z}, t) = 0$ for $\forall \, \vec{x} \neq \vec{z}$, we have a cont. process described by A_i & B_{ij}. Otherwise, we have jumps (discont. motion)

Ex. $\rightarrow$ show that higher-order coeffs. vanish [Gardiner]

Consider time evolution of a smooth f'n $f(\vec{x})$:

$$\partial_t \int d\vec{x} f(\vec{x}) \, p(\vec{x}, t | \vec{y}, t') = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int d\vec{x} f(\vec{x}) \times$$
$$\times [p(\vec{x}, t+\Delta t | \vec{y}, t') - p(\vec{x}, t | \vec{y}, t')] =$$

$$= \lim_{\Delta t \to 0} \frac{1}{\Delta t} \Big[\overbrace{\int d\vec{x} \int d\vec{z} \, f(x) \, p(\vec{x}, t+\Delta t | \vec{z}, t) \, p(\vec{z}, t | \vec{y}, t')}^{\text{apply CK eq'n}} - \int d\vec{z} \, f(\vec{z}) \, p(\vec{z}, t | \vec{y}, t') \Big] \quad (*)$$

$\vec{x} \to \vec{z} \Rightarrow$

Now, if $|\vec{x}-\vec{z}|<\epsilon$, we have

$$f(\vec{x}) \simeq f(\vec{z}) + \sum_i \underbrace{\frac{\partial f}{\partial z_i}}_{\equiv \left.\frac{\partial f}{\partial x_i}\right|_{x_i=z_i}} (x_i - z_i) + \frac{1}{2}\sum_{ij} \underbrace{\frac{\partial^2 f}{\partial z_i \partial z_j}}_{\equiv \left.\frac{\partial^2 f}{\partial x_i \partial x_j}\right|_{x_i=z_i,\, x_j=z_j}} (x_i - z_i)(x_j - z_j)$$

Substitute into (*):

$$\lim_{\Delta t\to 0} \frac{1}{\Delta t}\Big\{ \int_{|\vec{x}-\vec{z}|<\epsilon} d\vec{x}\, d\vec{z} \left[\sum_i (x_i - z_i)\frac{\partial f}{\partial z_i} + \frac{1}{2}\sum_{ij}(x_i-z_i)(x_j-z_j) \times \frac{\partial^2 f}{\partial z_i \partial z_j}\right] \times p(\vec{x}, t+\Delta t|\vec{z}, t)\, p(\vec{z}, t|\vec{y}, t') +$$

$$+ \int_{|\vec{x}-\vec{z}|\geq\epsilon} d\vec{x}\, d\vec{z}\, f(\vec{x})\, p(\underbrace{\vec{x}, t+\Delta t|\vec{z}}_{x\leftrightarrow z}, t)\, p(\vec{z}, t|\vec{y}, t') +$$

↑ no expansion here...

$$+ \int_{|\vec{x}-\vec{z}|<\epsilon} d\vec{x}\, d\vec{z}\, \underbrace{f(\vec{z})}_{\text{0th term in the expansion}}\, p(\vec{x}, t+\Delta t|\vec{z}, t)\, p(\vec{z}, t|\vec{y}, t') -$$

$$- \int d\vec{x}\, d\vec{z}\, f(\vec{z})\, p(\vec{x}, t+\Delta t|\vec{z}, t)\, p(\vec{z}, t|\vec{y}, t') \Big\}$$

Combine these 2

$$\int d\vec{x}\, p(\vec{x}, t+\Delta t|\vec{z}, t) = 1$$

Now,

$$\int d\vec{z} \left[\sum_i A_i(\vec{z}, t)\frac{\partial f}{\partial z_i} + \frac{1}{2}\sum_{ij} B_{ij}(\vec{z}, t)\frac{\partial^2 f}{\partial z_i \partial z_j}\right] p(\vec{z}, t|\vec{y}, t') +$$

$$+ \int_{|\vec{x}-\vec{z}|\geq\epsilon} d\vec{x}\, d\vec{z}\, f(\vec{z}) \left[W(\vec{z}|\vec{x}, t)\, p(\vec{x}, t|\vec{y}, t') - W(\vec{x}|\vec{z}, t)\, p(\vec{z}, t|\vec{y}, t')\right].$$

Now take $\epsilon\to 0$:

$$\partial_t \int d\vec{z}\, f(\vec{z})\, p(\vec{z}, t|\vec{y}, t') =$$

$$= \int d\vec{z} \left[\sum_i A_i \frac{\partial f}{\partial z_i} + \frac{1}{2}\sum_{ij} B_{ij}\frac{\partial^2 f}{\partial z_i \partial z_j}\right] p(\vec{z}, t|\vec{y}, t') +$$

$$+ \int d\vec{z}\, f(\vec{z}) \left[⨍ d\vec{x} \left[W(z|x, t)\, p(\vec{x}, t|\vec{y}, t') - \right.\right.$$

↑ principal value $\int$ (must be careful at $\vec{x}=\vec{z}$)

$\lim\limits_{\delta\to 0} \int_{|x-z|>\delta} d\vec{x}\, F(\vec{x}, \vec{z}) \equiv ⨍ d\vec{x}\, F(\vec{x}, \vec{z})$, usually exists

$- W(\vec{x}|\vec{z},t)\, p(\vec{z},t|\vec{y},t')\,]$

Finally, integrate by parts:

$$\int d\vec{z}\, f(\vec{z})\, \partial_t p(\vec{z},t|\vec{y},t') = \int d\vec{z}\, f(\vec{z}) \Big\{ -\sum_i \frac{\partial}{\partial z_i} \times$$

$$\times \left(A_i(\vec{z},t)\, p(\vec{z},t|\vec{y},t') \right) + \frac{1}{2} \sum_{ij} \frac{\partial^2}{\partial z_i \partial z_j} \times$$

$$\times \left(B_{ij}(\vec{z},t)\, p(\vec{z},t|\vec{y},t') \right) +$$

$$+ \int d\vec{x} \,[\, W(\vec{z}|\vec{x},t)\, p(\vec{x},t|\vec{y},t') -$$

$$- W(\vec{x}|\vec{z},t)\, p(\vec{z},t|\vec{y},t')\,] \Big\} + \text{surface terms}$$

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

$$+ \int d\vec{x} \,[\, W(\vec{z}|\vec{x},t)\, p(\vec{x},t|\vec{y},t') -$$

$$- W(\vec{x}|\vec{z},t)\, p(\vec{z},t|\vec{y},t')\,]$$

Differential CK eq'n

IC: $p(\vec{z},t|\vec{y},t) = \delta(\vec{z}-\vec{y})$

BCs: as appropriate

Interpretation of differential CK eq'n

(1.) Jump processes (ME)

$$A_i(\vec{z},t) = B_{ij}(\vec{z},t) = 0 \quad , \forall i,j$$

Then
$$\partial_t p(\vec{z},t|\vec{y},t') = \int d\vec{x}\,[W(\vec{z}|\vec{x},t)\,p(\vec{x},t|\vec{y},t') - W(\vec{x}|\vec{z},t)\,p(\vec{z},t|\vec{y},t')]$$

Discrete state space:
$$\partial_t P(\vec{n},t|\vec{n}',t') = \sum_{\vec{m}}[W(\vec{n}|\vec{m},t)\times P(\vec{m},t|\vec{n}',t') - W(\vec{m}|\vec{n},t)\times P(\vec{n},t|\vec{n}',t')]$$

$\theta(\Delta t)$: $t \to t+\Delta t$

$$p(\vec{z},t+\Delta t|\vec{y},t) = \underbrace{p(\vec{z},t|\vec{y},t)}_{\delta(\vec{x}-\vec{y})} + \Delta t\left[\int d\vec{x}\,[W(\vec{z}|\vec{x},t)\,p(\vec{x},t|\vec{y},t) - W(\vec{x}|\vec{z},t)\,\underbrace{p(\vec{z},t|\vec{y},t)}_{\delta(\vec{z}-\vec{y})}]\right] =$$

$$= \delta(\vec{z}-\vec{y}) + \Delta t\left[W(\vec{z}|\vec{y},t) - \delta(\vec{z}-\vec{y}) \times \int d\vec{x}\,W(\vec{x}|\vec{y},t)\right] =$$

$$= \delta(\vec{z}-\vec{y})\underbrace{\left[1 - \Delta t\int d\vec{x}\,W(\vec{x}|\vec{y},t)\right]}_{\text{prob. to stay @ } \vec{y} \text{ (s.t. } \vec{z}=\vec{y}\text{); 2nd term is "loss term"}} + \underbrace{\Delta t\,W(\vec{z}|\vec{y},t)}_{\text{prob. to jump from } \vec{y} \text{ to } \vec{z} \text{ in time } \Delta t\text{, "gain term"}}.$$

Paths are discontinuous at discrete points: trajectories are straight lines + discontinuous jumps

(2.) Diffusion processes (Fokker-Planck eq'n) [FP]

$W = 0$ (no jumps)

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

$\to$ path are continuous

$A_i = \text{const}$, $B_{ij} = \text{const}$ $\Rightarrow$ gaussian process,

i.e. $p(\vec{z}, t+\Delta t \mid \vec{y}, t)$ is given by a multi-D gaussian with mean $\vec{y} + \vec{A}\Delta t$

drift velocity

& variance given by $\begin{pmatrix} B_{11} & B_{12} & \dots \\ B_{21} & B_{22} & \\ \dots & & \end{pmatrix}$,

$\underbrace{\Delta t \mathbb{B}}_{\text{gaussian fluct'n}}$, where $\mathbb{B} \Rightarrow$ covariance matrix

In other words,

$$\vec{y}(t+\Delta t) = \underbrace{\vec{y}(t) + \vec{A}\Delta t}_{\text{deterministic part}} + \underbrace{\vec{\eta}(t)\,\Delta t^{1/2}}_{\text{random fluct's}} \qquad (*)$$

$\sqrt{\Delta t}$ since std $\sim \sqrt{\Delta t}$

$\langle \vec{\eta}(t) \rangle = 0$ (no drift)

$\langle \vec{\eta}(t)\,\vec{\eta}^T(t) \rangle = \mathbb{B}$

$$p(\vec{z}, t+\Delta t \mid \vec{y}, t) \sim \exp\left\{ - \frac{(\vec{z}-\vec{y}-\vec{A}\Delta t)^T \mathbb{B}^{-1} (\vec{z}-\vec{y}-\vec{A}\Delta t)}{2\Delta t} \right\}$$

From $(*)$: (i) $\Delta t \to 0 \Rightarrow \vec{y}(t+\Delta t) \to \vec{y}(t)$, paths are continuous

(ii) Paths are <u>not</u> differentiable:

$$\frac{\vec{y}(t+\Delta t) - \vec{y}(t)}{\Delta t} = \vec{A} + \frac{\vec{\eta}(t)}{\Delta t^{1/2}} \Leftarrow \text{diverges as } \Delta t \to 0$$

3. Deterministic process (Liouville eq'n)

$$W = 0, \quad B_{ij} = 0$$

So $$\frac{\partial p(\vec z, t \mid \vec y, t')}{\partial t} = -\frac{\partial}{\partial z_i}\left[A_i(\vec z, t)\, p(\vec z, t \mid \vec y, t')\right]$$

Deterministic motion:

if $p(\vec z, t' \mid \vec y, t') = \delta(\vec z - \vec y)$,

then $p(\vec z, t \mid \vec y, t') = \delta(\vec z - \vec x(\vec y, t))$, where

$$\frac{d\vec x^{\vec y}(t)}{dt} = \vec A(\vec x^{\vec y}(t), t) \quad \& \quad \underbrace{\vec x^{\vec y}(t') = \vec y}$$

initial condition, $\vec x$ @ t' is $= \vec y$ (t': init. time)

Indeed, $-\frac{\partial}{\partial z_i}\left[A_i(\vec z, t)\, \delta(\vec z - \vec x(\vec y, t))\right] =$

$$= -A_i(\vec x(\vec y, t), t)\frac{\partial}{\partial z_i}\delta(\vec z - \vec x(\vec y, t)). \quad (1)$$

Further, $$\frac{\partial}{\partial t}\delta(\vec z - \vec x(\vec y, t)) = -\frac{\partial}{\partial z_i}\delta(\vec z - \vec x(\vec y, t)) \times \frac{dx_i(\vec y, t)}{dt}. \quad (2)$$

(1) = (2) if $\frac{dx_i}{dt} = A_i$ ⇐ deterministic eq'n