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Stochastic differential equations

Stochastic analysis and simulation of reactive and diffusive systems

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Stochastic differential equations

Informal definition

SDEs | Informal definition

Consider the evolution of some variable $x(t) \in \mathbb{R}$ according to a differential equation

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = f\left(x(t), t\right), \qquad \text{with } f : \mathbb{R} \times [0, \infty) \to \mathbb{R}$$

Given the initial condition $x(t=0) = x_0$, we solve the ordinary differential equation

- The solution $(x(t))_{t \geq 0}$ exists if f is a 'well-behaved' function
- (Conditions for existence and uniqueness can be stated)

We can formally re-write the ordinary differential equation

$$\mathrm{d}x(t) = f\left(x(t), t\right) \mathrm{d}t$$

The infinitesimal change of variable x during $[t, t + \mathrm{d}t)$

$$\begin{aligned} x(t + \mathrm{d}t) - x(t) &= \mathrm{d}x(t) \\ &= f\left(x(t), t\right) \mathrm{d}t \end{aligned}$$

To solve the equation, we have the simple recursion

$$x(t + \mathrm{d}t) = x(t) + f\left(x(t), t\right) \mathrm{d}t$$

SDEs | Informal definition (cont.)

$$x(t + \mathrm{d}t) = x(t) + f\left(x(t), t\right) \mathrm{d}t$$

To compute the solution of the ODE, we consider a small time interval of duration Δt

$$x(t + \Delta t) = x(t) + f\left(x(t), t\right) \Delta t$$

Then, given some initial condition $x(0) = x_0$, we have the collection $\{x(k\Delta t)\}_{k=0}^{K}$

$$\begin{aligned} x(0 + 1\Delta t) &= x(0\Delta t) + f\left(x(0\Delta t), 0\Delta t\right) \Delta t \\ x(0 + 2\Delta t) &= x(1\Delta t) + f\left(x(1\Delta t), 1\Delta t\right) \Delta t \\ \cdots &= \cdots \\ x(0 + k\Delta t) &= x(k\Delta t) + f\left(x(k\Delta t), k\Delta t\right) \Delta t \\ \cdots &= \cdots \end{aligned}$$

The iterative scheme is the (explicit) Euler's method to approximate ODE's solutions

- The approximation gets better, the smaller the duration of the interval Δt

SDEs | Informal definition (cont.)

We can use an informal definition of a stochastic differential equation (SDE) as an ordinary differential equation with an additional term describing stochastic fluctuations

$$X(t+\Delta t) = X(t) + f\left(X(t), t\right)\Delta t + \underbrace{g\left(X(t), t\right)\sqrt{\Delta t}\mathcal{N}\left(0,1\right)}_{\text{additional term}}$$

We have the deterministic functions

$$\begin{cases} f : \mathbb{R} \times [0, 8) \to \mathbb{R} \\ g : \mathbb{R} \times [0, 8) \to \mathbb{R} \end{cases}$$

Function $g\left(\cdot\right)$ characterises the strength of the additive stochastic term, scaled by $\sqrt{\Delta t}$

Normally distributed numbers with zero-mean and unit-variance are easily simulated

$$\xi(t) \sim \mathcal{N}\left(0,1\right)$$

In terms of the Wiener increment $\Delta W(t)$ of the standard Brownian motion $W(t)$,

$$X(t+\Delta t) = X(t) + f\left(X(t), t\right)\Delta t + g\left(X(t), t\right)\underbrace{\sqrt{\Delta t}\xi(t)}_{\Delta W(t)}$$

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SDEs | Informal definition (cont.)

Given an initial condition $x\left(0\right) \sim p\left(X(0)\right)$, a $\xi(0) \sim \mathcal{N}\left(0,1\right)$, and small interval Δt

$$\begin{aligned} x(0+1\Delta t) &= x(0\Delta t) + f\left(x(0\Delta t), 0\Delta t\right) + g\left(x(0\Delta t), 0\Delta t\right)\underbrace{\sqrt{\Delta t}\xi(0\Delta t)}_{\Delta W(0\Delta t)} \\ x(0+2\Delta t) &= x(1\Delta t) + f\left(x(1\Delta t), 1\Delta t\right) + g\left(x(1\Delta t), 1\Delta t\right)\underbrace{\sqrt{\Delta t}\xi(1\Delta t)}_{\Delta W(1\Delta t)} \\ \cdots &= \cdots \\ x(0+k\Delta t) &= x(k\Delta t) + f\left(x(k\Delta t), k\Delta t\right) + g\left(x(k\Delta t), k\Delta t\right)\underbrace{\sqrt{\Delta t}\xi(k\Delta t)}_{\Delta W(k\Delta t)} \\ \cdots &= \cdots \end{aligned}$$

As a result of a single realisation of the recursion, we get the collection $\{x(k\Delta t)\}_{k=1}^{K}$

- The realisation scheme is the Euler-Maruyama method for simulating SDEs

SDEs | Informal definition (cont.)

$$X(t+\mathrm{d}t) = X(t) + f\left(X(t), t\right)\mathrm{d}t + g\left(X(t), t\right)\underbrace{\sqrt{\mathrm{d}t}\xi(t)}_{\mathrm{d}W(t)}$$

That is,

$$\mathrm{d}X(t) = f\left(X(t), t\right)\mathrm{d}t + g\left(X(t), t\right)\mathrm{d}W(t)$$

The solution of the differential equation is s stochastic process $(X(t))_{t\ \geq 0}$

$$X(t) = X(0) + \int_0^t f\left(x(s), s\right)\mathrm{d}s + \int_0^t g\left(x(s), s\right)\mathrm{d}W_s$$

Both function $f(\cdot,\cdot)$ and $g(\cdot,\cdot)$ are continuous functions of x and t

SDEs | Informal definition (cont.)

$$X(t) = X(t_0) + \int_0^t f\left(x(s), s\right)\mathrm{d}s + \int_0^t g\left(x(s), s\right)\mathrm{d}W_s$$

We can re-write the solution of the stochastic differential equation using summations,

$$X(t) = X(0) + \lim_{\Delta t_k \to 0}\sum_{0<t_k<t} f\left(X(t'_k), t'_k\right)\Delta t_k + \lim_{\Delta s_k \to 0}\sum_{0<s_k<t} g\left(X(s'_k), s'_k\right)\Delta W_{s_k}$$

We introduced two partitions $\{t_k\}_{k=0}^{K}$ and $\{s_k\}_{k=0}^{K}$ of the $[0,t]$ interval,

$$\underbrace{t_0}_{0}\cdots t_1\cdots\cdots\underbrace{t_{k-1}\cdots t_k}_{\Delta t_k}\underbrace{\cdots t_{k+1}}_{\Delta t_k}\cdots\cdots t_{K-1}\cdots\underbrace{t_K}_{t}$$

$$\underbrace{s_0}_{0}\cdots s_1\cdots\cdots\underbrace{s_{k-1}\cdots s_k}_{\Delta s_k}\underbrace{\cdots s_{k+1}}_{\Delta s_k}\cdots\cdots s_{K-1}\cdots\underbrace{s_K}_{t}$$

We introduced two interval points $t'_k \in \Delta t_k$ and $s'_k \in \Delta s_k$,

$$t_k \leq t'_k \leq t_{k+1}$$
$$s_k \leq s'_k \leq s_{k+1}$$

We also used $\Delta W_{s_k} = W(s_k + 1) - W(s_k)$

SDEs | Informal definition (cont.)

$$X(t) = X(0) + \lim_{\Delta t_k \to 0} \sum_{0<t_k<t} f\left(X(t'_k), t'_k\right) \Delta t_k + \underbrace{\lim_{\Delta s_k \to 0} \sum_{0<s_k<t} g\left(X(s'_k), s'_k\right) \Delta W_{s_k}}_{\text{A stochastic process } I(g(\cdot,\cdot),t)}$$

For $\Delta t_k \to 0$, the first sum converges to the Riemann integral regardless of $t'_k \in \Delta t_k$

$$\rightsquigarrow \quad \int_0^t f\left(X(s), s\right) \mathrm{d}s$$

For $\Delta s_k \to 0$, the value of the second sum may depend on the choice of $s'_k \in \Delta s_k$

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SDEs | Informal definition (cont.)

We can verify the dependence of the second integral on the actual choice of $s'_k \in \Delta s_k$

Consider the following integral

$$\int_0^t W(s)\mathrm{d}W_s \simeq \lim_{\Delta s_k \to 0} \sum_{0<s_k<t} W(s'_k)\Delta W_{s_k}$$

Introduce a partition $\{s_k\}_{k=0}^{K}$ of $[0, t]$,

$$\underbrace{s_0}_{0} \cdots s_1 \cdots\cdots \underbrace{s_{k-1} \cdots s_k}_{\Delta s_k} \underbrace{\cdots s_{k+1}}_{\Delta s_k} \cdots\cdots s_{K-1} \cdots \underbrace{s_K}_{t}$$

Introduce the points $s'_k \in \Delta s_k$,

$$s_k \leq s'_k \leq s_{k+1}$$

Again, we set

$$\Delta W_{s_k} = W(s_k + 1) - W(s_k)$$

We will consider three separate cases

- $s'_k = s_k$
- s'_k such that $W_{s'_k} = (W_{s_k+1+W_{s_k}})/2$

SDEs | Informal definition (cont.)

$$\int_0^t W(s)\mathrm{d}W_s \simeq \lim_{\Delta s_k \to 0} \sum_{0<s_k<t} W(s_k')\Delta W_{s_k}$$

Case I: $s_k' = s_k$

$$\begin{aligned}
\left\langle \int_0^t W_s \mathrm{d}W_s \right\rangle &= \left\langle \lim_{\Delta s_k \to 0} \sum_{0<s_k'<t} W(s_k')\Delta W_{s_k} \right\rangle \\
&= \left\langle \lim_{\Delta s_k \to 0} \sum_{s_k' \in \{s_k\}_{k=0}^{K-1}} W(s_k')\Delta W_{s_k} \right\rangle \\
&= \left\langle \lim_{\Delta s_k \to 0} \sum_{s_k=0}^{K-1} W(s_k)\Delta W_{s_k} \right\rangle \\
&= \left\langle \lim_{\Delta s_k \to 0} \sum_{s_k=0}^{K-1} W(s_k)\left(W(s_k+1) - W(s_k)\right) \right\rangle \\
&= \left\langle \lim_{\Delta s_k \to 0} \sum_{s_k=0}^{K-1} \left[\frac{1}{2}(W(s_k+1) + W(s_k)) - \frac{1}{2}(W(s_k+1) - W(s_k))\right] (W(s_k+1) - W(s_k)) \right\rangle \\
&= \frac{1}{2}\left\langle \lim_{\Delta s_k \to 0} \sum_{s_k=1}^{K-1} \left[W^2(s_k+1) - W^2(s_k)\right] \right\rangle - \frac{1}{2}\left\langle \lim_{\Delta s_k \to 0} \sum_{s_k=0}^{K-1} [W(s_k+1) - W(s_k)]^2 \right\rangle \\
&= \frac{1}{2}\left(\langle W^2(t)\rangle - \langle W^2(0)\rangle\right) - \frac{1}{2}t \\
&= 0
\end{aligned}$$

SDEs | Informal definition (cont.)

$$\int_0^t W(s)\mathrm{d}W_s \simeq \lim_{\Delta s_k \to 0} \sum_{0<s_k<t} W(s_k')\Delta W_{s_k}$$

Case III: s_k' such that $W_{s_k'} = (W_{s_k+1+W_{s_k}})/2$

$$\begin{aligned}
\left\langle \int_0^t W_s \mathrm{d}W_s \right\rangle &= \left\langle \lim_{\Delta s_k \to 0} \sum_{s_k=0}^{K-1} (W(s_k+1) - W(s_k))\,(W(s_k+1) - W(s_k)) \right\rangle \\
&= \frac{1}{2}\left\langle \sum_{\Delta s \to 0} \sum_{s_k=0}^{K-1} \left(W(s_k+1)^2 - W(s_k)^2\right) \right\rangle \\
&= \frac{1}{2}\left(\langle W(t)^2\rangle - \langle W(0)^2\rangle\right) \\
&= \frac{t}{2}
\end{aligned}$$

SDEs | Informal definition (cont.)

We show that there are different definitions of the stochastic integral

$$I\left(g(\cdot,\cdot),t\right)=\int_0^t g\left(X(s),s\right)\mathrm{d}W_s$$

There are two main types of definition of the stochastic integral

- The Itô integral

$$\rightsquigarrow \quad s_k' = s_k$$

- The Stratonovich integral

$$\rightsquigarrow \quad s_k' \text{ such that } g\left(X(s_k'),s_k'\right)=1/2\left[g\left(X(s_k),s_k\right)+g\left(X(s_k+1),s_k+1\right)\right]$$

SDEs | Informal definition (cont.)

Accordingly, we also have two interpretations of the stochastic differential equation

- The Itô equation

$$\mathrm{d}X(t)=f\left(X(t),t\right)\mathrm{d}t+g\left(X(t),t\right)\mathrm{d}W(t)$$

- The Stratonovich equation

$$\mathrm{d}X(t)=f\left(X(t),t\right)\mathrm{d}t+g\left(X(t),t\right)\circ\mathrm{d}W(t)$$

The Stratonovich equation is equivalent to the Itô equation of the form

$$\mathrm{d}X(t)=\left[f\left(X(t),t\right)+\frac{1}{2}\frac{\partial g\left(X(t),t\right)}{\partial x}g\left(X(t),t\right)\right]\mathrm{d}t+g\left(X(t),t\right)\mathrm{d}W(t)$$

SDEs | Informal definition (cont.)

For the somewhat general case of N_x Itô stochastic differential equations, we have

$$
\begin{aligned}
\mathrm{d}X_1(t) &= f_1\left(X_1(t),\dots,X_{N_x}(t),t\right)\mathrm{d}t + g_1\left(X_1(t),\dots,X_{N_x}(t),t\right)\mathrm{d}W_1(t)\\
\cdots &= \cdots\\
\mathrm{d}X_{N_x}(t) &= f_{N_x}\left(X_1(t),\dots,X_{N_x}(t),t\right)\mathrm{d}t + g_{N_x}\left(X_1(t),\dots,X_{N_x}(t),t\right)\mathrm{d}W_{N_x}(t)
\end{aligned}
$$

Equivalently, in computational form

$$
\begin{aligned}
\Delta X_1(t) &= f_1\left(X_1(t),\dots,X_{N_x}(t),t\right)\Delta t + g_1\left(X_1(t),\dots,X_{N_x}(t),t\right)\underbrace{\sqrt{\Delta t}\xi_1(t)}_{\Delta W_1(t)}\\
\cdots &= \cdots\\
\Delta X_{N_x}(t) &= f_{N_x}\left(X_1(t),\dots,X_{N_x}(t),t\right)\Delta t + g_{N_x}\left(X_1(t),\dots,X_{N_x}(t),t\right)\underbrace{\sqrt{\Delta t}\xi_{N_x}(t)}_{\Delta W_{N_x}(t)}
\end{aligned}
$$

SDEs | Informal definition (cont.)

In matrix form, for $X(t) = (X_1(t),\dots,X_{N_x}(t))$ we have

$$
\begin{bmatrix}\Delta X_1(t)\\ \vdots\\ \Delta X_{N_x}(t)\end{bmatrix} = \underbrace{\begin{bmatrix}f_1\left(X(t),t\right)\\ \vdots\\ f_{N_x}\left(X(t),t\right)\end{bmatrix}}_{N_x\times 1}\Delta t + \underbrace{\begin{bmatrix}g_1\left(X(t),t\right)\\ \vdots\\ g_{N_x}\left(X(t),t\right)\end{bmatrix}}_{N_x\times 1}\mathcal{N}\left(\underbrace{\begin{bmatrix}0\\ \vdots\\ 0\end{bmatrix}}_{N_x\times 1},\underbrace{\begin{bmatrix}\Delta t & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & \Delta t\end{bmatrix}}_{N_x\times N_x}\right)
$$

Note that the number of N_k of independent unit normals was constructed to be equal to the number N_x of process components, though nothing precludes the case $N_k \neq N_x$

SDEs | Informal definition (cont.)

For the more general case of N_x Itô equations and N_k Brownian motions, we have

$$
\begin{aligned}
\mathrm{d}X_1(t) &= f_1\left(X(t), t\right)\mathrm{d}t + \sum_{n_k=1}^{N_k} g_{1,n_k}\left(X(t), t\right)\mathrm{d}W_{n_k}(t) \\
\cdots &= \cdots \\
\mathrm{d}X_{N_x}(t) &= f_{N_x}\left(X(t), t\right)\mathrm{d}t + \sum_{n_k=1}^{N_k} g_{N_x,n_k}\left(X(t), t\right)\mathrm{d}W_{n_k}(t)
\end{aligned}
$$

Equivalently, in computational form

$$
\begin{aligned}
\Delta X_1(t) &= f_1\left(X(t), t\right)\Delta t + \sum_{n_k=1}^{N_k} g_{1,n_k}\left(X(t), t\right)\underbrace{\sqrt{\Delta t}\xi_1(t)}_{\Delta W_1(t)} \\
\cdots &= \cdots \\
\Delta X_{N_x}(t) &= f_{N_x}\left(X(t), t\right)\Delta t + \sum_{n_k=1}^{N_k} g_{N_x,n_k}\left(X(t), t\right)\underbrace{\sqrt{\Delta t}\xi_{N_k}(t)}_{\Delta W_{N_k}(t)}
\end{aligned}
$$

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SDEs | Informal definition (cont.)

In matrix form, for $X(t) = (X_1(t), \dots, X_{N_x}(t))$ we have

$$
\begin{bmatrix} \Delta X_1(t) \\ \vdots \\ \Delta X_{N_x}(t) \end{bmatrix} = \underbrace{\begin{bmatrix} f_1\left(X(t), t\right) \\ \vdots \\ f_{N_x}\left(X(t), t\right) \end{bmatrix}}_{N_x \times 1} \Delta t
$$

$$
+ \underbrace{\begin{bmatrix} g_{1,1}\left(X(t), t\right) & \cdots & g_{1,N_k}\left(X(t), t\right) \\ \vdots & \ddots & \vdots \\ g_{N_x,1}\left(X(t), t\right) & \cdots & g_{N_x,N_k}\left(X(t), t\right) \end{bmatrix}}_{N_x \times N_k} \mathcal{N}\left(\underbrace{\begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}}_{N_k \times 1}, \underbrace{\begin{bmatrix} \Delta t & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \Delta t \end{bmatrix}}_{N_k \times N_k} \right)
$$

That is,

$$
\mathrm{d}X(t) = f\left(X(t), t\right)\mathrm{d}t + G\left(X(t), t\right)\mathcal{N}\left(0, \mathrm{d}t I_{N_k}\right)
$$

SDEs | Informal definition (cont.)

$$\mathrm{d}X_{n_x}(t) = f_{n_x}(X(t), t)\,\mathrm{d}t + \sum_{n_k=1}^{N_k} g_{n_x,n_k}(X(t), t)\,\mathrm{d}W_{n_k}(t)$$

The n_x-th Itô equation is the standard-form Langevin equation for the Markov process

The corresponding Stratonovich equation,

$$\mathrm{d}X_{n_x}(t) = \left(f_{n_x}(X(t), t) + \frac{1}{2}\sum_{n_k=1}^{N_k}\sum_{n_x'=1}^{N_x}\frac{\partial g_{n_x,n_k}(X(t), t)}{\partial X^{n_x'}} g_{n_x,n_k}(X(t), t)\right)\mathrm{d}t + \sum_{n_k=1}^{N_k} g_{n_x,n_k}(X(t), t)\,\mathrm{d}W_{n_k}(t)$$

Stochastic differential equations

Examples

SDEs | Examples

Example

$$\mathrm{d}X(t) = f\left(X(t), t\right)\mathrm{d}t + g\left(X(t), t\right)\mathrm{d}W(t)$$

Let $f\left(X(t), t\right) = 0$ and $g\left(X(t), t\right) = 1$, we get the stochastic differential equation

$$X(t + \mathrm{d}t) = X(t) + \mathrm{d}W(t)$$

Using the informal treatment, we get the associated computational definition

$$X(t + \Delta t) = X(t) + \sqrt{\Delta t}\,\underbrace{\xi(t)}_{\mathcal{N}(0,1)}$$

We consider a time interval $\Delta t = 10^{-3}$ and an initial condition $X(0) = 0$

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Let $M_X(t)$ be the expected value of $X(t)$

$$M_X(t) = \left\langle X(t) \right\rangle$$

Let $V_X(t)$ be the variance of $X(t)$

$$\begin{aligned} V_X(t) &= \left\langle \left(X(t) - M_X(t)\right)^2 \right\rangle \\ &= \left\langle X(t)^2 \right\rangle - M_X(t)^2 \end{aligned}$$

From $X(t + \Delta t) = X(t) + \sqrt{\Delta t}\xi(t)$, we have

$$\begin{aligned} M_X(t + \Delta t) &= \left\langle X(t) + \sqrt{\Delta t}\xi(t) \right\rangle \\ &= \left\langle X(t) \right\rangle + \left\langle \sqrt{\Delta t}\xi(t) \right\rangle \\ &= \left\langle X(t) \right\rangle + \sqrt{\Delta t}\,\underbrace{\left\langle \xi(t) \right\rangle}_{=0} \\ &= \left\langle X(t) \right\rangle \\ &= M_X(t) \end{aligned}$$

Because $X(0) = 0$, we have that $\left\langle X(0) \right\rangle = 0$ and thus $M_X(0) = 0$ and also $M_X(t) = 0$

SDEs | Examples (cont.)

From $X(t+\Delta t) = X(t) + \sqrt{\Delta t}\xi(t)$, we also have

$$
\begin{aligned}
V_X(t+\Delta t) &= \left\langle \, (X(t+\Delta t) - M_X(t+\Delta t))^2 \, \right\rangle \\
&= \left\langle X(t+\Delta t)^2 \right\rangle - M_X(t+\Delta t)^2 \\
&= \left\langle X(t+\Delta t)^2 \right\rangle - \underbrace{M_X(t)^2}_{=0} \\
&= \left\langle X(t+\Delta t)^2 \right\rangle \\
&= \left\langle \, \left(X(t) + \sqrt{\Delta t}\xi(t) \right)^2 \, \right\rangle \\
&= \left\langle X(t)^2 + 2X(t)\sqrt{\Delta t}\xi(t) + \Delta t \xi(t)^2 \right\rangle \\
&= \left\langle X(t)^2 \right\rangle + 2\left\langle X(t) \right\rangle \sqrt{\Delta t} \underbrace{\left\langle \xi(t) \right\rangle}_{=0} + \Delta t \underbrace{\left\langle \xi(t)^2 \right\rangle}_{=1} \\
&= \left\langle X(t)^2 \right\rangle + \Delta t \\
&= \left\langle X(t)^2 \right\rangle - M_X(t)^2 + \Delta t \\
&= V_X(t) + \Delta t
\end{aligned}
$$

Because $X(0) = 0$, we have that $V_X(0 = 0$ and thus also $V_X(t) = 0$

SDEs | Examples (cont.)

We have that both expected value and variance of $(X(t))_{t\geq 0}$ do not depend on Δt

- It can be shown that higher-order moments are also independent of Δt

SDEs | Examples (cont.)

Example

Consider a diffusing particle whose position in time is $(X(t), Y(t), Z(t))$ for $t \geq 0$

We will show that the position at time $(t + \mathrm{d}t)$ is related to position at time t

$$X(t + \mathrm{d}t) = X(t) + (2D)^{1/2}\,\mathrm{d}W_x(t)$$
$$Y(t + \mathrm{d}t) = Y(t) + (2D)^{1/2}\,\mathrm{d}W_y(t)$$
$$Z(t + \mathrm{d}t) = Z(t) + (2D)^{1/2}\,\mathrm{d}W_z(t)$$

Quantities $\mathrm{d}W_x(t)$, $\mathrm{d}W_y(t)$, and $\mathrm{d}W_z(t)$ are increments of Brownian motions

Quantity $D = 10^{-4}$ mm^{2}sec^{-1} is the diffusion constant

Using the informal treatment, we get the associated computational definitions

$$X(t + \Delta t) = X(t) + (2D)^{1/2}\sqrt{\Delta t}\xi_x(t)$$
$$Y(t + \Delta t) = Y(t) + (2D)^{1/2}\sqrt{\Delta t}\xi_y(t)$$
$$Z(t + \Delta t) = Z(t) + (2D)^{1/2}\sqrt{\Delta t}\xi_z(t)$$

We consider an interval $\Delta t = 10^{-2}$ and initial condition $(X(0), Y(0), Z(0)) = (0, 0, 0)$

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Example

$$\mathrm{d}X(t) = f(X(t), t)\,\mathrm{d}t + g(X(t), t)\,\mathrm{d}W(t)$$

Let $f(X(t), t) = 1$ and $g(X(t), t) = 1$, we get the stochastic differential equation

$$X(t + \mathrm{d}t) = X(t) + \mathrm{d}t + \mathrm{d}W(t)$$

Using the informal treatment, we get the associated computational definition

$$X(t + \Delta t) = X(t) + \Delta t + \sqrt{\Delta t}\underbrace{\xi(t)}_{\mathcal{N}(0,1)}$$

We consider a time interval $\Delta t = 10^{-3}$ and an initial condition $X(0) = 0$

SDEs | Examples (cont.)

Let $M_X(t)$ be the expected value of $X(t)$

$$M_X(t) = \langle X(t) \rangle$$

Let $V_X(t)$ be the variance of $X(t)$

$$\begin{aligned} V_X(t) &= \left\langle \, (X(t) - M_X(t))^2 \, \right\rangle \\ &= \left\langle X(t)^2 \right\rangle - M_X(t)^2 \end{aligned}$$

From $X(t + \Delta t) = X(t) + \Delta t + \sqrt{\Delta t}\xi(t)$, we have

$$\begin{aligned} M_X(t + \Delta t) &= \left\langle X(t) + \Delta t + \sqrt{\Delta t}\xi(t) \right\rangle \\ &= \left\langle X(t) \right\rangle + \underbrace{\left\langle \Delta t \right\rangle}_{\Delta t} + \left\langle \sqrt{\Delta t}\xi(t) \right\rangle \\ &= \left\langle X(t) \right\rangle + \Delta t + \sqrt{\Delta t} \underbrace{\left\langle \xi(t) \right\rangle}_{=0} \\ &= \left\langle X(t) \right\rangle + \Delta t \\ &= M_X(t) + \Delta t \end{aligned}$$

Because $X(0) = 0$, we have that $\langle X(0) \rangle = 0$ and thus $M_X(0) = 0$ and also $M_X(t) = t$

SDEs | Examples (cont.)

From $X(t + \Delta t) = X(t) + \Delta t + \sqrt{\Delta t}\xi(t)$, we have

$$V_X(t) = t$$

The Fokker-Planck equation

Stochastic differential equations

Fokker-Planck equation

Consider a system that evolves according to an Itô stochastic differential equation

$$\mathrm{d}X(t) = f\left(X(t), t\right) + g\left(X(t), t\right)\mathrm{d}W(t)$$

We let the probability density function of the process be $p(x, t)$

The probability that $x \leq X(t) \leq x + \mathrm{d}x$ is thus $p(x, t)\mathrm{d}x$, at t

$$\int_{\Omega_x \equiv \mathbb{R}} p(x, t)\mathrm{d}x = 1$$

We can determine $p(x, t)$ empirically, after computing a large number of realisations

- The fraction of realisations that arrived at $[x, x + \Delta x]$ at $t = 1$

It is possible to determine the equation of motion for the probability density $p(x, t)$

Fokker-Planck equation (cont.)

$$\mathrm{d}X(t) = f\left(X(t), t\right) + g\left(X(t), t\right)\mathrm{d}W(t)$$

It can be shown that density $p(x, t)$ evolves according to a partial differential equation

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}\left(\frac{1}{2}g^2(x,t)p(x,t)\right) - \frac{\partial}{\partial}\left(f(x,t)p(x,t)\right)$$

This partial differential equation is the Fokker-Planck or Kolmogorov forward equation

It useful to understand the PFE as a master equation for certain process $(X(t))_{t\geq 0}$

- Any Markov processes whose individual jumps are very small
- (Sample paths of $(X(t))_{t\geq 0}$ are continuous functions of t)

Fokker-Planck equation (cont.)

$$\frac{\partial p(x,t)}{\partial t} = \underbrace{\frac{\partial^2}{\partial x^2}\left(\frac{1}{2}g^2(x,t)p(x,t)\right)}_{\text{Diffusion}} - \underbrace{\frac{\partial}{\partial}\left(f(x,t)p(x,t)\right)}_{\text{Drift}}$$

The FP/KF equation is a convection–diffusion equation for the transfer of probability

- ⇝ The first term has been called the ‘transport-’, ‘convection-’, or ‘drift-’ term
- ⇝ The second term has been called the ‘diffusion-’ or ‘fluctuation-’ term

The FPE is a continuity equation for the probability density

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial J\left(x,t\right)}{\partial x}$$

The Fickian probability flux $J\left(x,t\right)$

$$J\left(x,t\right) = f\left(x,t\right)p(x,t) - \frac{1}{2}\frac{\partial}{\partial x}\left(g\left(x,t\right)p(x,t)\right)$$

Fokker-Planck equation (cont.)

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x}$$

An equilibrium steady-state solution corresponds to the conditions

$$\frac{\partial p(x,t)}{\partial t} = 0$$
$$J(x,t) \equiv 0$$

This leads to a first-order ODE for the equilibrium density $p_{\mathrm{SS}}(x)$

$$f(x)\, p_{\mathrm{SS}}(x) - \frac{1}{2}\frac{\partial}{\partial x}\left(g(x)\, p_{\mathrm{SS}}(x)\right) = 0$$

Fokker-Planck equation (cont.)

$$\mathrm{d}X(t) = f(X(t),t) + g(X(t),t)\,\mathrm{d}W(t)$$

For the special case of $f(x,t) = 0$ and $g(x,t) = 1$, we get the differential equation

$$\mathrm{d}X(t) = \mathrm{d}W(t)$$

The associated Fokker-Planck equation is the diffusion equation

$$\frac{\partial p(x,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 p(x,t)}{\partial^2 x^2}$$

For the Fickian probability flux $J(x,t)$, we get

$$J(x,t) = -\frac{1}{2}\frac{\partial}{\partial x}(p(x,t))$$

Fokker-Planck equation (cont.)

At equilibrium, the steady-state solution for the probability density $p(x)$

$$p_{\mathrm{SS}}(x) = C \frac{1}{g^2(x)} \exp\left[\int_0^x 2 \frac{f(x')}{g^2(x')} \mathrm{d}x'\right] \qquad (C > 0)$$

Constant C is whatever number makes p_{SS} integrate to one

$$C = \left(\int_{\Omega_x \equiv \mathbb{R}} \frac{1}{g^2(x)} \exp\left[\int_0^x 2 \frac{f(x')}{g^2(x)} \mathrm{d}x'\right]\right)^{-1}$$

Fokker-Planck equation | Derivation

How to derive the equation of motion for the probability density function $p(x,t)$?

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}\left(\frac{1}{2} g^2(x,t) p(x,t)\right) - \frac{\partial}{\partial x}\left(f(x,t)p(x,t)\right)$$

We let $p(x,t|y,s)\mathrm{d}x$ be the probability that $X(t) \in [x, x+\mathrm{d}x]$, given $X(s) = y$

$$\cdots\cdots \underbrace{s \cdots t} \cdots\cdots$$

Now, we want to consider a future time $t + \Delta t$, such that $s < t < t + \Delta t$

$$\cdots\cdots \underbrace{s \cdots t} \underbrace{\cdots t + \Delta t} \cdots\cdots$$

Given $X(s) = y$, the probability that $X(t + \Delta t) \in [z, z + \Delta z]$ is $p(z, t + \Delta t|y, s)\mathrm{d}z$

Fokker-Planck equation | Derivation (cont.)

$$\cdots\cdots\underbrace{\overbrace{s}^{y}\ \cdots}\ \overbrace{t}^{X(t)}\ \underbrace{\cdots\overbrace{t+\Delta t}^{z}}\cdots\cdots$$

We are interested in the probability that X moves from y at time s, to z at $t + \Delta t$

We sum the probabilities of all possible paths through intermediate points $x(t)$

$$p(z, t + \Delta t \mid y, s) = \int_{\Omega_x} p(z, t + \Delta t \mid x, t) p(x, t \mid y, s) \mathrm{d}x$$

To derive the Fokker-Planck equation, we consider a vanishingly small Δt

Fokker-Planck equation | Derivation (cont.)

$$p(z, t + \Delta t \mid y, s) = \int_{\Omega_x} p(z, t + \Delta t \mid x, t) p(x, t \mid y, s) \mathrm{d}x$$

To proceed, we firstly multiply both sides by some smooth function $\varphi : \Omega_x \to \mathbb{R}$

$$p(z, t + \Delta t \mid y, s)\varphi(z) = \int_{\Omega_x} p(z, t + \Delta t \mid x, t)\varphi(z) p(x, t \mid y, s) \mathrm{d}x$$

The integrating over Ω_x and rearranging, we get

$$\begin{aligned}\int_{\Omega_x} p(z, t + \Delta t \mid y, s)\varphi(z)\mathrm{d}z &= \int_{\Omega_x}\int_{\Omega_x} p(z, t + \Delta t \mid x, t)\varphi(z) p(x, t \mid y, s)\mathrm{d}x\mathrm{d}z \\ &= \int_{\Omega_x}\left[\int_{\Omega_x} p(z, t + \Delta t \mid x, t)\varphi(z)\mathrm{d}z\right] p(x, t \mid y, s)\mathrm{d}x\end{aligned}$$

Fokker-Planck equation | Derivation (cont.)

Function $\varphi(\cdot)$ is chosen to be any arbitrary smooth function over the domain Ω_x

Thus, it has a Taylor's expansion about any point $z_0 \in \Omega_x$

$$\begin{aligned}\varphi(z) &= \sum_{k=0}^{\infty} \frac{1}{k!}\frac{\mathrm{d}\varphi(z)}{\mathrm{d}z}\Big|_{z=z_0}(z-z_0)^k \\ &= \varphi(z_0) + \varphi'(z_0)(z-z_0) + \frac{1}{2}\varphi''(z_0)(z-z_0)^2 + \cdots\end{aligned}$$

We expand $\varphi(\cdot)$ about point $x \in \Omega_x$ and truncate, to get

$$\varphi(z) \approx \varphi(x) + \varphi'(x)(z-x) + \frac{1}{2}\varphi''(x)(z-x)^2$$

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Fokker-Planck equation | Derivation (cont.)

Substituting, we get

$$\begin{aligned}&\int_{\Omega_x} p(x, y+\Delta t \mid y, s)\varphi(x)\mathrm{d}x \\ &= \int_{\Omega_x}\left[\int_{\Omega} p(z, t+\Delta t|x,t)\underbrace{\varphi(z)}_{\text{Taylor}}\mathrm{d}z\right]p(x,t|y,s)\mathrm{d}x \\ &= \int_{\Omega_x}\left[\int_{\Omega} p(z, t+\Delta t|x,t)\left(\varphi(x) + \varphi'(x)(z-x) + \varphi''(x)\frac{(z-x)^2}{2}\right)\mathrm{d}z\right]p(x,t|y,s)\mathrm{d}x\end{aligned}$$

Rearranging, we get

$$\begin{aligned}&\int_{\Omega_x} p(x, t+\Delta t \mid y, s)\varphi(x)\mathrm{d}x \\ &= \int_{\Omega_x}\left[\int_{\Omega_x}\varphi(x)p(z,t+\Delta t \mid x,t)\mathrm{d}z\right]p(x,t \mid y,s)\mathrm{d}x \\ &+ \int_{\Omega_x}\left[\int_{\Omega_x}\varphi'(x)(z-x)p(z,t+\Delta t \mid x,t)\mathrm{d}z\right]p(x,t \mid y,s)\mathrm{d}x \\ &+ \int_{\Omega_x}\left[\int_{\Omega_x}\varphi''(x)\frac{(z-x)^2}{2}p(z,t+\Delta t \mid x,t)\mathrm{d}z\right]p(x,t \mid y,s)\mathrm{d}x\end{aligned}$$

Fokker-Planck equation | Derivation (cont.)

Further rearranging terms, we get

$$
\begin{aligned}
&\int_{\Omega_x} p(x, t+\Delta t \mid y, s)\varphi(x)\mathrm{d}x \\
&= \int_{\Omega_x} \left[\varphi(x) \int_{\Omega_x} p(z, t+\Delta t \mid x, t)\mathrm{d}z\right] p(x, t \mid y, s)\mathrm{d}x \\
&+ \int_{\Omega_x} \left[\varphi'(x) \int_{\Omega_x} (z-x)p(z, t+\Delta t \mid x, t)\mathrm{d}z\right] p(x, t \mid y, s)\mathrm{d}x \\
&+ \int_{\Omega_x} \left[\frac{1}{2}\varphi''(x) \int_{\Omega_x} (z-x)^2 p(z, t+\Delta t \mid x, t)\mathrm{d}z\right] p(x, t \mid y, s)\mathrm{d}x
\end{aligned}
$$

We recognise the following identity,

$$\int_{\Omega_x} p(z, t+\Delta t \mid x, t)\mathrm{d}z = 1$$

Fokker-Planck equation | Derivation (cont.)

$$
\begin{aligned}
&\int_{\Omega_x} p(x, t+\Delta t \mid y, s)\varphi(x)\mathrm{d}x \\
&= \int_{\Omega_x} \left[\varphi(x) \underbrace{\int_{\Omega_x} p(z, t+\Delta t \mid x, t)\mathrm{d}z}_{=1}\right] p(x, t \mid y, s)\mathrm{d}x \\
&+ \int_{\Omega_x} \left[\varphi'(x) \int_{\Omega_x} (z-x)p(z, t+\Delta t \mid x, t)\mathrm{d}z\right] p(x, t \mid y, s)\mathrm{d}x \\
&+ \int_{\Omega_x} \left[\frac{1}{2}\varphi''(x) \int_{\Omega_x} (z-x)^2 p(z, t+\Delta t \mid x, t)\mathrm{d}z\right] p(x, t \mid y, s)\mathrm{d}x
\end{aligned}
$$

We also recognise another identity,

$$\int_{\Omega_x} (z-x)p(z, t+\Delta t \mid x, t)\mathrm{d}z = \langle X(t+\Delta t) - \underbrace{x(t)}_{z} \rangle$$

We need the expected displacement,

$$X(t+\Delta t) - x(t) = \Delta x(t)$$

Fokker-Planck equation | Derivation (cont.)

Using the Itô stochastic differential equation, we get

$$\underbrace{X(t+\Delta t) - x(t)}_{\Delta x(t)} = f\left(x(t), t\right)\Delta t + g\left(x(t), t\right)\Delta W(t)$$

For the expected displacement, we get

$$\begin{aligned}\left\langle \Delta x(t) \right\rangle &= \left\langle f\left(x(t), t\right)\Delta t + g\left(x(t), t\right)\Delta W(t) \right\rangle \\ &= \left\langle f\left(x(t), t\right)\Delta t \right\rangle + \underbrace{\left\langle g\left(x(t), t\right) \underbrace{\Delta W(t)}_{\sqrt{\Delta t}\xi(t)} \right\rangle}_{g(x(t),t)\times 0} \\ &= f\left(x(t), t\right)\Delta t\end{aligned}$$

Thus, for the integral we have

$$\int_{\Omega_x} (z-x) p(z, t+\Delta t \mid x, t) \mathrm{d}z = f\left(x(t), t\right)\Delta t$$

Fokker-Planck equation | Derivation (cont.)

$$\begin{aligned}&\int_{\Omega_x} p(x, t+\Delta t \mid y, s)\varphi(x)\mathrm{d}x \\ &= \int_{\Omega_x} \left[\varphi(x) \underbrace{\int_{\Omega_x} p(z, t+\Delta t \mid x, t)\mathrm{d}z}_{=1}\right] p(x, t \mid y, s)\mathrm{d}x \\ &+ \int_{\Omega_x} \left[\varphi'(x) \underbrace{\int_{\Omega_x} (z-x) p(z, t+\Delta t \mid x, t)\mathrm{d}z}_{=f(x(t),t)\Delta t}\right] p(x, t \mid y, s)\mathrm{d}x \\ &+ \int_{\Omega_x} \left[\frac{1}{2}\varphi''(x) \int_{\Omega_x} (z-x)^2 p(z, t+\Delta t \mid x, t)\mathrm{d}z\right] p(x, t \mid y, s)\mathrm{d}x\end{aligned}$$

We recognise one last identity for the squared displacement

$$\int_{\Omega_x} (z-x)^2 p(z, t+\Delta t \mid x, t)\mathrm{d}z = \left\langle \left(X(t+\Delta t) - \underbrace{x(t)}_{z} \right)^2 \right\rangle$$

Fokker-Planck equation | Derivation (cont.)

Using again the stochastic differential equation, we have

$$\underbrace{X(t+\Delta t) - x(t)}_{\Delta x(t)} = f(x(t),t)\,\Delta t + g(x(t),t)\,\Delta W(t)$$

For the expected squared displacement, we get

$$\begin{aligned}\langle(\Delta x(t))^2\rangle &= \left\langle \left(f(x(t),t)\,\Delta t + g(x(t),t)\,\Delta W(t)\right)^2 \right\rangle \\ &= \underbrace{\left\langle (f(x(t),t)\,\Delta t)^2 \right\rangle}_{f(x(t),t)^2\Delta t^2} + \underbrace{\left\langle (2f(x(t),t)\,\Delta t)\left(g(x(t),t)\,\underbrace{\Delta W(t)}_{\sqrt{\Delta t}\xi(t)}\right)\right\rangle}_{2f(x(t),t)g(x(t),t)\Delta t^{3/2}\times 1} \\ &\quad + \underbrace{\left\langle (g(x(t),t)\,\Delta W(t))^2 \right\rangle}_{g(x(t),t)^2\times\Delta t\times 1} \\ &= g(x(t),t)^2\,\Delta t + \mathcal{O}(\Delta t^2)\end{aligned}$$

Thus, for the integral we have

$$\int_{\Omega_x} (z-x)^2 p(z,t+\Delta t \mid x,t)\mathrm{d}z = g(x(t),t)^2\,\Delta t$$

Fokker-Planck equation | Derivation (cont.)

$$\begin{aligned}&\int_{\Omega_x} p(x,t+\Delta t \mid y,s)\varphi(x)\mathrm{d}x \\ &= \int_{\Omega_x}\left[\varphi(x)\underbrace{\int_{\Omega_x} p(z,t+\Delta t \mid x,t)\mathrm{d}z}_{=1}\right] p(x,t \mid y,s)\mathrm{d}x \\ &+ \int_{\Omega_x}\left[\varphi'(x)\underbrace{\int_{\Omega_x} (z-x)p(z,t+\Delta t \mid x,t)\mathrm{d}z}_{=f(x(t),t)\Delta t}\right] p(x,t \mid y,s)\mathrm{d}x \\ &+ \int_{\Omega_x}\left[\frac{1}{2}\varphi''(x)\underbrace{\int_{\Omega_x} (z-x)^2 p(z,t+\Delta t \mid x,t)\mathrm{d}z}_{=g(x(t),t)^2\Delta t}\right] p(x,t \mid y,s)\mathrm{d}x\end{aligned}$$

Fokker-Planck equation | Derivation (cont.)

After substituting those integrals, we get

$$\int_{\Omega_x} p(x, t+\Delta t \mid y, s)\varphi(x)\mathrm{d}x = \int_{\Omega_x} [\varphi(x)1]\, p(x, t \mid y, s)\mathrm{d}x + \int_{\Omega_x} [\varphi'(x) f\,(x(t), t)\, \Delta t]\, p(x, t \mid y, s)\mathrm{d}x + \int_{\Omega_x} \left[\frac{1}{2}\varphi''(x) g\,(x(t), t)^2\, \Delta t\right] p(x, t \mid y, s)\mathrm{d}x$$

After some manipulations, we get

$$\int_{\Omega_x} p(x, t+\Delta t \mid y, s)\varphi(x)\mathrm{d}x = \int_{\Omega_x} p(x, t \mid y, s)\varphi(x)\mathrm{d}x + \Delta t \int_{\Omega_x} \varphi'(x) f\,(x(t), t) p(x, t \mid y, s)\mathrm{d}x + \Delta t \int_{\Omega_x} \left[\frac{1}{2}\varphi''(x) g\,(x(t), t)^2\right] p(x, t \mid y, s)\mathrm{d}x$$

Fokker-Planck equation | Derivation (cont.)

Reordering some terms, we get

$$\int_{\Omega_x} \frac{p(x, t+\Delta t \mid y, s) - p(x, t \mid y, s)}{\Delta t}\varphi(x)\mathrm{d}x = \int_{\Omega_x} \varphi'(x) f\,(x,)\, p(x, t \mid y, s)\mathrm{d}x + \int_{\Omega_x} \varphi''(x)\frac{g\,(x, t)^2}{2} p(x, t \mid y, s)\mathrm{d}x$$

Then, integrating by parts

$$\int_{\Omega_x} \frac{p(x, t+\Delta t \mid y, s) - p(x, t \mid y, s)}{\Delta t}\varphi(x)\mathrm{d}x = - \int_{\Omega_x} \varphi(x)\frac{\partial}{\partial x}\left(f(x, t) p(x, t \mid y, s)\right)\mathrm{d}x + \int_{\Omega_x} \varphi(x)\frac{\partial^2}{\partial x^2}\left(\frac{g(x, t)^2}{2} p(x, t \mid y, s)\right)\mathrm{d}x$$

Fokker-Planck equation | Derivation (cont.)

Collecting terms and joining the integrals, we get

$$0 = \int_{\Omega_x} \varphi(x) \times \{-\frac{p(x, t + \Delta t \mid y, s) - p(x, t \mid y, s)}{\Delta t} - \frac{\partial}{\partial x}\left(f(x, y)p(x, t \mid y, s)\right) + \frac{\partial^2}{\partial x^2}\left(\frac{g(x, t)^2}{2} p(x, t \mid y, s)\right) \mathrm{d}x\}$$

As the function $\varphi(\cdot)$ is arbitrary (non-zero), the term within brackets must be zero

$$\frac{p(x, t + \Delta t \mid y, s) - p(x, t \mid y, s)}{\Delta t} = \frac{\partial^2}{\partial x^2}\left(\frac{g(x, t)^2}{2} p(x, t \mid y, s)\right) - \frac{\partial}{\partial x}\left(f(x, t)p(x, t \mid y, s)\right)$$

Taking the limit $\Delta t \to 0$, we obtain the Fokker-Planck equation

$$\frac{\partial}{\partial t} p(x, t \mid y, s) = \frac{\partial^2}{\partial x^2}\left(\frac{g(x, t)}{2} p(x, t \mid y, s)\right) - \frac{\partial}{\partial x}\left(f(x, t)p(x, t \mid y, s)\right)$$