Diffusion processes

Consider the motion of a Brownian walker, e.g., a colloidal particle suspended in a fluid. The particle is being bombarded by lots of collisions with the solvent molecules:

\[ m \left[ v(t+\Delta t) - v(t) \right] = \int_{t'=t}^{t+\Delta t} F_{\text{ext}}(r(t')) \, dt + \sum_{\text{collisions}} \Delta p_i \]

We could do MCMC to simulate this, but there will be lots of transitions (collisions) to process. Can we approximate?
Assume that the dynamics of a system follows a continuous time continuous space Markov chain, without jumps. This means that we can define moments of the local dynamics over a short interval $\Delta t$: 

$$M_1 = \langle x(t+\Delta t) - x(t) \rangle = \langle \Delta x \rangle$$

$$M_2 = \langle [x(t+\Delta t) - x(t)]^2 \rangle = \langle \Delta x^2 \rangle$$

i.e. mean displacement and mean square displacement.
More generally,

\[ M_n(t; x_0, t_0) = \left< (x-x_0)^n \right> \]

\[ = \int (x-x_0)^n \, P(x, t \mid x_0, t_0) \, dx \]

\[ \uparrow \]

transition probability

The moments fully define \( P(x, t \mid x_0, t_0) \)

specifically

\[ P(x, t \mid x_0, t_0) = \sum_{n=0}^{\alpha} \frac{(-1)^n}{n!} \, M_n \, \frac{\partial^n}{\partial x^n} \, \delta(x-x_0) \]

\[ \uparrow \]

formal moment expansion (moments match on two sides)
For small time intervals

\[ M_n(\Delta t) = n! \cdot D \cdot \Delta t + \text{terms of order higher than linear} \]

Then

\[ \frac{\partial P(x,t)}{\partial t} = \sum_{n=0}^{\infty} (-1)^n \frac{a^n}{2 \pi x^n} \left[ D(x,t) P(x,t) \right] \]

**Proof:**

\[ P(x,t+\Delta t) = \int P(x,t+\Delta t | x',t) P(x',t) \, dx' \]

and then integrate by parts.
Pawula theorem: Either all terms have to be included or only the first two!

\[
\frac{\partial P(x,t)}{\partial t} = - \frac{\partial}{\partial x} \left[ A(x) P(x,t) \right] + \frac{\partial^2}{\partial x^2} \left[ B(x) P(x,t) \right]
\]

\text{Fokker-Planck equation}

Recall \( A(x) \cdot \Delta t = \langle \Delta x \rangle \cdot \Delta t = \langle \Delta x^2 \rangle \) (velocity) \[2B(x) \cdot \Delta t = \langle \Delta x^2 \rangle \) (diffusion)
The Fokker-Planck equation is the extension of the Master equation to diffusion processes, which are the limit where transitions are very small (local) jumps.

Multi variable generalization:

\[ \frac{\partial P(x,t)}{\partial t} = - \sum_{x_i} \frac{\partial}{\partial x_i} \left[ A_{ij}(x) P(x,t) \right] \]

\[ + \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} \left[ B_{ij}(x) P(x,t) \right] \]

\[ \langle \Delta x_i \Delta x_j \rangle = 2 B_{ij} \Delta t \]
If one looks at a small interval $\Delta t$ over which $A$ and $B$ are held fixed at their initial values, then $P(x, t+\Delta t)$ is a Gaussian centered around $x_0 + A \cdot \Delta t$ with covariance matrix $2B \Delta t$.

In one dimension, this gives for $A=0$ Brownian motion, or the Wiener process, $X(t)$.
This suggests the following numerical scheme or approximation:

\[ X(t + \Delta t) = X(t) + A \left[ X(t), t \right] \Delta t + \]

\[ + (2BA\Delta t)^{1/2} \cdot N(0,1) \]

Denote \( \sim \)

\[ W(t) \equiv N(0,1) \]

Going back to the Brownian walker:

\[ m \left[ \frac{\theta(t + \Delta t) - \theta(t)}{\Delta t} \right] \sim F[\theta(t)] \Delta t \cdot W(t) \]

\[ \Gamma(t + \Delta t) = \Gamma(t) + \theta(t) \cdot \Delta t \]
In the limit $\alpha \to 0$, this gives rise to a stochastic differential equation

$$
\dot{x}(t) = \alpha \left[ x(t) \right] + \beta \left[ x(t) \right] W(t)
$$

where $W(t)$ formally denotes the time derivative of Brownian motion (does not exist classically), and is termed white noise. It is a Gaussian process with mean and covariance

$$
\begin{align*}
\langle W_i(t) \rangle &= 0 \\
\langle W_i(t) W_j(t') \rangle &= \delta(t-t')
\end{align*}
$$

\textit{Dirac "function" (distribution)}
Stochastic differential equations are often written in differential form to avoid derivatives of the nowhere differentiable white noise:

\[ d\hat{x}(t) = a[\hat{x}(t)] \, dt + \theta [\hat{x}(t)] \, dB_{\text{Brownian motion}}(t) \]

But physicists will usually write it as a differential equation.

In math, \( W(t) \) often denotes a Wiener process and \( \hat{W}(t) \) denotes white noise, so watch out for notation.
A. Donev

What we have so far is an Ito differential equation, which means that

\[ \dot{x} = a(x,t) + \mathcal{B}(x,t) \, \mathcal{W}(t) \]

is the limit as \( \Delta t \to 0 \) of the Euler–Maruyama numerical method

\[ x(t + \Delta t) = x(t) + a[x(t),t] \, \Delta t \]

\[ + \mathcal{B}[x(t),t] \, \sqrt{\Delta t} \cdot \mathcal{N}(0,1) \]

"discrete" while noise denote as

\[ \left( \frac{\mathcal{W}}{\sqrt{\Delta t}} \right) \cdot \Delta t \]
Recall that the Fokker–Planck equation associated with this Itô equation is

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

Itô here refers to the convention that the noise covariance is evaluated at the beginning of a timestep, keeping the Markov character (non-anticipatory).
Its calculus does not, however, follow
the ordinary rules of calculus, notably,
the chain rule.

For example, what SODE does
\[ f \left( x(t) \right) \] follow? Ordinary calculus
would say
\[ \dot{x} = f' \cdot x = f' \left[ a + b W \right], \]
but in fact because of the \( \sqrt{dt} \) one
must keep second order terms in
the Taylor expansion for the
noise terms.
Drift for \( t [x(t)] \)

\[
\begin{align*}
\langle t [x(t + \Delta t)] - t [x(t)] \rangle &= \\
&= \langle t' [x(t)] \Delta x + \frac{1}{2} t'' [x(t)] \Delta x^2 + O(\Delta x^3) \rangle \\
&= t' \langle a \Delta t + b \Delta \sqrt{t} \rangle + O(\Delta t) \\
&\quad + \frac{1}{2} t'' \langle b^2 \Delta t \widetilde{W}^2 \rangle \\
&= (t' a + \frac{1}{2} t'' b^2) \Delta t
\end{align*}
\]

extra or "spurious" drift
2) Diffusion for $t \{ x(t) \}$:

$$
\left\langle \left[ f(t + \Delta t) - f(t) \right]^2 \right\rangle = (f')^2 \left\langle \mathcal{E}^2 \Delta t \right\rangle
$$

new diffusion coefficient

In summary, the SODE for $t \{ x(t) \}$ is:

$$
\dot{f} \{ x(t) \} = (a f' + \frac{b^2}{2} f''\dot{f}) + b f' \dot{W}(t)
$$

This is one version of "Ito's" formula
Now, what if we had interpreted the SDE

\[ \dot{x} = a(x, t) + b(x, t) \cdot W(t) \]

in the Stratonovich sense, meaning, we used a midpoint rule to integrate the stochastic term:

\[ x(t + \Delta t) = x(t) + a \left[ x(t), t \right] \Delta t + b \left[ \frac{x(t + \Delta t) + x(t)}{2}, t + \frac{\Delta t}{2} \right] \sqrt{\Delta t} \]

Ignore dependence on time.

\[ b \left[ x(t) \right] + \frac{1}{2} b \cdot \Delta x \]
Look now at the drift of the new Stratonovich interpretation:

\[
\langle x(t+\Delta t) - x(t) \rangle = \alpha \langle x(t) \rangle \Delta t \\
+ \langle \frac{1}{2} \beta' \Delta x \tilde{W} \sqrt{\Delta t} \rangle
\]

But note that

\[
\text{extra drift} = \langle \frac{1}{2} \beta' (\alpha \Delta t + \beta \tilde{W} \sqrt{\Delta t}) \tilde{W} \sqrt{\Delta t} \rangle \\
+ \mathcal{O}(\Delta t)
\]

\[= \frac{1}{2} \beta' \beta \Delta t\]

The extra terms only appear in the drift.
Yet another, less common in math, but very important for Langevin equations, is a non-

ito interpretation, which means we use a backward Euler implicit method:

\[ x(t + \Delta t) = x(t) + a [x(t)] \Delta t + b [x(t + \Delta t)] \dot{w} \sqrt{\Delta t} \]

giving extra drift \( b' \Delta t \)

explicit integrator "Fixman" method

\[ \begin{cases} \dot{x} = x(t) + a [x(t)] \Delta t + b [x(t)] \dot{w} \sqrt{\Delta t} \\ x(t + \Delta t) = x(t) + a [x(t)] \Delta t + b [\hat{\dot{x}}] \dot{w} \sqrt{\Delta t} \end{cases} \]
Therefore, the Stratonovich equation

\[ x = a(x) + \mathbf{b}(x) \circ W(t) \]

is equivalent to the Itô equation:

\[ x = [a(x) + \frac{1}{2} \mathbf{b} \mathbf{b}'] + \mathbf{b}(x) \cdot W(t) \]

Similarly, if we had adopted a non-Itô interpretation, we would have obtained

\[ x = [a(x) + \mathbf{b} \mathbf{b}'] + \mathbf{b}(x) \cdot W(t) \]

Observe: if \( \mathbf{b}(x) = \mathbf{b}_0 = \text{const} \) then all interpretations are equivalent.
The Stratonovich interpretation follows the rules of ordinary calculus and can be seen as the limit of smooth noise with a very short correlation time (so more physical).

So, the Stratonovich SDE for $f[X(t)]$ is:

$$\dot{f} = a f' + (b f') \cdot \mathcal{W}(t)$$

To see this, rewrite as $I_t$ to via

$$\frac{d(e f')}{df} = e' + e \frac{f''}{f'} \Rightarrow \frac{1}{2} (b f') \frac{1}{dt} (b f') = \left( \frac{1}{2} b e' \right) f' + \left( \frac{1}{2} e \right)^2 f'$$
therefore the Ito equation for $f(x(t))$ is

$$\dot{f} = \left[ a \dot{f} + \frac{1}{2} \sigma \sigma' \sigma f' \right] + \frac{\sigma^2}{2} f'' + (f + \sigma') \cdot W(t)$$

which is indeed the transformed version of the Ito equation

$$x = \left[ a + \frac{1}{2} \sigma \sigma' \right] t + \sigma \cdot W(t)$$

as we derived earlier.

The non-Ito or anti-Ito interpretation will become important when looking at overdamped Langevin equations (Brownian dynamics).