Ito calculus of diffusion — two-page-tutorial

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For those who know nothing about the Ito differential calculus (i.e., Langevin's approach extended for space-dependent diffusion/drift coefficients), a quick guide is offered from classical bases even until a Schrödinger-Ito equation.

I. WIENER STOCHASTIC PROCESSES

We call x_t a stochastic process if x is a function of time t and for each t the value x_t is a stochastic (i.e. random) variable. The process x_t is Markovian if the probability distribution of $x_{t+\Delta t}$ for all *positive* Δt depends on the current value x_t and does not depend on the previous values $x_s; s < t$. All the Ito stuff is about the non-linear Wiener (diffusion) processes which form an important sub-class of Markovian processes.

Consider $\Delta x_t = x_{t+\Delta t} - x_t$ (recall $\Delta t > 0$) and suppose that

$$\lim_{\Delta t \to +0} \mathrm{M}[\Delta x_t/\Delta t] = V_t(x_t) ,$$

$$\lim_{\Delta t \to +0} \mathrm{M}[(\Delta x_t)^2/\Delta t] = 2D_t(x_t) ,$$

$$\lim_{\Delta t \to +0} \mathrm{M}[(\Delta x_t)^n/\Delta t] = 0, \quad n > 2 .$$

where M stands for stochastic mean. Then x_t is a generalized Wiener (or diffusion) process which is determined by two functions: V_t is the drift and D_t is the diffusion.

The standard Wiener process W_t is a stationary stochastic process of zero drift and 'unit' diffusion: $V_t = 0$ and $D_t = 1/2$. Its formal time-derivative is the standard white-noise w_t:

$$dW_t/dt = w_t, \qquad \mathrm{M}[w_t] = 0, \quad \mathrm{M}[w_t w_s] = \delta(t-s) .$$

Technically, there are many equivalent tools to treat Wiener processes. Our choice may depend on the details of the task. The traditional tool is Fokker-Planck partial differential equations, its perfect alternative is Ito stochastic differential equations. These tools are time-local. We dont learn about but mention the integral methods that are based on functional probability distributions, also called path integrals in physics, whose perfect equivalent is Ito stochastic integral calculus.

II. CLASSICAL FOKKER-PLANCK VS ITO-LANGEVIN

Given a stochastic process x_t, we introduce the normalized probability density $\rho_t(x)$ of x_t at a given time t:

$$\rho_t(x) = \mathrm{M}[\delta(x - x_t)] .$$

For its time-derivative, using Taylor expansion and the definitive eqs. of our Wiener process, we obtain the Fokker-Planck eq. (FPE):

$$\frac{d\rho}{dt} = (D\rho)'' - (V\rho)' .$$

If, the other way around, we start from this FPE, we arrive at the less familiar notion of the Ito stochastic eqs. through the widely known Langevin eqs. There is a further pedagogical hint for those of Monte Carlo (MC) numeric experience: they know that the solutions of the FPE can be MC-simulated via the random trajectories x_t. If D and V are independent of x, the trajectories are governed by the linear Langevin eq.

$$\frac{dx}{dt} = V + \sqrt{2D}w .$$

In the general case, the above naive Langevin eq. does not work (some MC experts and some theoreticians are aware of it). One must learn the Ito-Langevin eq. which uses the notion of the Ito differential dx. This latter is defined as the r.h.s.-differential of the process x, i.e.:

$$dx_t = \lim_{\Delta t \to \text{infinitesimal}} (x_{t+\Delta t} - x_t), \qquad \Delta t > 0 ,$$

to the contrary of the Stratonowitch differential which is the symmetric differential (i.e.: limes of $x_{t+\Delta t/2} - x_{t-\Delta t/2}$) or to the common differential which assumes x_t is smooth — that's not true for Wiener x_t. From now on, all differentials denote Ito differentials. The standard Wiener process satisfies the rules:

$$\mathrm{M}[dW] = 0, \qquad (dW)^2 = dt, \quad (dW)^n = 0 \ \ for\ n > 2 .$$

Observe(!!!): the first identity is valid in mean, all the others are valid without the mean, i.e., in a stronger sense. Don't ask why, just do it! There are favorable properties like

$$\mathrm{M}[WdW] = 0 .$$

The reason of this identity is that the r.h.s.-differential dW_t is independent of W_t.

Each generalized Wiener process satisfies the Ito-Langevin eq.:

$$dx = Vdt + \sqrt{2D}dW .$$

This eq. is equivalent with the FPE and can be directly used for MC-generating the trajectories x: you generate the random process W while the Ito differentials dW, dx are approximated by the numeric increments between the present and the next time-step. Ito favors numerics!

While all generalized Wiener processes are of the above standard 'W-driven' form, it is crucial to know that we can eliminate the auxiliary noise W from the Ito eq. if we just write:

$$\mathrm{M}[dx] = Vdt, \quad (dx)^2 = 2Ddt \ ,$$

while higher powers of dx are always zero. Any given Wiener process x is fully characterized by the above two Ito eqs. which are equivalent with the previous single W-driven eq. as well as with the FPE.

Notes and Exercises

Vector valued Wiener process.— If x is a vector then D becomes nonnegative matrix and V becomes vector. The process is defined by the Ito eqs.:

$$\mathrm{M}[dx_n] = V_n dt, \quad dx_n dx_m = 2D_{nm} dt \ ,$$

or, equivalently, through the W-driven eqs.:

$$dx_n = V_n dt + \sqrt{2}(D^{1/2})_{nm} dW_m \ ,$$

where the Einstein convention of index-summation is understood and W_n are independent standard Wiener processes satisfying $\mathrm{M}[dW_n] = 0$, $dW_n dW_m = \delta_{nm} dt$. Of course, the FPE is also valid and can be used alternatively to the Ito eqs.:

$$\frac{d\rho}{dt} = \partial_n \partial_m (D_{nm}\rho) - \partial_n (V_n \rho) \ .$$

Later you must get accostumed to the abstract notation (i.e., without the vector and matrix indices). You also need to accept (or inspect for yourself) the same structure of eqs. with complex valued vectors, where, e.g. $x = |\psi\rangle_t$.

Transformation of variables.— Suppose $f(x)$ is a smooth function. Then $y = f(x)$ is also a generalized Wiener process hence y must satisfy the same form of Ito eq. as x, with some other diffusion G and drift U:

$$dy = Udt + \sqrt{2G} dW$$

where, and this is the point:

$$dy = df = dxf' + \frac{1}{2}(dx)^2 f'' = (Vdt + \sqrt{2D}dW)f' + Ddtf''$$

leading to $G = D(f')^2$ and $U = Vf' + Df''$. Observe(!!!): Exact Taylor expansion in Ito differential dx needs zeroth, first and second order terms where the latter ones are always proportional to dt hence never contribute to diffusion but to drift.

Exercise: Change the variable x of the FPE for $y = f(x)$ and inspect that the new diffusion and drift are the above G, U, resp.

Ito-corrected Leibniz rule.— Suppose x and y are any two (maybe correlated) Wiener processes. Then, by Taylor expansion of xy, we get:

$$d(xy) = xdy + ydx + dxdy \ ,$$

where the third term on the r.h.s. is the Ito correction with respect to the common Leibniz rule.

The bonus of Ito.— Prove that

$$\mathrm{M}[xdy] = \mathrm{M}[x]\mathrm{M}[dy] \ .$$

This compensates us for the brake-down of the usual Leibniz rule. (For Stratonowitch differentials, Leibniz rule is maintained and $\mathrm{M}[xdy]$ needs the 'Stratonowitch correction'.)

Your first Schrödinger-Ito eq.— The naive Schrödinger eq. of an electronic spin state $|\psi\rangle_t$ in white-noise external magnetic field $H_z(t) = 2w_t$ would be $d|\psi\rangle_t/dt = -iw_t\hat{\sigma}_z|\psi\rangle_t$. Realize that you are in trouble to preserve the norm of the state. Turn to the Ito calculus and start from:

$$|\psi\rangle_{t+dt} = exp\left[-i\hat{\sigma}_z dW_t\right]|\psi\rangle_t \ ,$$

expressing the same dynamics.

Exercise: Using Taylor expansion, derive the Ito-Schrödinger eq. $d|\psi\rangle_t = \ldots$. Then prove that it preserves the norm, i.e., calculate the Ito differential $d[{}_t\langle\psi|\psi\rangle_t]$ and show it vanishes identically. Moreover, you should derive the Ito-von-Neumann eq., too, which is the same as the Ito-Schrödinger just expressed for the pure state projector $\hat{P}_t = |\psi\rangle_t\,{}_t\langle\psi|$.