THE COVARIANT LANGEVIN EQUATION OF DIFFUSION ON RIEMANNIAN MANIFOLDS

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The covariant form of the multivariable diffusion-drift process is described by the covariant Fokker–Planck equation using the standard toolbox of Riemann geometry. The covariant form of the adapted Langevin stochastic differential equation is long sought after in both physics and mathematics. We show that the simplest covariant Stratonovich stochastic differential equation depending on the local orthogonal frame (cf. vielbein) becomes the desired covariant Langevin equation provided we impose an additional covariant constraint: the vectors of the frame must be divergence-free.

Keywords: Fokker–Planck equation, stochastic differential equation, Riemann geometry.

1. Introduction

Differential geometric studies of stochastic differential equations (SDEs) of diffusion go back to Dynkin [1] and Ito [2]. Diffusion on Riemannian manifolds described by the Fokker–Planck equation (FPE) and the celebrated Eells–Elworthy–Malliavin construction [3–5] yields the adapted diffeomorphism invariant stochastic process. But its 'canonical' SDE (i.e. covariant in local coordinates) is notoriously missing. In physics, Graham studied diffeomorphism invariant diffusion on the thermodynamic state space in seminal papers [6–9], searching in vain for the covariant Langevin SDE. The need for a solution has recently re-emerged in the theory of hybrid classical-quantum dynamics [10, 11]. Our work finds a simple construction of the covariant Langevin SDE adapted to the covariant FPE and we conjecture that it is the missing 'canonical' SDE.

Differently from the typical mathematical literature which defines the Riemannian manifold first and introduces the natural diffusion equation on it, here we define the diffusion equation on a manifold first and impose the natural Riemannian structure afterwards. Accordingly, Section 2 recapitulates the usual FPEs and Langevin SDEs first, then Section 3 adds the Riemannian structure and transforms the FPE and SDE into their equivalent covariant forms, utilizing our finding: a mandatory covariant constraint on the Langevin SDE's covariant parameters. Comparisons with previous mathematical works are postponed to Section 4, also containing our conclusions.

2. Fokker–Planck vs Langevin equation

The most common irreversible phenomena in physics are diffusive ones, modelled mathematically by the FPE. If $P(x)$ is the normalized probability distribution of an abstract particle of coordinates $x = (x^1, x^2, \ldots, x^n)$ then the FPE reads [12]

$$\frac{\partial P}{\partial t} = \tfrac{1}{2}\big(g^{ab}P\big)_{,ab} - \big(\widetilde{V}^a P\big)_{,a}. \tag{1}$$

Here $g^{ab}(x)$ is the positive diffusion matrix and $\widetilde{V}^a(x)$ is the drift, defined respectively by the expectation value of diffusion and velocity if the particle is at the position x,

$$g^{ab}(x) = \frac{d}{dt}\langle x^a x^b\rangle_{P(z)=\delta(z-x)}, \tag{2}$$

$$\widetilde{V}^a(x) = \frac{d}{dt}\langle x^a\rangle_{P(z)=\delta(z-x)}. \tag{3}$$

With one eye on forthcoming considerations of covariance, we use the formalism of general relativity: summation of identical labels is understood, partial derivatives $\partial/\partial x^a$ are denoted by lower label a with the comma.

The same diffusive phenomena can alternatively be represented by the adapted stochastic processes x_t satisfying Langevin SDEs. The equivalence between the FPE and the SDE means the following relationship,

$$P_t(x) = \big\langle \delta(x - x_t)\big\rangle, \tag{4}$$

where $\langle \ldots \rangle$ stands for averaging over the stochastic x_t. With n independent Wiener processes W^A, the Ito form of the Langevin SDE of x_t is the following [12],

$$dx^a = e^a_A dW^A + \widetilde{V}^a dt. \tag{5}$$

Summation from 1 to n over repeated labels A is understood and the matrices $e^a_A(x)$ satisfy

$$\delta^{AB} e^a_A e^b_B = g^{ab}. \tag{6}$$

This condition allows for a local orthogonal gauge-freedom,

$$e^a_A \Rightarrow O^B_A e^a_B \tag{7}$$

with orthogonal matrices $O^B_A(x)$. The form of the SDE (5) is gauge-dependent but the stochastic process x_t is unique.

Using the method e.g. in [10], we verify the relationship (4). Suppose it holds at time t, then we have to show that $dP_t(x) = \langle d\delta(x - x_t)\rangle$ is satisfied if the l.h.s. is given by the FPE (1) and the r.h.s. is given by the SDE (5).

Let us workout the r.h.s.,

$$
\begin{aligned}
\frac{1}{dt}\langle d\delta(x-x_t)\rangle &= \frac{1}{dt}\langle -\delta_{,a}(x-x_t)dx_t^a + \tfrac{1}{2}\delta_{,ab}(x-x_t)dx_t^a dx_t^b\rangle \\
&= \langle -\delta_{,a}(x-x_t)\widetilde{V}^a(x_t) + \tfrac{1}{2}\delta_{,ab}(x-x_t)g^{ab}(x_t)\rangle \\
&= -\big(\langle\delta(x-x_t)\rangle\widetilde{V}^a(x)\big)_{,a} + \tfrac{1}{2}\big(\langle\delta(x-x_t)\rangle g^{ab}(x)\big)_{,ab} \\
&= -\big(P(x)\widetilde{V}^a(x)\big)_{,a} + \tfrac{1}{2}\big(P(x)g^{ab}(x)\big)_{,ab}.
\end{aligned} \tag{8}
$$

First we calculated $d\delta(x-x_t)$ with the Ito correction, then inserted dx^a from the SDE (5). Next, we moved derivations in front of the expressions so that we could replace the argument x_t of both $\widetilde{V}^a$ and of g^{ab} by x, thanks to the δ-function. Finally, we inserted our initial assumption that (4) holds at t. The result coincides with $dP_t(x)/dt$ calculated from the FPE (1).

3. Covariance

Neither the FPE (1) nor the Ito–Langevin SDE (5) are covariant under general transformations of the coordinates x^a. The common reason of their non-covariance is the non-covariance of the drift vector (3). For example, if the velocity $\widetilde{V}^a$ vanishes in Euclidean coordinates it becomes nonzero in curvilinear ones.

The desired covariant FPE is easily achieved. We borrow the toolbox of Riemann geometry well known from general relativity [13]. Accordingly, we impose a Riemann geometry structure on the manifold of coordinates x by identifying the diffusion matrix g^{ab} with the contravariant metric tensor and we introduce the scalar probability density $\rho = P/\sqrt{g}$ of covariant normalization

$$\int \rho(x)\sqrt{g}dx = 1. \tag{9}$$

The covariant form of the FPE (1) follows,

$$\frac{d\rho}{dt} = \tfrac{1}{2}g^{ab}\rho_{;ab} - (V^a\rho)_{;a}, \tag{10}$$

where semicolons denote covariant derivatives and V^a is the co(ntra)variant drift

$$V^a = \widetilde{V}^a - \frac{1}{2\sqrt{g}}(\sqrt{g}g^{ab})_{,b}. \tag{11}$$

As a price of its covariance, this velocity *parameter* is different from the *true* but noncovariant drift velocity $\widetilde{V}^a$ defined by (3).

Now we propose the covariant Langevin equation. The matrix e_A^a, introduced for the noncovariant Ito–Langevin SDE (5), is standard in Riemann geometry. It is called *frame* (or vielbein, also tetrad in the four-dimensional pseudo-Riemann space of general relativity). The condition (6) is called the frame's orthogonality condition. And now we impose our *new covariant constraint* on the frame. Namely, the covariant divergence of the frame's n orthogonal vectors should vanish,

$$(e^a_A)_{;a} = 0. \tag{12}$$

We mention that the choice of the frame still has a gauge-freedom which is a restriction of (7), not detailed here.

The covariant form of the noncovariant Ito–Langevin SDE (5) is, as we prove below, simple enough,

$$dx^a = e^a_A \circ dW^A + V^a dt, \tag{13}$$

where $\circ$ means Stratonovich product instead of Ito's. The r.h.s. is explicit covariant. This is compatible with the covariance of the l.h.s. since the Stratonovich differentials satisfy the chain rule exactly like common differentials. In our case, if we change the coordinates for y^a then the Stratonovich differentials transform covariantly,

$$dy^a = \frac{\partial y^a}{\partial x_b} dx^b. \tag{14}$$

Now we prove that the covariant Stratonovich–Langevin SDE (13) is equivalent indeed with the noncovariant SDE (5). The Ito form of a Stratonovich SDE, like our (13), reads [12] as

$$\begin{aligned} dx^a &= e^a_A dW^A + \frac{1}{2}\delta^{AB}(e^a_A)_{,b} e^b_B dt + V^a dt \\ &= e^a_A dW^A + \frac{1}{2}\delta^{AB}(e^a_A)_{,b} e^b_B dt + \left(\widetilde{V}^a - \frac{(\sqrt{g} g^{ab})_{,b}}{2\sqrt{g}}\right) dt. \end{aligned}$$

Observe that the new drift term contains the standard partial derivatives of the frame, not the covariant ones. We are going to work it out,

$$\begin{aligned} \delta^{AB}(e^a_A)_{,b} e^b_B &= g^{ab}_{,b} - e^a_A (e^b_A)_{,b} \\ &= g^{ab}_{,b} + e^a_A \Gamma^b_{bc} e^c_A \\ &= g^{ab}_{,b} + g^{ac}\Gamma^b_{bc} \\ &= \frac{1}{\sqrt{g}}(\sqrt{g} g^{ab})_{,b}. \end{aligned} \tag{15}$$

In the four steps we used the orthogonality (6) of the frame, the constraint (12) on its covariant divergence, then (6) again, and the identity $\Gamma^b_{ab} = (\log\sqrt{g})_{,a}$. If we insert the result in the SDE (15) we recognize the coincidence with the noncovariant SDE (5).

We have not yet asked if divergence-free frames e^a_A exist at all. The answer is reassuring [14]. They exist — at least locally — for $n > 2$. Interestingly enough, they do not exist for $n = 2$ unless the geometry is flat. Construction of the divergence-free frames is trivial on flat Riemannian manifolds. Then the coordinates x^a can be functions of Euclidean coordinates y^A. Accordingly, $x^a = f^a(y)$ and the map from Euclidean to curvilinear coordinates satisfies the relationship between the Euclidean

δ^{AB} and the curvilinear metric tensors,

$$\delta^{AB} f^a_{,A} f^b_{,B} = g^{ab}. \tag{16}$$

The frame's orthogonality condition (6) is then satisfied if we choose the frame as

$$e^a_A = f^a_{,A}. \tag{17}$$

This frame is divergence-free. Indeed, the covariant divergence $(e^a_A)_{;a}$ vanishes in any curvilinear coordinates because it vanishes in the particular Euclidean coordinates where $e^a_A = \delta^a_A$.

4. Discussion

The covariant Langevin equation (13), known in itself by both Ito [2] and Graham [7], is describing a frame dependent stochastic process generically different from the adapted process to the given covariant FPE (10). Obviously, the choice of the orthogonal frames must not be left completely free. Originally, Ito [2] proposed that the frame follows stochastic parallel transport along the stochastic trajectory x_t, the covariant derivative of the frame along the trajectory be vanishing. In other words,

$$de^a_A = -\Gamma^a_{bc} e^b_A \circ dx^c, \tag{18}$$

which is a second SDE coupled to the Langevin equation (13) of dx^a, see also Eq. (3.3.9) in [5]. With Ito's stochastic parallel transport, the covariant SDE (13) becomes a bit more involved than with our deterministic constraint $e^a_{A;a} = 0$ but obtains the same stochastic process x_t. The frame is defined on the stochastic trajectory only, differently from our proposal where the frame e^a_A is a given smooth function on the whole Riemannian manifold.

In the mathematical literature of diffusion on Riemannian manifolds, the lack of 'canonical' SDE is explained by the fact that the Laplace-Beltrami operator Δ_{LB} is not a sum of operator squares, cf. p. 75 in [5] or in [15] most recently. That seems to contradict to the existence of the covariant Langevin SDE. Fortunately, there is no contradiction. We can always write Δ_{LB} as sum of operator squares (at least locally and unless $n = 2$),

$$\Delta_{LB} \equiv \nabla_a g^{ab} \nabla_b = \delta^{AB}(e^a_A \nabla_a)(e^b_B \nabla_b), \tag{19}$$

where ∇_a means the covariant derivative. The proof is easy if we substitute $g^{ab} = \delta^{AB} e^a_A e^b_B$ and use the constraint $\nabla_a e^a_A = 0$.

In summary, we have proved that once the covariant Fokker–Planck equation is given, the long-sought stochastic differential equation of the adapted process, i.e. the covariant Langevin equation is the Stratonovich stochastic differential equation (13) containing covariant objects only, as it should, while our main result is that the covariant divergence of the orthogonal frame e^a_A must be set vanishing (12). Our result can and should be refined by more rigorous methods of probability theory and differential geometry.

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