Open system dynamics: the nature of stochastics

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A prototype of closed system

Let $h > 0$ be given and consider the time set $T_h = \{t_k = kh : \ k \in \mathbb{N}\}$ (discrete times). We denote by $q(nh)$ the position of a particle at time nh. So that,

$$q(t_n) = q(t_n) - q(t_{n-1}) + q(t_{n-1}) - q(t_{n-2}) + \ldots + q(t_1) - q(0) + q(0).$$

That is,

$$q(t_n) = q(0) + \sum_{k=1}^{n} \Delta q(t_k), \tag{1}$$

where $\Delta q(t_k) = q(t_k) - q(t_{k-1})$. Notice that $\Delta t_k = h$.

Let assume that the mass of the particle is m. So that, according to Newtonian mechanics, the velocity $\Delta q(t_k)/\Delta t_k$ coincides with $p(t_k)/m$, where $p(t_k)$ is the momentum at time t_k.

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Replacing p en (1), yields

$$q(t_n) = q(0) + \frac{1}{m}\sum_{k=1}^{n} p(t_k)\Delta t_k, \tag{2}$$

which shows the convenience of calling $x(t) = (q(t), p(t))$ the state of the particle at time t.

Moreover,

$$p(t_n) = p(0) + \sum_{k=1}^{n} \Delta p(t_k) = p(0) + \sum_{k=1}^{n} F(t_k)\Delta t_k, \tag{3}$$

To completely determine $x(t)$ at any time t we need to know the initial state $x(0) = (q(0), p(0))$ and the force $F(t)$. This is the fundamental paradigm of classical mechanics after Newton, describing the evolution of a closed or isolated system.

For $x = (q, p)$, let us define the vector function:

$$b(x,t) = \begin{pmatrix} \frac{p}{m} \\ F(t) \end{pmatrix},$$

which allows to write both (2), and (3) in a single equation:

$$x(t_n) = x(0) + \sum_{k=1}^{n} b(x(t_k), t_k)\Delta t_k. \tag{4}$$

The above relation can be written as a system of finite-difference equations too:

$$\begin{cases} \Delta q(t_n) = \frac{1}{m} p(t_n) \Delta t_n \\ \Delta p(t_n) = F(t_n) \Delta t_n \\ q(0) = q_0 \\ p(0) = p_0. \end{cases} \tag{5}$$

Or,

$$\begin{cases} \Delta x(t_n) = b(x(t_n), t_n) \Delta t_n \\ x(0) = x_0. \end{cases} \tag{6}$$

The flow of solutions

Let assume b known, and denote by $t \mapsto \theta_t(x_0)$ the unique solution which starts from x_0, that is, $\theta_0(x_0) = x_0$. This map will be called the flow of solutions to Newton equations.

$$\theta_{t_n}(x_0) = x_0 + \sum_{k=1}^{n} b(\theta_{t_k}(x_0), t_k)\Delta t_k.$$

Notice that x_0 becomes a parameter which completely determines the function $t \mapsto \theta_t(x_0)$ (a trajectory on the state space) as soon as one knows its value.

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Thus, $\omega(t)$ is a couple $\omega(t) = (\omega_q(t), \omega_p(t))$, where $\omega_q(t)$ is the position

of the particle at time t when it follows the trajectory ω; while $\omega_p(t)$ is its momentum at time t.

The stochastic processes appear

Let ω be fixed and we observe the motion following this trajectory. We define a functional to inform the state in which we are at time t.

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As mentioned before, any solution of (2), (3), is a function $\omega \in \Omega$, which is completely determinde once one fixes the initial conditions. Thus, Ω contains all possible solutions to the above equations. In Probability Theory Ω is called the sample space and $X = (X_t; t \in T_h)$, $Q = (Q_t; t \in T_h)$, $P = (P_t; t \in T_h)$, are stochastic processes defined on the space Ω. Newton equations become stochastic.

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So that, (4) for instance, is now written

$$X_{t_n}(\omega) = X_0(\omega) + \sum_{k=1}^{n} b(X_{t_k}(\omega), t_k)\Delta t_k,$$

and we often omit the reference to ω for simplicity.

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For instance, if we want to start from a fixed value $X_0 = x$, we know that $\theta_\bullet(x) : t \mapsto \theta_t(x)$ is the unique function of t solving (4) and starting from x. That is, $\theta_t(x)$ is the state of the particle at time t, when it follows the trajectory $\theta_\bullet(x)$

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$$\delta_{\theta_\bullet(x)}(A) = \begin{cases} 1 & \text{si } \theta.(x) \in A \\ 0 & \text{otherwise,} \end{cases}$$

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So that, the state $\theta_t(x)$ is in turn identifiable to a Dirac measure $\delta_{\theta_t(x)}$ on the space Σ as well.

Opening the system

Once fixed our main one-particle system, suppose it is immersed in an environment of smaller particles. These small particles hit the big one, changing its momentum at each time $t \in T_h$.

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The collisions depend on the trajectory ω followed by the big particle on the real line. We denote $\xi_k(\omega) \in \{-1, 1\}$ the direction in which the main system is collided at each instant t_k.

$$Q_{t_n} = Q_0 + \sum_{k=1}^{n} \frac{P_{t_k}}{m} \Delta t_k \tag{7}$$

$$P_{t_n} = P_0 + \sum_{k=1}^{n} F(t_k)\Delta t_k + \sigma_h \sum_{k=1}^{n} \xi_k. \tag{8}$$

Or, in vector form

$$X_{t_n} = X_0 + \sum_{k=1}^{n} b(X_{t_k}, t_k)\Delta t_k + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \sigma_h \sum_{k=1}^{n} \xi_k. \tag{9}$$

Additional hypothesis on the environment

We assume that the environment is in equilibrium. To represent this idea,we suppose that both hitting directions are equiprobable. That is,

$$\mathbb{P}(\xi_k = 1) = \frac{1}{2} = \mathbb{P}(\xi_k = -1). \tag{10}$$

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Moreover, the hypothesis on the independence of collisions implies that

$S^h_{t_n}(\omega) := \sum_{k=1}^n \xi_k(\omega)$ satisfies:

$$\mathbb{E}\left(S^h_{t_n}\right) = 0 \tag{11}$$

$$\mathbb{E}\left(S^{h\,2}_{t_n}\right) = \sum_{k=1}^{n} \mathbb{E}\left(\xi_k^2\right) = n, \tag{12}$$

for all $t \in T_h$.

The distribution of the random variable S_{t_n} is binomial $B(n, 1/2)$.

Changing scales

Now, we assume that $h \downarrow 0$. Writing $[t]$ the integer part of a real number t, one has:

$$\left[\frac{t}{h}\right] h \leq t < \left(\left[\frac{t}{h}\right] + 1\right) h.$$

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And the equation of the open system becomes,

$$X_t = X_0 + \sum_{k=1}^{[t/h]} b(X_{kh}, kh)h + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \sigma_h S_t^h. \tag{14}$$

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Does $\sigma_h S^h$ converge?

Asking for help to Nature

Notice that if σ_h is constant, then S^h explodes.

For each integer k, $\sigma_h \xi_k$ represents the moemntum variation. Thus, $\sigma_h^2 \xi_k^2$ corresponds to a kinetic energy variation (dissipated through collisions). But $\xi_k^2 = 1$, therefore the sum of dissipated energies is given by

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Einstein postulóated that this quantity should have a finite limit, proportional

to time t. This implies that σ_h be of the form

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Calling $W_t^h = \sqrt{h}\sum_{k=1}^{[t/h]} \xi_k$, we obtain

$$\Delta W_t^h = \sqrt{h}\xi_{[t/h]},$$

and

$$\left(\Delta W_t^h\right)^2 = h = \Delta t. \tag{16}$$

All these processes converge in distribution towards a process W which satisfies the following properties.

The Brownian Motion

- W_t follows a normal distribution with mean 0 and variance t, and it coincides with the distribution of $W_{t+s} - W_s$.
- For each $0 \leq s \leq t$, $W_t - W_s$ is independent of W_s.
- W has continuous trajectories, but they are not differentiable!

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The open system dynamics, at a mesoscale, is then represented by the

stochastic equation

$$X_t = X_0 + \int_0^t b(X_s, s)ds + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \sigma W_t. \tag{17}$$

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The informal notation of the above equation is:

$$dX_t = b(X_t, t)dt + \sigma dW_t. \tag{18}$$

but beware of interpreting dW_t as a differential which DOES NOT EXIST!.

The birth of Stochastic Analysis

The non differentiability of W has been a crucial mathematical problem, and motivated new research in integration theory. One cannot define an integral with respect to W following the usual procedure of Riemann or Lebesgue. A new object, the stochastic integral, and a new calculus have been developed so as to have a correct interpretation of expressions like

$$\int_0^t H_s(\omega) dW_s(\omega).$$

Let us illustrate briefly a particular case of stochastic integral. If σ is a bounded

continuous function, one can give a rigorous meaning to an equation like

$$X_t = X_0 + \int_0^t b(X_s, s)ds + \int_0^t \sigma(X_s, s)dW_s, \tag{19}$$

where the integral with respect to the Brownian Motion is interpreted as a limit **in probability** of sums

$$\sum_{t_k^n, t_{k+1}^n \in \pi_n} \sigma(X_{t_k^n}, t_k^n) \left(W_{t_{k+1}^n} - W_{t_k^n} \right),$$

where π_n is a partition of $[0, t]$ such that $\max \left| t_{k+1}^n - t_k^n \right|$ tends to 0.

A little formal algebra of integrals

Equation (16) inspires a formalism of differentials summarizing a number of properties of stochastic integrals which can be rigorously proved otherwise. This formalism is expressed via a "multiplication table of differentials", which is indeed a mnemotecnic rule.

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Consider a function f twice differentiable with continuous derivatives. A formal

limited Taylor development until the second order of $df(W_t)$ gives

$$\begin{aligned} df(W_t) &= f'(W_t)dW_t + \frac{1}{2}f''(W_t)dW_t^2 \\ &= f'(W_t)dW_t + \frac{1}{2}f''(W_t)dt, \end{aligned}$$

This is rigorously written as

Theorem 1. *Given a twice differentiable function f with continuous derivatives, the following formula due to Itô holds:*

$$f(W_t) = f(W_0) + \int_0^t f'(W_s)dW_s + \frac{1}{2}\int_0^t f''(W_s)ds. \tag{20}$$

Notice that a formal computation of $dX_t dY_t$ for

$$dX_t = a(t)dt + b(t)dW_t,$$

$$dY_t = \alpha(t)dt + \beta(t)dW_t,$$

gives:

$$dX_t dY_t = b(t)\beta(t)dt.$$

Langevin equations

This is a model of an open system dynamics frequently used in Physics. The force is assumed to be the derivative of a potential U that is, Newton equations are written after Langevin in the form

$$\begin{cases} dQ_t = \dfrac{P_t}{m} dt \\ \\ dP_t = -\dfrac{\partial U}{\partial q}(Q_t) + \sigma dW_t. \end{cases} \tag{21}$$

The energy functional

The above system of equations can be written introducing a Hamiltonian or energy functional:

$$H(x) = H(q,p) = \frac{p^2}{2m} + U(q).$$

So that,

$$\frac{p}{m} = \frac{\partial H}{\partial p}(x); \quad \frac{\partial U}{\partial q}(q) = \frac{\partial H}{\partial q}(x),$$

and the gradient of H is

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If the environment changes the position of the main system, one can introduce the energy of interaction $K(x)$, so that

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In Physics this class of equations are usually obtained through the so called Weak Coupling Limit which is nothing more than a sinonymous of the Central Limit Theorem.

Basic concepts of Open System Theory

To write down a model of an open system dynamics the analysis needs to precise the following concepts

1. The main system and the environment (sometimes referred as "the heat bath").
2. The states of the main system and the environment.
3. The observables of the phenomenon under study.
4. The evolution equations of both, states and observables.
5. The different space and time scales where the above equations hold.

Main system and the environment

Matter is always moving, so that to study a part of Nature one needs to focus on a piece of this motion. One cannot embrace the whole Universe! Thus, the main system contains the part of the matter flow that will be transformed by our observations or experiences, while the environment represents the unobserved elements of it.

The states

A state is the probability distribution of the matter flow. For instance, the process $X_t = (Q_t, P_t)$ introduced in our previous mechanical examples, corresponds to the flow of matter. Its probability distribution gives us the state of the system at time t. In classical Newtonian mechanics (or closed system), the state was considered as the couple $X_t = (Q_t, P_t)$ simply. But that is equivalent to work with the Dirac measure supported by X_t.

The observables

Observables are functions $f(X_t)$ of the matter flow. The function f is referred sometimes as the instrument used to perform the observation of X_t.

If μ_t is the distribution of X_t, that is, the state at time t, the mean value

$$\mathbb{E}(f(X_t)) = \int_\Sigma f(x)\mu_t(dx),$$

corresponds to an observation or measurement of the system at time t in the state μ_t.

Space and time scales

The deep unity of Nature allows us to move our analysis through a diversity of space and time scales. The interaction main system–environment considers an agglomeration of dynamics, producing different paces in their evolution.

Moreover, sometimes is possible to refine an analysis to go into observations at a finer space scale. For instance, in Ecology, the number of individuals (an integer valued flow) distribution is considered as *a state* of a system. A more detailed analysis, should consider this as a function of biomass, so becoming an *observable* in another model.

The low density limit

Consider again a main dynamics described by

$$dX_t = J\nabla H(X_t)dt.$$

Assume that this system is perturbed by impulses occurring at random times $(T_n)_{n\in\mathbb{N}}$, such that the differences $T_{n+1} - T_n$ are distributed according to an exponential law of parameter $\lambda > 0$. That is, for a constant c,

$$X_t = X_0 + \int_0^t J\nabla H(X_s)ds + \begin{pmatrix} 0 \\ 1 \end{pmatrix} cN_t, \text{ with}$$

$$N_t(\omega) = n, \text{ si } T_n(\omega) \leq t < T_{n+1}(\omega). \tag{24}$$

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N is a Poisson Process characterized as follows:

- The random variables $N_{t+h} - N_t$ have the same distribution as N_h,
- For each sequence $0 \leq t_1 < t_2 < \ldots < t_n$, the increments $N_{t_{k+1}} - N_{t_k}$ are independent,
- $\mathbb{P}(N_t = n) = e^{-\lambda t} \frac{(\lambda t)^n}{n!}$.

Typically, this kind of processes is used to model a situation in which the main dynamics run faster than that of perturbations, which are considered as rare events. For instance, it is the case of great earthquakes.

Changing scales

A Central Limit Theorem for the Poisson Process works as follows.

One introduces a change in time and space scales taking $\epsilon \downarrow 0$ and defining:

$$M_t^\epsilon = \sqrt{\epsilon\lambda^{-1}} \left(N_{\epsilon^{-1}t} - \lambda\epsilon^{-1}t \right),$$

this family of processes converges in distribution towards a Brownian Motion W.

Thus, if we arrange the initial equation by writing $X_t^\epsilon = \sqrt{\epsilon\lambda^{-1}} X_{\epsilon^{-1}t}$, we

obtain

$$\begin{aligned} X_t^\epsilon &= X_0^\epsilon + \sqrt{\epsilon\lambda^{-1}} \int_0^{\epsilon^{-1}t} J\nabla H(X_s) ds \\ &+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} cM_t^\epsilon \\ &+ \frac{t}{\sqrt{\epsilon\lambda^{-1}}} \end{aligned}$$

If the intensity of the Poisson Process is changed to $\lambda \sim 1/\epsilon$, then X^ϵ can be approached by a diffusion process.

Multiscale dynamics

Brownian Motion and Poisson Processes are particular cases of a Lévy process. This class is defined así follows.

X is a Lévy process if

- The random variables have $X_{t+h} - X_t$ have the same distribution as N_h,
- For each collection $0 \leq t_1 < t_2 < \ldots < t_n$ of times, the increments $X_{t_{k+1}} - X_{t_k}$ are independent.

Lévy processes representation

Any Lévy process can be decomposed in a continuous (Brownian) component and a discontinuous (Poissonian) one. More precisely,

$$X_t = \sigma W_t + \int_{\{|x|<1\}} x(N_t(dx) - t\nu(dx)) + \sum_{0<s\leq t} \Delta X_s 1_{\{|\Delta X_s|\geq 1\}}. \quad (25)$$