Lecture 4a

Equations of motion for stochastic processes

CONTENTS

I. INTRODUCTION

There are two ways to describe how stochastic processes evolve over time:

- Time evolution of probability distributions $P(x,t)$ (continuous or discrete) in probability space $(\Omega, \mathcal{A}, P)$.
- Time evolution of random variables $X(t)$ in sample space Ω.

Last lecture, we have considered the first case, and derived the master equation and the Fokker-Planck equation for a specific class of stochastic processes, the Markovian processes. Here we consider the time evolution of random variables $X(t)$ that describe the time evolution of physical processes, e.g. the time evolution of a Brownian particle or a random walk, and derive a stochastic differential equation. For this purpose, two strategies are possible:

- We can derive a phenomenological stochastic equation of motion, i.e. we guess how the equation should be constructed based on our experience.
- We construct a stochastic equation of motion from first principles, i.e. from a purely deterministic model.

II. PHENOMENOLOGICAL LANGEVIN DYNAMICS

The first route, is the one taken by Paul Langevin in 1908 [1] to describe the Brownian motion of particles suspended in a fluid. Consider a particle of mass M in a fluid, then the equation of motion of the particle can be written as

$$M\ddot{Q} = -\frac{dV(Q)}{dQ} - M\gamma\dot{Q}(t) + f_r(t)\,, \tag{1}$$

or equivalently

$$\dot{P} = -\frac{dV(Q)}{dQ} - \gamma P(t) + f_r(t)\,, \tag{2}$$

where

- Q is the position of the particle.
- $P = M\dot{Q}$ is the momentum of the particle.
- $V(Q)$ is an external potential energy function that depends on the position, for example the gravitational potential or the Lennard-Jones potential;
- $\gamma P(t)$ is a frictional force due to the fluid that dissipates the energy of the particle;
- γ is a friction constant with units $[\text{time}]^{-1}$.
- $f_r(t)$ is a random kick that the particle receives when it collides with the fluid's molecules.

Here the notation $\dot{f} = {}^{df}/_{dt}$ denotes the time derivative of a function f. The force f_r is a stochastic process, but how can be modelled? We expect that

$$\langle f_r(t)\rangle = 0\,, \tag{3}$$

$$\langle f_r(t),\, f_r(t')\rangle = \delta(t-t')\,, \tag{4}$$

i.e. the average is zero and the action of the random force on the system does not have memory, then $f_r(t)$ is a Markovian process.

III. DERIVATION OF THE GENERALIZED LANGEVIN EQUATION

In what follows, we derive the a stochastic differential equation from a purely deterministic system. This model, known as the Kac–Zwanzig model, studies the dynamics of a particle coupled with a heat bath represented by a set of oscillators that exchange energy with the particle.

Consider a particle of mass M governed by the one-dimensional potential energy function $V(Q) : \Omega \subset \mathbb{R} \to \mathbb{R}$. The dynamics of the particle is fully described by the pair of time-dependent variables $\{Q(t),\, P(t)\}$, where Q denotes the position, and P denotes the moment $P = M\dot{Q}$. Assume that the particle can interact with N one-dimensional oscillators of mass m_i, position q_i and momentum p_i, with $i = 1, 2, \ldots, N$, through a potential $0.5k_i(Q - q_i)^2$, where k_i is a spring constant with units $[\mathrm{N\,m^{-1}}]$.

The complete Hamiltonian that describes the dynamics of the system is written as

$$H(Q, P; q_1, p_1; q_2, p_2, \ldots; Q_N, P_N) = \frac{P^2}{2M} + \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + V(Q) + \frac{1}{2}\sum_{i=1}^{N} k_i(q_i - Q)^2\,, \tag{5}$$

the equations of motion of the particle are

$$\begin{cases} \dot{Q} &= \dfrac{P}{M}\,, \\ \dot{P} &= -\nabla V(Q) - \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} k_i(Q - q_i)\,, \end{cases} \tag{6}$$

the equations of motion of the oscillators are

$$\begin{cases} \dot{q}_i &= \dfrac{p_i}{m_i}\,, \\ \dot{p}_i &= k_i(Q - q_i)\,, \end{cases} \qquad \forall i = 1...N\,. \tag{7}$$

For the entire system, we need to solve $2N + 2$ equations. However, typically, the trajectories of the oscillators which represent the environment in which the system is immersed, are of little interest. Thus, we are really only interested in solving eq. 6. The question is, is it possible to solve eq. 6 without also solving eq. 7 directly?

For this purpose, we first differentiate with respect to time the first eq. 7

$$\dot{q}_i = \frac{p_i}{m_i}\,, \tag{8}$$

obtaining

$$\ddot{q}_i = \frac{\dot{p}_i}{m_i}\,, \tag{9}$$

$$m_i\ddot{q}_i = \dot{p}_i \tag{10}$$

Inserting eq. 10 into the second equation of eq. 7 yields

$$m_i \ddot{q}_i = k_i(Q - q_i) \tag{11}$$

$$\ddot{q}_i = \omega_i^2 (Q - q_i) \tag{12}$$

$$\ddot{q}_i + \omega_i^2 q_i = \omega_i^2 Q\,, \tag{13}$$

where $\omega_i = \sqrt{k_i/m_i}$ is the angular frequency of the ith oscillator. Eq. 13 is a non-homogeneous, second-order differential equation. It can be solved using the method of variation of parameters: (i) first, we find the general solution assuming $\omega_i^2 Q = 0$; (ii) then, we find a particular solution of the non-homogeneous equation. The general solution of the homogeneous part is

$$q_i^H(t) = c_1 \cos(\omega_i, t) + c_2 \sin(\omega_i, t)\,, \tag{14}$$

A particular solution is obtained by varying the parameters c_1 and c_2:

$$q_i^P(t) = c_1(t) \cos(\omega_i, t) + c_2(t) \sin(\omega_i, t)\,. \tag{15}$$

To determine $c_1(t)$ and $c_2(t)$, we solve the system of differential equations,

$$\begin{cases} \dot{c}_1(t) \cos(\omega_i t) + \dot{c}_2(t) \sin(\omega_i t) = 0\,, \\ \dot{c}_1(t) \dfrac{d}{dt} \cos(\omega_i t) + \dot{c}_2(t) \dfrac{d}{dt} \sin(\omega_i t) = 0\,, \end{cases} \tag{16}$$

and find the solutions

$$\begin{cases} c_1(t) = -\displaystyle\int_0^t ds\, \omega_i Q(s) \sin(\omega_i s)\,, \\ c_2(t) = \displaystyle\int_0^t ds\, \omega_i Q(s) \cos(\omega_i s)\,. \end{cases} \tag{17}$$

Inserting eqs. 17 into eq. 15 and applying trigonometric rules, we obtain

$$q_i^P(t) = \int_0^t ds\, \omega_i Q(s) \sin(\omega_i (t - s))\,. \tag{18}$$

Finally the solution of eq. 13 is written as

$$q_i(t) = q_i^H(t) + q_i^P(t)\,, \tag{19}$$

$$= c_1 \cos(\omega_i, t) + c_2 \sin(\omega_i, t) + \int_0^t ds\, \omega_i Q(s) \sin(\omega_i (t - s))\,. \tag{20}$$

The integral in eq. 20 contains the variable $Q(s)$, i.e. the position of the particle, which is the solution of the first equation in eq. 6. Applying integration by parts, and bringing on the left-hand side $Q(t)$, we have

$$\begin{aligned} &q_i(t) - Q(t) \\ &= q(0)\cos(\omega_i t) + \frac{p_i(0)}{\omega_i m_i}\sin(\omega_i t) - Q(0)\cos(\omega_i t) - \int_0^t ds\, \dot{Q}(s)\cos(\omega_i(t-s)) \end{aligned} \tag{21}$$

Finally, inserting eq. 21 into the second equation of eq. 6 yields the Generalized Langevin Equation (GLE):

$$\dot{P} = -\nabla V(Q(t)) - \int_0^t ds\, \dot{Q} K(t-s) + R(t)\,, \tag{22}$$

where

$$K(t) = \sum_{i=1}^{N} k_i \cos(\omega_i t)\,, \tag{23}$$

and

$$R(t) = \sum_{i=1}^{N} k_i \left[q_i(0) - Q(0)\right]\cos(\omega_i t) + \frac{k_i}{m_i\omega_i} p_i(0)\sin(\omega_i t)\,. \tag{24}$$

The GLE is made of three terms:

- A Markovian term that depends on the external potential $V(Q)$.
- A memory kernel which conserves the story of $Q(t)$.
- A noise term that depends on the initial conditions and physical properties of the oscillators.

Given specific physical characteristics, initial momenta and initial positions of the oscillators, eq. 22, which is purely deterministic, can be replaced by eq. 2, which is a stochastic differential equation.

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[1] P. Langevin, Sur la theorie du mouvement brownien, C. R. Acad. Sci. **146**, 530–533 (1908).