Basic properties of stochastic processes

Now that we have gained a little intuition about stochastic processes and discussed different methods to analyze their properties, we will further formalize the discussion of stochastic processes

So far we always looked at individual microscopic realizations of the stochastic process and subsequently performed averages over the ensemble of all possible microscopic realizations.

Now instead, we will look directly at the ensemble of all microscopic realizations as described by

<u>probability distribution</u> $p_1(t,v)$

such that

$$\langle v(t)\rangle = \int dv \, v \, p_1(t,v)$$

or more generally a set of

n-point probability distributions $p_n(t_1, v_1, \ldots, t_n, v_n)$

such that

$$\langle v(t_1) \ldots v(t_n) \rangle = \int dv_1 \ldots dv_n \, (v_1 \ldots v_n) \, p_n(t_1 v_1, \ldots t_n v_n)$$

where in analogy to n-body phase space distribution, the lower order distributions can be obtained by marginalizing over one of the variables

$$\underset{\text{``} \quad n-1}{p}(t_1 v_1, \ldots t_{n-1}, v_{n-1}) = \int dv_n \, p_n(t_1 v_1, \ldots, t_n, v_n)$$

Now in addition to the probability distributions p_n that describe state of the system at different times, we are interested in the dynamics of the system as described by conditional probability distributions

$$P_{m|n-m}(t_1 v_1, \ldots t_m, v_m | t_{m+1}, v_{m+1}, \ldots, t_n, v_n)$$

which describe the probability for $t_1, v_1 \ldots t_n, v_n$ knowing $t_{m+1}, v_{m+1} \ldots t_n, v_n$, such that the likelihood $p_n(t_1, v_1, \ldots, t_n, v_n)$ that all values are taken is given by

$$p_n(t_1 v_1 \ldots t_n v_n) = p_{m|n-m}(t_1 v_1 \ldots t_m v_m | t_{m+1} v_{m+1} \ldots t_n v_n) \times$$
$$p_{n-m}(t_{m+1} v_{m+1} \ldots t_n v_n)$$

and to a certain extent $p_{m|n-m}$ describe the dynamics of the stochastic process

Markov processes

Now in principle the dynamics of a stochastic process can be arbitrarily complicated, however there is an important class of processes called "Markov processes" which has some nice features and is particularly relevant for many physical applications

Stochastic process is Markovian, if and only if for $t_1 < t_2 < \dots < t_n < t_{n+1}$

$$P_{1|n}(t_{n+1}, v_{n+1} \mid t_1, v_1 \dots t_n, v_n)$$

$$= P_{1|1}(t_{n+1}, v_{n+1} \mid t_n, v_n)$$

i.e. the evolution of the probability distribution is completely determined by $P_{1|1}$ and the last known state of the system t_n, v_n and there is no memory of the past evolution

It follows immediately that for Markovian process and $t_1 < t_2 < \dots < t_n < t_{n+1}$

$$P_n(t_1 v_1 \dots t_n v_n) = P_{1|1}(t_n v_n \mid t_{n-1} v_{n-1}) \dots P_{1|1}(t_2 v_2 \mid t_1 v_1)\, P_1(t_1 v_1)$$

such that only P_1 and $P_{1|1}$ are needed in the description

Moreover for a Markov process the transition probabilities $P_{1|1}$ satisfy a composition relation, known as the Chapman-Kolmogorov relation, which can easily be derived as follows

Consider $t_1 < t_2 < t_3$ such that

a) $P_2(t_1 v_1, t_3 v_3) = P_{1|1}(t_3 v_3 | t_1 v_1)\, P_1(t_1 v_1)$

but also

b) $P_2(t_1 v_1, t_3 v_3) = \int dv_2 \; P_3(t_1 v_1, t_2 v_2, t_3 v_3)$

with $P_3(t_1 v_1, t_2 v_2, t_3 v_3) = P_{1|1}(t_3 v_3 | t_2 v_2)\, P_{1|1}(t_2 v_2 | t_1 v_1)\, P_1(t_1 v_1)$

By comparison of a) and b)

$$P_{1|1}(t_3 v_3 | t_1 v_1) = \int dv_2 \; P_{1|1}(t_3 v_3 | t_2 v_2)\, P_{1|1}(t_2 v_2 | t_1 v_1)$$

which allows to split an arbitrary time interval $t_3 - t_1$ into many small pieces

//

Brownian motion as a Markov process

Now generally speaking Brownian motion is not a Markov process, as of finite auto-correlation time of the stochastic force implies a memory of the past evolution of the system

However on macroscopic scales $\Delta t \gg \tau_{coll}$ the forces are uncorrelated, and the Brownian motion can be treated as a Markov process in the spirit of coarse grained description.

Now in order to determine the evolution of the n-point probability distributions for we need the conditional probabilities $P_{1|1}$ for Brownian motion on macroscopic time scales

//

We consider the evolution of P_1 for $\Delta t \gg \tau_{coll}$

$$P_1(t+\Delta t, v) = \int dv' \, P_{1|1}(t+\Delta t, v | t, v') \, P_1(t, v')$$

setting $v - v' = \Delta v$

$$= \int d\Delta v \, P_{1|1}(t+\Delta t, v+\Delta v-\Delta v | t, v-\Delta v) \, P_1(t, v-\Delta v)$$

we can expand this into a Taylor series in Δv, anticipating that for $\Delta t \ll \frac{1}{\gamma}$ the typical change Δv is small compared to gradients of $P_1(t,v)$ wrt v

$$= \int d\Delta v \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \Delta v^n \frac{\partial^n}{\partial v^n}$$

$$P_{1|1}(t+\Delta t, v+\Delta v | t, v) \, P_1(t, v)$$

Now we recognize that the Δv dependence only appears in $P_{1|1}$ and we can define moments

$$M_n(t, t+\Delta t, v) = \int d\Delta v \, \Delta v^n \, P_{1|1}(t+\Delta t, v+\Delta v | t, v)$$

where in particular for $n=0$ we have

$$M_0(t, t+\Delta t, v) = \int d\Delta v \, P_{1|1}(t+\Delta t, v+\Delta v | t, v) = 1$$

due to probability conservation.

Splitting this term off the sum, we obtain

$$P_1(t+\Delta t, v) - P_1(t, v) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial v^n} M_n(t, t+\Delta t, v) \, P_1(t, v)$$

Now if we divide by Δt and take the limit $\Delta t \to 0$, the LHS becomes a derivative wrt to t, while on the RHS, we only need to worry about terms for which the limit

$$\lim_{\Delta t \to 0} \frac{M_n(t, t+\Delta t, v)}{\Delta t} = M_n(t, v)$$

is non-zero, i.e. the moments increase linearly with Δt for sufficiently small Δt

Collecting everything, we obtain the

<u>Kramers-Moyal expansion</u>

$$\boxed{\partial_t \, \rho_1(t,v) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial v^n}\left(M_n(t,v)\, \rho_1(t,v)\right)}$$

In particular if only M_1 and M_2 are non-zero, one obtains

<u>Fokker-Planck equation:</u>

$$\partial_t \, \rho_1(t,v) = -\frac{\partial}{\partial v}\left[M_1(t,v)\, \rho_1(t,v)\right] + \frac{1}{2}\frac{\partial^2}{\partial v^2}\left[M_2(t,v)\, \rho_1(t,v)\right]$$

//

Now lets calculate the moments for Brownian motion, where based on the definition

$$M_n(t,v) = \lim_{\Delta t \to 0} \int d\Delta v \, \Delta v^n \frac{P_{1|1}(t+\Delta t, v+\Delta v | t, v)}{\Delta t}$$

we can calculate

$$M_n(t, v(t)) = \lim_{\Delta t \to 0} \frac{\langle (v(t+\Delta t) - v(t))^n \rangle_{Noise}}{\Delta t}$$

with

$$v(t+\Delta t) = e^{-\gamma \Delta t} v(t) + \frac{1}{M} \int_t^{t+\Delta t} ds \, e^{-\gamma(t+\Delta t - s)} F_c(s)$$

Now for the one-point function $\langle F_c(s) \rangle_{Noise} = 0$

$$M_1(t, v(t)) = \lim_{\Delta t \to 0} \frac{e^{-\gamma \Delta t} - 1}{\Delta t} v(t) = -\gamma v(t)$$

Similarly we can evaluate the two point function

$$M_2(t,v(t)) = \lim_{\Delta t\to 0}\left[\underbrace{\frac{\left(e^{-\gamma\Delta t}-1\right)^2}{\Delta t}}_{\to 0} v(t)^2 + \frac{1}{M^2}\int_t^{t+\Delta t} ds \int_t^{t+\Delta t} ds' \, \frac{e^{-\gamma(t+\Delta t-s)}\, e^{-\gamma(t+\Delta t-s')}}{\Delta t} \underbrace{\langle F_L(s) F_L(s')\rangle_{Noise}}_{=2D_v M^2 \delta(s-s')}\right]$$

So upon performing integrals and taking limits

$$M_2(t,v(t)) = 2D_v$$

Since it can easily be shown that all higher order moments vanish in this particular case, we obtain a Fokker-Planck equation for the evolution of the probability distribution.

$$\frac{\partial P_1}{\partial t}(t,v) = \gamma \frac{\partial}{\partial v}\left(v P_1(t,v)\right) + D_v \frac{\partial^2}{\partial v^2} P_1(t,v)$$

where we can directly attribute the different terms on the RHS to the physical effects of Drag (γ) and velocity diffusion (D_v)

//

Similarly if we look at the Brownian motion in phase-space (t, x, v) this is described by SDE

$$\frac{d}{dt}\begin{pmatrix} x(t) \\ v(t) \end{pmatrix} = \begin{pmatrix} v(t) \\ -\gamma v(t) + \frac{1}{m} F_{ext}(t) \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{1}{m} F_C(t) \end{pmatrix}$$

and the associated Fokker-Planck equation for the probability distribution $P_1(t,x,v) = f(t,x,v)$

$$\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial x} + F_{ext}\frac{\partial}{\partial v}\right) f(t,x,v) = \gamma \frac{\partial}{\partial v} v f(t,x,v) + D_v \frac{\partial^2}{\partial v^2} f(t,x,v)$$

takes the form of a Boltzmann type equation with the collision integral approximated by (momentum) diffusion approximation

//

Properties & Solution of Fokker-Planck equation

Since FPE is an evolution equation for the probability, we expect the conservation of probability to manifest itself at the level of FPE

$$\frac{\partial \rho_1}{\partial t}(t,v) = \gamma \frac{\partial}{\partial v}\left(v \rho_1(t,v)\right) + D_v \frac{\partial^2}{\partial v^2} \rho_1(t,v)$$

$$= \frac{\partial}{\partial v} \gamma \left[v \rho_1(t,v) + \frac{D_v}{\gamma} \frac{\partial}{\partial v} \rho_1(t,v) \right]$$

Can express as continuity equation

$$\frac{\partial \rho_1(t,v)}{\partial t} + \frac{\partial}{\partial v} J_v(t,v) = 0$$

with probability current J_v

$$J_v(t,v) = -\gamma \left[v \rho_1(t,v) + \frac{D_v}{\gamma} \frac{\partial}{\partial v} \rho_1(t,v) \right]$$

in velocity space.

Based on FPE, we can also read off the equilibrium solution for the probability distribution, obtained by

$$J_v(t,v) = 0 \Rightarrow \frac{\partial}{\partial v} \rho_1^{eq}(t,v) = -\frac{\gamma}{D_v} v \, \rho_1^{eq}(t,v)$$

such that $\rho_1^{eq}(v) = \sqrt{\frac{\gamma}{2\pi D_v}} \, e^{-\frac{\gamma}{2D_v} v^2}$

where the pre-factor is determined by the normalization condition.

Since $\frac{D_v}{\gamma} = \frac{k_B T}{M}$ this corresponds to the Maxwell-Boltzmann distribution

Now let's have a look at time dependent solutions of FPE.

$$\frac{\partial p_1}{\partial t}(t,v) = \gamma \frac{\partial}{\partial v}\left(v\, p_1(t,v)\right) + D_v \frac{\partial^2}{\partial v^2} p_1(t,v)$$

Since FPE is a linear PDE, the general solution can be constructed as linear superposition of elementary solutions and we will consider for simplicity

$$p_1(t=0,v) = \delta(v-v_0)$$

Next in order to eliminate derivatives wrt to v, we perform a Fourier transform

$$\tilde{p}_1(t,k) = \int_{-\infty}^{+\infty} dv\; p_1(t,v)\, e^{ikv}$$

Such that the initial conditions are given by

$$\tilde{p}(t=0,k) = e^{ikv_0}$$

and a Fourier transform of the FPE results in the replacements

$$\frac{\partial}{\partial v} \to -ik \quad , \quad v \to -i \frac{\partial}{\partial k}$$

such that

$$\frac{\partial}{\partial t} \tilde{\rho}_1(t,k) = \left(-\gamma k \frac{\partial}{\partial k} - D_v k^2 \right) \tilde{\rho}_1(t,k)$$

which is now a linear first order PDE.

Even though the solution is not obvious at this point, linear first order PDEs can be solved in general using the method of characteristics.

We first re-express the equation as

$$\left(\frac{\partial}{\partial t} + \gamma k \frac{\partial}{\partial k}\right) \tilde{\rho}_1(t,k) = -D_v k^2 \tilde{\rho}_1(t,k)$$

bringing all derivatives to the LHS.

Now the basic idea is to introduce a new variable s, describing a trajectory $t(s), k(s)$ in order to re-write the LHS as a total derivative wrt to s.

$$\frac{d}{ds} \tilde{\rho}_1(t(s), k(s)) = \frac{dt}{ds} \frac{\partial}{\partial t} \tilde{\rho}_1(t(s), k(s)) + \frac{dk}{ds} \frac{\partial}{\partial k} \tilde{\rho}_1(t(s), k(s))$$

Such that by comparison, we infer

$$\frac{dt}{ds} = 1 \Rightarrow s = t \quad (\text{+ const set to zero})$$

$$\frac{dk}{ds} = \gamma k(s) \quad \Rightarrow \quad k(s) = k(s=0)\, e^{\gamma s}$$

and the PDE becomes

$$\frac{d}{ds} \tilde{\rho}_1(t(s), k(s)) = - D_r k(s)^2 \tilde{\rho}_1(t(s), k(s))$$

Since $k(s)$ is already known from matching of the differentials, we can now infer the solution as

$$\tilde{\rho}_1(t(s), k(s)) = \exp\left(-D_r \int_0^s ds'\, k^2(s')\right) \tilde{\rho}_1(t(s=0), k(s=0))$$

Now performing the integral

$$\int_0^s ds'\, k^2(s'=0)\, e^{2\gamma s'} = \frac{k^2(s=0)}{2\gamma}\left(e^{2\gamma s} - 1\right)$$

we get

$$\tilde{\rho}_1\big(t(s), k(s)\big) = \exp\left(-\frac{D_v k^2(s=0)}{2\gamma}\left(e^{2\gamma s}-1\right)\right)\tilde{\rho}_1\big(t(s=0), k(s=0)\big)$$

where $t(s) = s$ and $k(s) = k(s=0)\, e^{\gamma s}$, so to obtain the solution for general k, we have to invert the solution and determine $k(s=0) = e^{-\gamma s} k(s)$ as a function of $k(s)$ on the LHS. Denoting then $t(s) = t$, $k(s) = k$

$$\tilde{\rho}_1(t, k) = \exp\left(-\frac{D_v k^2}{2\gamma}\left(1-e^{-2\gamma t}\right)\right)\tilde{\rho}_1\left(t=0, k e^{-\gamma t}\right)$$

$$= \exp\left(-\frac{D_v k^2}{2\gamma}\left(1-e^{-2\gamma t}\right) + i k e^{-\gamma t} v_0\right)$$

Now to obtain the final result we simply need to perform the inverse Fourier transformation

$$P_1(t,v) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \, \tilde{P}_1(t,k) \, e^{-ikv}$$

$$= \sqrt{\frac{\gamma}{2\pi D_v (1-e^{-2\gamma t})}} \exp\left(-\frac{\gamma}{2D_v} \frac{(v - v_0 e^{-\gamma t})^2}{1-e^{-2\gamma t}} \right)$$

yielding a Gaussian probability distribution with mean

$$\langle v(t) \rangle = v_0 e^{-\gamma t}$$

and variance

$$\sigma_v^2(t) = \frac{D_v}{\gamma} \left(1 - e^{-2\gamma t}\right)$$

in line with our previous analysis of the stochastic differential equation

Based on the probability $P_1(t,v)$ distribution and the conditional probability $P_{1|1}(t,v)$ or respectively its moments, one can then compute all equal and unequal time correlation functions