

Lecture 3

From Chapman-Kolmogorov equation to master equation and Fokker-Planck equation

CONTENTS

I.	Stochastic processes	1
II.	The Chapman-Kolmogorov equation	2
III.	The differential Chapman-Kolmogorov equation	4
	A. Derivation of the Master equation	5
	B. Derivation of the Kramers-Moyal expansion	6
IV.	Pawula theorem	8
V.	The Fokker-Planck equation	10
	A. The Liouville's equation	10
	References	11

I. STOCHASTIC PROCESSES

Consider a probability space (Ω, \mathcal{F}, P) and an n -dimensional time-dependent random variable $X : \Omega \subset \mathbb{R}^n \rightarrow \mathbb{R}$, i.e. a real-valued function that maps elements of the sample space to real numbers associated to the outcomes of a random experiment.

Assume now that the random variable is time-dependent: $X(t) : \Omega \subset \mathbb{R}^n \rightarrow \mathbb{R}$, then, given a sequence of timesteps t_1, t_2, \dots, t_N with $t_1 < t_2 < \dots < t_N$, we can write

$$\{X(t_1) = x_1, X(t_2) = x_2, \dots, X(t_N) = x_N\} , \quad (1)$$

where $x_1, x_2, \dots, x_N \in \Omega$. The sequence defined in eq. 1 is a stochastic process if the joint probability density

$$p(x_1, t_1, ; x_2, t_2, ; \dots x_N, t_N) , \quad (2)$$

fully describes the system. Depending on how the joint probability density is defined, we can classify the stochastic processes. Here, we consider two cases.

- Purely random process or separable stochastic process [1]. If successive values of $X(t)$ are statistically independent, then the joint probability density is written as

$$p(x_1, t_1, ; x_2, t_2, ; \dots x_N, t_N) = \prod_{i=1}^N p(x_i, t_i). \quad (3)$$

The underlying idea is that the probability of an event x_i occurring at a time t_i does not depend on the past and in no way determines the future. In terms of conditional probabilities, we can write

$$p(x_N, t_N | x_1, t_1, ; x_2, t_2, ; \dots x_{N-1}, t_{N-1}) = p(x_N, t_N). \quad (4)$$

- A second example of a stochastic process of particular relevance to many applications in physics and chemistry is the Markov process, whose joint probability density is written as

$$p(x_1, t_1, ; x_2, t_2, ; \dots x_N, t_N) = \prod_{i=2}^N p(x_i, t_i | x_{i-1}, t_{i-1}) p(x_1, t_1), \quad (5)$$

or in terms of conditional probabilities as

$$p(x_N, t_N | x_1, t_1, ; x_2, t_2, ; \dots x_{N-1}, t_{N-1}) = p(x_N, t_N | x_{N-1}, t_{N-1}). \quad (6)$$

In other words, a Markovian process is a process without memory, whose temporal evolution depends only on the present state, not on the past.

II. THE CHAPMAN-KOLMOGOROV EQUATION

From this point on, we consider Markov processes. Eq. 6 fully defines a Markov process, but it does not say anything about the probability density function p . The Chapman-Kolmogorov Equation (CKE) states the property that the function p must satisfy to describe a Markov process. To derive the CKE, we proceed as follows. Consider two values x_1 and

x_3 of the random variable $X(t) : \Omega \subset \mathbb{R} \rightarrow \mathbb{R}$, measured at times t_1 and t_3 with $t_1 < t_3$, then from eq. 5 we obtain

$$p(x_1, t_1; x_3, t_3) = p(x_3, t_3 | x_1, t_1) p(x_1, t_1). \quad (7)$$

Integrating over x_1 , we define the marginal density

$$p(x_3, t_3) := \int_{\Omega} dx_1 p(x_1, t_1; x_3, t_3) = \int_{\Omega} dx_1 p(x_3, t_3 | x_1, t_1) p(x_1, t_1) \quad (8)$$

Consider now an intermediate point x_2 , then the joint probability is

$$p(x_1, t_1; x_2, t_2; x_3, t_3) = p(x_3, t_3 | x_2, t_2) p(x_2, t_2 | x_1, t_1) p(x_1, t_1). \quad (9)$$

We integrate over x_2 and applying the definition in eq. 8, we obtain

$$\begin{aligned} \int_{\Omega} dx_2 p(x_1, t_1; x_2, t_2; x_3, t_3) &= \int_{\Omega} dx_2 p(x_3, t_3 | x_2, t_2) p(x_2, t_2 | x_1, t_1) p(x_1, t_1) \\ p(x_1, t_1; x_3, t_3) &= p(x_1, t_1) \int_{\Omega} dx_2 p(x_3, t_3 | x_2, t_2) p(x_2, t_2 | x_1, t_1) \\ \frac{p(x_1, t_1; x_3, t_3)}{p(x_1, t_1)} &= \int_{\Omega} dx_2 p(x_3, t_3 | x_2, t_2) p(x_2, t_2 | x_1, t_1). \end{aligned} \quad (10)$$

The left-hand side of eq. 10 is by definition a conditional probability, thus we obtain the Chapman-Kolmogorov equation

$$\boxed{p(x_3, t_3 | x_1, t_1) = \int_{\Omega} dx_2 p(x_3, t_3 | x_2, t_2) p(x_2, t_2 | x_1, t_1).} \quad (11)$$

Remarks:

- The conditional probability defined in eq. 11 is a transition probability (unit less).
- The CKE fully determines a Markov process, but it does not provide the time evolution of the probability.
- The CKE satisfies the normalization conditions

$$\int_{\Omega} dx_1 p(x_3, t_3 | x_1, t_1) = 1, \quad (12)$$

and

$$\int_{\Omega} dx_3 p(x_3, t_3 | x_1, t_1) = 1. \quad (13)$$

- If $t_3 \rightarrow t_1$, then $p(x_3, t_3|x_1, t_1) = \delta(x_3 - x_1)$.
- For discrete variables $n_1, n_2, \dots, n_N \in \mathbb{Z}$, the CKE is written as

$$p(n_3, t_3|n_1, t_1) = \sum_{n_2} p(n_3; t_3|n_2; t_2) p(n_2; t_2|n_1; t_1). \quad (14)$$

- The CKE of the Brownian motion has the explicit form

$$p(x_3, t_3|x_1, t_1) = \frac{1}{\sqrt{4\pi D(t_3 - t_1)}} \exp\left(-\frac{(x_3 - x_1)^2}{4D(t_3 - t_1)}\right), \quad (15)$$

where D is the diffusion constant.

III. THE DIFFERENTIAL CHAPMAN-KOLMOGOROV EQUATION

In order to find how the conditional probability defined in eq. 11 evolves with time, we need a differential equation. For this purpose, we make the following change of notation:

$$\begin{cases} (x_1, t_1) \rightarrow (x_0, t_0) \\ (x_2, t_2) \rightarrow (x', t) \\ (x_3, t_3) \rightarrow (x, t + \Delta t), \end{cases} \quad (16)$$

and rewrite eq. 11 as

$$p(x, t + \Delta t|x_0, t_0) = \int_{\Omega} dx' p(x, t + \Delta t|x', t) p(x', t|x_0, t_0). \quad (17)$$

We now introduce the time derivative of $p(x, t|x_0, t_0)$:

$$\frac{\partial}{\partial t} p(x; t|x_0, t_0) = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \left[\underline{p(x, t + \Delta t|x_0, t_0)} - p(x; t|x_0, t_0) \right] \right\}. \quad (18)$$

Inserting eq. 17 into eq. 18 yields

$$\begin{aligned} \frac{\partial}{\partial t} p(x; t|x_0, t_0) &= \\ &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[\underline{\int_{\Omega} dx' p(x, t + \Delta t|x', t) p(x', t|x_0, t_0)} - \underline{1 \cdot p(x; t|x_0, t_0)} \right]. \end{aligned} \quad (19)$$

The second term in the inner integral in the right-hand side of eq. 19 is multiplied by **1**. Then, rewriting the normalization condition defined in eqs. 12, 13 with the coordinates x and x' as

$$\int_{\Omega} dx' p(x', t + \Delta t|x; t) = \underline{1}, \quad (20)$$

eq. 21 yields

$$\begin{aligned} & \frac{\partial}{\partial t} p(x; t | x_0, t_0) = \\ & = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[\int_{\Omega} dx' p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) - \right. \\ & \quad \left. - \int_{\Omega} dx' p(x', t + \Delta t | x, t) p(x; t | x_0, t_0) \right]. \end{aligned} \quad (21)$$

A. Derivation of the Master equation

Let us now consider the case of a discontinuous stochastic process (also called a jump process), e.g. the random walk on a grid. For convenience, we rewrite here the differential CKE (eq. 21)

$$\begin{aligned} & \frac{\partial}{\partial t} p(x; t | x_0, t_0) = \\ & = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[\int_{\Omega} dx' \underline{p(x, t + \Delta t | x', t) p(x', t | x_0, t_0)} - \right. \\ & \quad \left. - \int_{\Omega} dx' \underline{p(x', t + \Delta t | x, t) p(x; t | x_0, t_0)} \right]. \end{aligned} \quad (22)$$

Then, we introduce the terms:

$$\begin{aligned} W(x, t | x', t) &= \underline{\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} p(x, t + \Delta t | x', t)} \\ W(x', t | x, t) &= \underline{\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} p(x', t + \Delta t | x, t)}, \end{aligned} \quad (23)$$

with $x \neq x'$. $W(x, t | x', t)$ and $W(x', t | x, t)$, with units $[\text{time}^{-1}]$, are called transition rates. From a physical point of view, these are transition probabilities in the unit time Δt , i.e. they describe the transition probability from x to x' (either from x' to x) in a infinitesimal timestep.

In this way, we obtain the master equation:

$$\boxed{\frac{\partial}{\partial t} p(x, t | x_0, t_0) = \int_{\Omega} dx' [W(x, t | x', t) p(x', t | x_0, t_0) - W(x', t | x, t) p(x, t | x_0, t_0)]} \quad (24)$$

In the case of discrete variables $n_0, n_1, n_2, \dots, n_N \in \mathbb{Z}$, the master equation is written as

$$\frac{\partial}{\partial t} p(n, t | n_0, t_0) = \sum_{n'} [W(n, t | n', t) p(n', t | n_0, t_0) - W(n', t | n, t) p(n, t | n_0, t_0)] \quad (25)$$

Note that, since eq. 24 (or 25) are valid for any x_0 (or n_0), the dependence on x_0 (or n_0) can be omitted:

$$\frac{\partial}{\partial t} p(x, t) = \int_{\Omega} dx' [W(x, t | x', t) p(x', t) - W(x', t | x, t) p(x, t)] \quad (26)$$

B. Derivation of the Kramers-Moyal expansion

Consider now the case of continuous stochastic processes, e.g. Brownian motion of pollen grains in water. Eq. 21 is rewritten here:

$$\begin{aligned} & \frac{\partial}{\partial t} p(x; t | x_0, t_0) = \\ &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[\int_{\Omega} dx' p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) - \right. \\ & \quad \left. - \int_{\Omega} dx' p(x', t + \Delta t | x, t) p(x, t | x_0, t_0) \right]. \end{aligned} \quad (27)$$

We now multiply both sides of eq. 27 by a test function $\varphi : \Omega \rightarrow \mathbb{R}$ and integrate over x :

$$\begin{aligned} & \frac{\partial}{\partial t} \int_{\Omega} dx \varphi(x) p(x, t | x_0, t_0) = \\ &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{\Omega} dx \int_{\Omega} dx' \varphi(x) p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) - \right. \\ & \quad \left. - \int_{\Omega} dx \int_{\Omega} dx' \varphi(x) p(x', t + \Delta t | x, t) p(x, t | x_0, t_0) \right\}. \end{aligned} \quad (28)$$

Consider now the Taylor expansion around x' of the test function φ :

$$\varphi(x) = \varphi(x') + \sum_{m=1}^{\infty} (x - x')^m \frac{1}{m!} \left. \frac{\partial^m \varphi}{\partial x^m} \right|_{x=x'}. \quad (29)$$

Inserting eq. 29 into the first inner integral of eq. 28 yields

$$\begin{aligned} & \frac{\partial}{\partial t} \int_{\Omega} dx \varphi(x) p(x, t | x_0, t_0) = \\ &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{\Omega} dx \left[\int_{\Omega} dx' \varphi(x') p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) + \right. \right. \\ & \quad \left. + \int_{\Omega} dx' \sum_{m=1}^{\infty} (x - x')^m \frac{1}{m!} \left. \frac{\partial^m \varphi}{\partial x^m} \right|_{x=x'} p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) - \right] \\ & \quad \left. - \int_{\Omega} dx \int_{\Omega} dx' \varphi(x) p(x', t + \Delta t | x, t) p(x, t | x_0, t_0) \right\}. \end{aligned} \quad (30)$$

The last integral is a double integral over $\Omega \times \Omega$, however the order of integration does not matter. Then, it is convenient to swap the variables $x \leftrightarrow x'$:

$$\begin{aligned}
& \frac{\partial}{\partial t} \int_{\Omega} dx \varphi(x) p(x, t | x_0, t_0) = \\
& = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{\Omega} dx \left[\int_{\Omega} dx' \varphi(x') p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) + \right. \right. \\
& \quad \left. \left. + \int_{\Omega} dx' \sum_{m=1}^{\infty} (x - x')^m \frac{1}{m!} \frac{\partial^m \varphi}{\partial x^m} \Big|_{x=x'} p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) - \right. \right. \\
& \quad \left. \left. - \int_{\Omega} dx \int_{\Omega} dx' \varphi(x') p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) \right] \right\}. \tag{31}
\end{aligned}$$

Rearranging the integrals, we have

$$\begin{aligned}
& \frac{\partial}{\partial t} \int_{\Omega} dx \varphi(x) p(x, t | x_0, t_0) = \\
& = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{\Omega} dx' \left[\int_{\Omega} dx \varphi(x') p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) + \right. \right. \\
& \quad \left. \left. + \int_{\Omega} dx \sum_{m=1}^{\infty} (x - x')^m \frac{1}{m!} \frac{\partial^m \varphi}{\partial x^m} \Big|_{x=x'} p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) - \right. \right. \\
& \quad \left. \left. - \int_{\Omega} dx \varphi(x') p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) \right] \right\}. \tag{32}
\end{aligned}$$

Then, we obtain:

$$\begin{aligned}
& \frac{\partial}{\partial t} \int_{\Omega} dx \varphi(x) p(x, t | x_0, t_0) = \\
& = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{\Omega} dx' \int_{\Omega} dx \sum_{m=1}^{\infty} (x - x')^m \frac{1}{m!} \frac{\partial^m \varphi}{\partial x^m} \Big|_{x=x'} p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) \right\}. \tag{33}
\end{aligned}$$

We now define the coefficients

$$D_m(x', t) = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{\Omega} dx (x - x')^m p(x, t + \Delta t | x', t), \tag{34}$$

and eq. 33 is rewritten as

$$\begin{aligned}
& \frac{\partial}{\partial t} \int_{\Omega} dx \varphi(x) p(x, t | x_0, t_0) = \\
& = \int_{\Omega} dx' \left[\sum_{m=1}^{\infty} D_m(x', t) \frac{1}{m!} \frac{\partial^m \varphi}{\partial x^m} \Big|_{x=x'} p(x', t | x_0, t_0) \right]. \tag{35}
\end{aligned}$$

Consider now the generalized rule for integration by parts

$$\int_{\Omega} dx \frac{\partial^m f}{\partial x^m} g = \sum_{k=0}^{m-1} (-1)^k \frac{\partial^k g}{\partial x^k} \frac{\partial^{m-1-k} f}{\partial x^{m-1-k}} \Big|_{\partial \Omega} + (-1)^m \int_{\Omega} dx f \frac{\partial^m g}{\partial x^m}, \tag{36}$$

where the sum \sum_k term is a sum of derivatives calculated at the boundary $\partial\Omega$ of Ω . We now assume that the stochastic process is confined in Ω , then p and its m th derivatives are zero on $\partial\Omega$ and the \sum_k term can be canceled. Finally we obtain

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\Omega} dx \varphi(x) p(x, t | x_0, t_0) &= \\ &= \sum_{m=1}^{\infty} \frac{(-1)^m}{m!} \int_{\Omega} dx' \left[\varphi(x') \frac{\partial^m}{\partial x'^m} [D_m(x', t) p(x', t | x_0, t_0)] \right]. \end{aligned} \quad (37)$$

Because eq. 37 holds for any test function φ , we obtain

$$\boxed{\frac{\partial}{\partial t} p(x, t | x_0, t_0) = \sum_{m=1}^{\infty} \frac{(-1)^m}{m!} \frac{\partial^m}{\partial x^m} [D_m(x, t) p(x, t | x_0, t_0)]}, \quad (38)$$

which is known as Kramers-Moyal Expansion (KME). Because eq. 38 does not depend not (x_0, t_0) , if the initial condition is fixed, then, we can write

$$p(x, t | x_0, t_0) = p(x, t), \quad (39)$$

and

$$\frac{\partial}{\partial t} p(x, t) = \sum_{m=1}^{\infty} \frac{(-1)^m}{m!} \frac{\partial^m}{\partial x^m} [D_m(x, t) p(x, t)]. \quad (40)$$

IV. PAWULA THEOREM

The Kramers-Moyal expansion defined in eq. 38 is an infinite-order partial differential equation, but in practical applications, we cannot handle an infinite sum of terms. The Pawula theorem, using a logical argument states that, for a given problem, only one of the following situation is valid:

- The KME is truncated at the first term (Liouville's equation);
- The KME is truncated at the second term (Fokker-Planck equation);
- The KME cannot be truncated, it must include all infinite terms.

Then, if we assume that a certain even term is zero, it is correct to assume all the terms with $m \geq 3$ equal to zero. Note that this is not a physical argument, then there is no guarantee that the Fokker-Planck equation is a correct approximation of the Kramer-Moyal expansion.

The Pawula theorem is based on the following

Lemma [2, 3]: Consider the Kramers-Moyal coefficients as defined in eq. 34 (exchanging x and x' for convenience):

$$D_m(x, t) = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{\Omega} dx' (x' - x)^m p(x', t + \Delta t | x, t) \quad (41)$$

$$= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \mathbb{E} [(x' - x)^m | x, t] . \quad (42)$$

If $D_m < \infty$ for all m , and if $D_m = 0$ for some even m , then $D_m = 0$ for all $n \geq 3$.

Proof. First, we recall the Cauchy-Schwarz inequality for two arbitrary functions $f, g : \Omega \rightarrow \mathbb{R}$ applied to random variables X and Y with probability density $p : \Omega \rightarrow \mathbb{R}$:

$$\mathbb{E} [f(X)g(Y)]^2 \leq \mathbb{E} [f(X)^2] \mathbb{E} [g(Y)^2] . \quad (43)$$

Inserting eq. 34 (omitting the $\lim_{\Delta t \rightarrow 0}$ part for brevity) into eq. 43 yields and distinguishing between odd and even m :

- if m is odd and $m \geq 3$:

$$\mathbb{E} [(x' - x)^m]^2 = \mathbb{E} \left[(x' - x)^{\frac{m-1}{2}} (x' - x)^{\frac{m+1}{2}} \right]^2 \leq \mathbb{E} [(x' - x)^{m-1}] \mathbb{E} [(x' - x)^{m+1}] \quad (44)$$

- if m is even and $m \geq 4$:

$$\mathbb{E} [(x' - x)^m]^2 = \mathbb{E} \left[(x' - x)^{\frac{m-2}{2}} (x' - x)^{\frac{m+2}{2}} \right]^2 \leq \mathbb{E} [(x' - x)^{m-2}] \mathbb{E} [(x' - x)^{m+2}] \quad (45)$$

In short notation:

$$D_m^2 \leq D_{m-1} D_{m+1} \quad m \text{ odd}, m \geq 3; \quad (46)$$

$$D_m^2 \leq D_{m-2} D_{m+2} \quad m \text{ even}, m \geq 4. \quad (47)$$

Consider now an even number $r \geq 4$ such that $D_r = 0$, i.e. consider the hypothesis of the lemma, and applying the inequalities defined in eqs. 46 and 47, we check whether the terms $D_m \forall m \geq 0$. First, we consider the term with m odd. If r is even, then $m = r \pm 1, r \pm 3, \dots$ are odd. Consider the first two cases:

$$m = \begin{cases} r - 1 \geq 3 \rightarrow D_{r-1}^2 \leq D_{(r-1)-1} D_{(r-1)+1} = D_{r-2} D_r \\ r + 1 \geq 3 \rightarrow D_{r+1}^2 \leq D_{(r+1)-1} D_{(r+1)+1} = D_r D_{r+2} \end{cases} \quad (48)$$

Likewise, to build m even, we add and subtract multiples of 2, for example:

$$m = \begin{cases} r - 2 \geq 4 \rightarrow D_{r-2}^2 \leq D_{(r-2)-2} D_{(r-2)+2} = D_{r-4} D_r \\ r + 2 \geq 4 \rightarrow D_{r+2}^2 \leq D_{(r+2)-2} D_{(r+2)+2} = D_r D_{r+4} \end{cases} \quad (49)$$

Since $D_m < \infty$ for all m and $D_r = 0$, then from eqs. 48 and 49 follows that D_{r-1} , D_{r+1} , D_{r-2} and D_{r+2} must vanish. Repeating this argument iteratively, one finds that $D_m = 0 \forall m \leq 3$. ■

From ref. [2]: *Note that the above lemma does not guarantee that the Fokker-Planck equation will be a good approximation to the linear Boltzmann equation. We should in general expect to obtain different solutions from each equation. The lemma merely leads to the conclusion that the probability density function of a random process cannot be correctly described by a finite number, greater than two, of terms of the Kramers-Moyal expansion.*

V. THE FOKKER-PLANCK EQUATION

By truncating the KME after the second term, one gets the Fokker-Planck Equation (FPE)

$$\frac{\partial p(x, t)}{\partial t} = -\frac{\partial}{\partial x} [D_1(x, t) p(x, t)] + \frac{\partial^2}{\partial x^2} [D_2(x, t) p(x, t)] . \quad (50)$$

where $D_1(x, t)$ is the drift, and $D_2(x, t)$ is the diffusion.

A. The Liouville's equation

If there is no diffusion, then the Fokker-Planck equation reduces to the Liouville's equation for deterministic processes:

$$\frac{\partial p(x, t)}{\partial t} = -\frac{\partial}{\partial x} [D_1(x, t) p(x, t)] . \quad (51)$$

Given the initial condition

$$p(x, 0) = \delta(x - x_0) , \quad (52)$$

The solution is

$$p(x, t) = \delta(x - x(t)) . \quad (53)$$

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