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Chapter 1

Chapmann Kolmogorov equation

In the chapter on stochastic processes we have have seen that if a stochastic process has the Markov property the $1|1$ conditional probability density $p(x_2, t_2|x_1, t_1)$, satisfies the Chapman-Kolmogorov equation

$$\boxed{p(x_3, t_3|x_1, t_1) = \int_{\mathbb{R}} p(x_3, t_3|x_2, t_2)p(x_2, t_2|x_1, t_1)dx_2} \tag{1.1}$$

In the above form the CK equation is an integral equation but, under suitable conditions it can be rewritten in a differential form. Let us consider $(t_1, x_1) \equiv (t_0, x_0)$ the initial state of a given Markov process. Moreover $(t_2, x_2) \equiv (t, x')$ is the state at time t and $(t_3, x_3) \equiv (t + \Delta t, x)$ the state at time $t + \Delta t$. In this case eq. (1.1) becomes:

$$p(x, t + \Delta t|x_0, t_0) = \int_{\mathbb{R}} p(x, t + \Delta t|x', t)p(x', t|x_0, t_0)dx' \tag{1.2}$$

Remark. From a rigorous point of view the conditional probabilities $p(..|..)$ are not function but distributions and in that sense they need to be supported by well behaving functions (test functions) to be properly defined. For example in the general theory of distributions belonging to the so called D' space the test functions $\varphi \in D$ are functions that are C^∞ and with compact support.

Also here we need the use of test functions $\varphi \in S$ such that the distribution $p(x, t|x_0, t_0)$ is defined through the integral (or more generally trough a linear operator T acting on φ) as:

$$\int_{\mathbb{R}} dx\varphi(x)p(x, t|x_0, t_0) \equiv \langle p, \varphi\rangle \tag{1.3}$$

If we then multiply eq. (1.2) by a test function $\varphi(x)$ and integrate both sides with respect to x we obtain the so called *smeared* Chapmann-Kolmogorov equation

$$\int_{\mathbb{R}} dx\varphi(x)p(x, t + \Delta t|x_0, t_0) = \int_{\mathbb{R}} dx\varphi(x) \int_{\mathbb{R}} p(x, t + \Delta t|x', t)p(x', t|x_0, t_0)dx' \tag{1.4}$$

The time derivative of the above quantity is then, by definition,

$$\partial_t \int_{\mathbb{R}} dx\varphi(x)p(x, t|x_0, t_0) = \lim_{\Delta t\to 0} \frac{1}{\Delta t} \left\{ \int_{\mathbb{R}} dx\varphi(x) \left[p(x, t + \Delta t|x_0, t_0) - p(x, t|x_0, t_0)\right] \right\} \tag{1.5}$$

and by using eq.(1.2) for $p(x, t + \Delta t|x_0, t_0)$ we have

$$\begin{aligned}
\partial_t & \int_{\mathbb{R}} dx\varphi(x)p(x, t|x_0, t_0) \\
= & \lim_{\Delta t\to 0} \frac{1}{\Delta t} \left\{ \int_{\mathbb{R}} dx\varphi(x) \left[p(x, t + \Delta t|x_0, t_0) - p(x, t|x_0, t_0)\right] \right\} \\
= & \lim_{\Delta t\to 0} \frac{1}{\Delta t} \left\{ \left[\int_{\mathbb{R}^2} dxdx'\varphi(x)p(x, t + \Delta t|x', t)p(x', t|x_0, t_0) \right] - \left[\int_{\mathbb{R}} dxp\varphi(x)(x, t|x_0, t_0) \right] \right\}
\end{aligned} \tag{1.6}$$

On the other hand

$$\int_{\mathbb{R}} dx' p(x', t + \Delta t | x, t) = 1 \tag{1.7}$$

and by inserting this identity in the second term of the integral (1.6) one obtains:

$$\begin{aligned} \partial_t &\int_{\mathbb{R}} dx \varphi(x) p(x, t | x_0, t_0) \qquad (1.8) \\ = &\lim_{\Delta t \to 0} \frac{1}{\Delta t} \left\{ \int_{\mathbb{R}^2} dx dx' \varphi(x) \left[p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) - p(x', t + \Delta t | x, t) p(x, t | x_0, t_0) \right] \right\}. \end{aligned}$$

We now observe that in the term

$$\int_{\mathbb{R}} dx \varphi(x) p(x, t | x_0, t_0) p(x', t + \Delta t | x, t) \tag{1.9}$$

we can change the name of the integration variable x (since we are summing over it) into x' giving:

$$\int_{\mathbb{R}} dx' \varphi(x') p(x', t | x_0, t_0) p(x, t + \Delta t | x', t) \tag{1.10}$$

Eq.(1.9) then becomes:

$$\begin{aligned} \partial_t &\int_{\mathbb{R}} dx \varphi(x) p(x, t | x_0, t_0) = \\ &\lim_{\Delta t \to 0} \frac{1}{\Delta t} \left\{ \int_{\mathbb{R}^2} dx dx' p(x, t + \Delta t | x', t) \left[\varphi(x) p(x', t | x_0, t_0) - \varphi(x') p(x', t | x_0, t_0) \right] \right\} \end{aligned} \tag{1.11}$$

If the paths (sampling) are continuous one should expect that, as $\Delta t \to 0$, $x \to x'$. Hence for Δt small enough and for continuous paths the distance $|x - x'|$ is sufficiently small i.e. $|x - x'| < \epsilon$. For non continuous paths this is not any more true in general and it is possible that $|x - x'| > \epsilon$. To separate the equation into these two different cases it is then convenient to split the integrals over x between the ones performed over the region $|x - x'| \leq \epsilon$ and $|x - x'| > \epsilon$:

$$\begin{aligned} \partial_t &\int_{\mathbb{R}} dx \varphi(x) p(x, t | x_0, t_0) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \Bigg\{ \\ &\int_{\mathbb{R}} dx' \int_{|x - x'| \leq \epsilon} dx \varphi(x) p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) \\ + &\int_{\mathbb{R}} dx' \int_{|x - x'| > \epsilon} dx \varphi(x) p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) \\ - &\int_{\mathbb{R}} dx' \int_{\mathbb{R}} dx \varphi(x') p(x, t + \Delta t | x', t) p(x', t | x_0, t_0) \Bigg\} \end{aligned} \tag{1.12}$$

On the other hand, if $|x - x'| \leq \epsilon$ it is possible to expand $\varphi(x)$ in the neighborhood of x' i.e.

$$\varphi(x) = \varphi(x') + \sum_{m=1}^{N} (x - x')^m \frac{1}{m!} \left. \frac{\partial^m \varphi(x)}{\partial x^m} \right|_{x = x'} + R_N(x), \tag{1.13}$$

where

$$R_N(x) = \frac{1}{(N+1)!} \left. \frac{\partial^{N+1} \varphi(x)}{\partial x^{N+1}} \right|_{x = y \in |x - x'|} (x - x')^{N+1} \tag{1.14}$$

is the remainder in the Lagrange form. Inserting eq. (1.13) in (1.12) one obtains:

$$
\begin{aligned}
\partial_t \quad & \int_{\mathbb{R}} dx\varphi(x)p(x,t|x_0,t_0) = \lim_{\Delta t\to 0}\frac{1}{\Delta t}\Bigg\{ \\
& \int_{\mathbb{R}} dx' \int_{|x-x'|\le\epsilon} dx\varphi(x')p(x,t+\Delta t|x',t)p(x',t|x_0,t_0) \\
+ \quad & \int_{\mathbb{R}} dx' \int_{|x-x'|\le\epsilon} dx \sum_{m=1}^{N}(x-x')^m\frac{1}{m!}\left.\frac{\partial^m\varphi(x)}{\partial x^m}\right|_{x=x'} p(x,t+\Delta t|x',t)p(x',t|x_0,t_0) \\
+ \quad & \int_{\mathbb{R}} dx' \int_{|x-x'|\le\epsilon} dx R_N(x)p(x,t+\Delta t|x',t)p(x',t|x_0,t_0) \\
+ \quad & \int_{\mathbb{R}} dx' \int_{|x-x'|>\epsilon} dx\varphi(x)p(x,t+\Delta t|x',t)p(x',t|x_0,t_0) \\
- \quad & \int_{\mathbb{R}} dx' \int_{\mathbb{R}} dx\varphi(x')p(x,t+\Delta t|x',t)p(x',t|x_0,t_0)\Bigg\}. \qquad (1.15)
\end{aligned}
$$

By adding together the second and the last line one gets

$$
\begin{aligned}
\partial_t \quad & \int_{\mathbb{R}} dx\varphi(x)p(x,t|x_0,t_0) = \lim_{\Delta t\to 0}\frac{1}{\Delta t}\Bigg\{ \\
& \int_{\mathbb{R}} dx' \int_{|x-x'|\le\epsilon} dx \sum_{m=1}^{N}(x-x')^m\frac{1}{m!}\left.\frac{\partial^m\varphi(x)}{\partial x^m}\right|_{x=x'} p(x,t+\Delta t|x',t)p(x',t|x_0,t_0) \\
+ \quad & \int_{\mathbb{R}} dx' \int_{|x-x'|\le\epsilon} dx R_N(x)p(x,t+\Delta t|x',t)p(x',t|x_0,t_0) \\
+ \quad & \int_{\mathbb{R}} dx' \int_{|x-x'|>\epsilon} dx\varphi(x)p(x,t+\Delta t|x',t)p(x',t|x_0,t_0) \\
- \quad & \int_{\mathbb{R}} dx' \int_{|x-x'|>\epsilon} dx\varphi(x')p(x,t+\Delta t|x',t)p(x',t|x_0,t_0)\Bigg\} \qquad (1.16)
\end{aligned}
$$

The integral of line 4 can be rewritten by interchanging x with x' (this can be done since we are summing over these variables). Moreover, since $|x-x'|>\epsilon$, (i.e. what it counts is the distance) we can still integrate x' over $\mathbb{R}$ and x over $|x-x'|>\epsilon$. This gives:

$$
\begin{aligned}
\partial_t \quad & \int_{\mathbb{R}} dx\varphi(x)p(x,t|x_0,t_0) = \lim_{\Delta t\to 0}\frac{1}{\Delta t}\Bigg\{ \\
& \int_{\mathbb{R}} dx' \int_{|x-x'|\le\epsilon} dx \sum_{m=1}^{N}(x-x')^m\frac{1}{m!}\left.\frac{\partial^m\varphi(x)}{\partial x^m}\right|_{x=x'} p(x,t+\Delta t|x',t)p(x',t|x_0,t_0) \\
+ \quad & \int_{\mathbb{R}} dx' \int_{|x-x'|\le\epsilon} dx R_N(x)p(x,t+\Delta t|x',t)p(x',t|x_0,t_0) \\
+ \quad & \int_{\mathbb{R}} dx' \int_{|x-x'|>\epsilon} dx\varphi(x')p(x',t+\Delta t|x,t)p(x,t|x_0,t_0) \\
- \quad & \int_{\mathbb{R}} dx' \int_{|x-x'|>\epsilon} dx\varphi(x')p(x,t+\Delta t|x',t)p(x',t|x_0,t_0)\Bigg\} \qquad (1.17)
\end{aligned}
$$

For fixed $\epsilon>0$ we now take the $\Delta t\to 0$ limit inside the integral by assuming that:

1. $\forall\epsilon>0$

$$
\begin{aligned}
\lim_{\Delta t\to 0}\frac{p(x,t+\Delta t|x',t)}{\Delta t} &= w(x,t|x',t) \\
\lim_{\Delta t\to 0}\frac{p(x',t+\Delta t|x,t)}{\Delta t} &= w(x',t|x,t) \qquad (1.18)
\end{aligned}
$$

uniformly in x, x', t and for $|x - x'| > \epsilon$.

2. For each $m \geq 1$ and $\forall \epsilon > 0$

$$\frac{1}{m!} \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{|x-x'| \leq \epsilon} dx (x - x')^m p(x, t + \Delta t | x', t) = D_\epsilon^{(m)}(x', t), \tag{1.19}$$

uniformly in x', ϵ and t. We further assume that for any $\epsilon > 0$ the relation

$$\frac{1}{m!} \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{|x-x'| > \epsilon} dx (x - x')^m p(x, t + \Delta t | x', t) = 0 \tag{1.20}$$

holds. This last condition strengthen the continuity condition and allows to extend the definition of $D_\epsilon^{(m)}(x', t)$ to the whole space.

On the other hand for the analytic functions $\varphi(x)$ the following inequality holds

$$\sup_{y \in |x-x'|} \left| \frac{\partial^k \varphi(y)}{\partial x^k} \right| \leq (M_x)^k \qquad \forall k \in \mathbb{N} \bigcup \{0\} \tag{1.21}$$

giving

$$\begin{aligned}
& \left| \frac{1}{\Delta t} \int_{|x-x'| < \epsilon} dx R_N(x') p(x, t + \Delta t | x', t) \right| \\
\leq \quad & \frac{1}{\Delta t} \int_{|x-x'| < \epsilon} dx \, |R_N(x')| \, p(x, t + \Delta t | x', t) \\
\leq \quad & \frac{1}{(N+1)!} \left[\frac{1}{\Delta t} \int_{|x-x'| < \epsilon} dx |x - x'|^{N+1} p(x, t + \Delta t | x', t) \right] (M_x)^{N+1} \\
\to_{\Delta t \to 0} \quad & \left[D_\epsilon^{(N+1)}(x', t) (M_x)^{N+1} \right]
\end{aligned} \tag{1.22}$$

and when we will take the limit $\epsilon \to 0$ this term goes to 0. We can the omit it from the equation. If we use the above assumptions and we change, in the left hand size term, the integration variable x with x', we then have:

$$\begin{aligned}
& \partial_t \int_{\mathbb{R}} dx' \varphi(x') p(x', t | x_0, t_0) = \\
& \int_{\mathbb{R}} dx' \sum_{m=1}^{N} D_\epsilon^{(m)}(x', t) \left. \frac{\partial^m \varphi(x)}{\partial x^m} \right|_{x=x'} p(x', t | x_0, t_0) \\
+ \quad & \int_{\mathbb{R}} dx' \varphi(x') \int_{|x-x'| > \epsilon} dx \left[w(x', t | x, t) p(x, t | x_0, t_0) - w(x, t | x', t) p(x', t | x_0, t_0) \right]
\end{aligned} \tag{1.23}$$

By taking the limit $\epsilon \to 0$ we have:

$$\begin{aligned}
& \partial_t \int_{\mathbb{R}} dx' \varphi(x') p(x', t | x_0, t_0) = \\
& \int_{\mathbb{R}} dx' \sum_{m=1}^{N} D^{(m)}(x', t) \left. \frac{\partial^m \varphi(x)}{\partial x^m} \right|_{x=x'} p(x', t | x_0, t_0) \\
+ \quad & \int_{\mathbb{R}} dx' \varphi(x') \int_{\mathrm{PV}} dx \left[w(x', t | x, t) p(x, t | x_0, t_0) - w(x, t | x', t) p(x', t | x_0, t_0) \right]
\end{aligned} \tag{1.24}$$

where

$$\lim_{\epsilon \to 0} \int_{|x-x'| > \epsilon} dx F(x, x') \equiv \int_{\mathrm{PV}} dx F(x, x') \tag{1.25}$$

is the principal value of the integral. Indeed, by assumption (1.18), the quantity $w(x,t|x',t)$ is defined only for $x \neq x'$ and it possible that $w(x,t|x',t)$ is infinite for $x = x'$. This is, for example, the case of a Cauchy process where:

$$p(x, t + \Delta t|, x', t) = \frac{\Delta t/\pi}{(x - x')^2 + (\Delta t)^2} \tag{1.26}$$

In an homogeneous process with discontinuous paths and

$$w(x, t|x', t) = \frac{1}{\pi(x - x')^2}. \tag{1.27}$$

If, on the other hand $p(x,t|x_0,t_0)$ is continuous and differentiable the principal value of the integral exits. The final step consists in moving the derivatives from the test functions to the conditional probabilities by integrating by parts the integrals of the second line. In doing that, integrals over the boundaries (surface integrals) do appear and we need to better specify the domain of integration. Let us suppose that the process is confined in a region Ω with boundary $\partial\Omega$. In other words we assume

$$p(x, t|x, t') = 0 \qquad \forall x, x' \notin \Omega \tag{1.28}$$

and

$$w(x, t|x', t) = 0, \qquad \text{if either} \quad x \quad \text{or} \quad x' \notin \Omega \tag{1.29}$$

Note that the coefficients $D^{(m)}(x',t)$ could present discontinuities at $\partial\Omega$ since $p(x, t + \Delta t|x', t)$ can change in a discontinuous manner as we cross Ω. For a safer situation it usually assumed that the support Ω' of the test function $\varphi(x)$ is included in Ω (i.e. $\Omega' \subset \Omega$. Hence, for values of $x' \in \Omega' \subset \Omega$ we can interchange the derivative operator between the test functions and the distribution by using the well known rule

$$\langle \partial^m T, \varphi \rangle = (-1)^m \langle T, \partial^m \varphi \rangle. \tag{1.30}$$

This gives

$$\begin{aligned}
&\partial_t \int_\Omega dx' \varphi(x') p(x', t|x_0, t_0) = \\
&\sum_{m=1}^{N} (-1)^m \int_\Omega dx' \varphi(x') \frac{\partial^m}{\partial x^m} \left[D^{(m)}(x', t) p(x', t|x_0, t_0) \right] \\
+ &\int_\Omega dx' \varphi(x') \int_{\mathrm{PV}} dx \left[w(x', t|x, t) p(x, t|x_0, t_0) - w(x, t|x', t) p(x', t|x_0, t_0) \right]
\end{aligned} \tag{1.31}$$

Since the above equation is true for any test function φ it can be written formally as

$$\begin{aligned}
&\partial_t p(x', t|x_0, t_0) = \\
&\sum_{m=1}^{N} (-1)^m \frac{\partial^m}{\partial x'^m} \left[D^{(m)}(x', t) p(x', t|x_0, t_0) \right] \\
+ &\int_{\mathrm{PV}} dx \left[w(x', t|x, t) p(x, t|x_0, t_0) - w(x, t|x', t) p(x', t|x_0, t_0) \right]
\end{aligned} \tag{1.32}$$

The above equation is called the differential form of the CK backward equation and describes the time evolution of the distribution function for general Markov Processes whose paths can be piecewise continuous . Let us now consider particular cases.

Chapter 2

Chapman-Kolmogorov for jump processes: Master equation

Suppose first for each $m \geq 1$ and $\forall \epsilon > 0$

$$D_\epsilon^{(m)}(x',t) = \frac{1}{m!} \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{|x-x'|\leq\epsilon} dx(x-x')^m p(x,t+\Delta t|x',t) = 0, \qquad \text{uniformly in} \quad x', \epsilon, t. \tag{2.1}$$

In this case the CK differential equation simplifies to

$$\begin{aligned} &\partial_t p(x',t|x_0,t_0) = \\ +\quad &\int_{\mathrm{PV}} dx \left[w(x',t|x,t)p(x,t|x_0,t_0) - w(x,t|x',t)p(x',t|x_0,t_0) \right] \end{aligned} \tag{2.2}$$

This is what usually is called the *Master Equation* for jump Markov processes.

Either if the Markov process $X(t)$ is stationary (i.e. $X(t)$ and $X(t+\epsilon)$ share the same statistics) or if it is homogeneous in time (i.e. the two point $p(x_2,t_2|x_1,t_1)$ depends only on $\tau = t_2 - t_1$), to simplify notations we can write $p(x_2,t_2|x_1,t_1) = p_\tau(x_2|x_1)$ and the original C-K equation becomes

$$p_{\tau+\tau'}(x_3|x_1) = \int_{\mathbb{R}} dx_2 p_{\tau'}(x_3|x_2)p_\tau(x_2|x_1). \tag{2.3}$$

With these assumptions the master equation for jump processes simplifies to

$$\frac{\partial p_\tau(x|x_0)}{\partial \tau} = \int_{\mathbb{R}} dx' \left[w(x|x')p_\tau(x'|x_0) - w(x'|x)p_\tau(x|x_0) \right] \tag{2.4}$$

Since the above equation is valid for any x_0 we can safely omit the dependence on x_0 (or we can integrate over $dx_0 p(x_0)$) to get the master equation for the one-point distribution function

$$\boxed{\frac{\partial p_\tau(x)}{\partial \tau} = \int_{\mathbb{R}} dx' \left[w(x|x')p_\tau(x') - w(x'|x)p_\tau(x) \right].} \tag{2.5}$$

In the case in which the state space is discrete (i.e. $X : \Omega \to \mathbb{Z}$) the Master equation may be written as

$$\partial_t P(n,t|n',t') = \sum_m \left[w(n,t|m,t)P(m,t|n',t') - w(m,t|n,t)P(n,t|n',t') \right] \tag{2.6}$$

and, if the process is stationary or homogeneus,

$$\boxed{\partial_t P(n|n',t) = \sum_m \left[w(n|m,t)P(m|n',t) - w(m|n,t)P(n|n',t) \right]} \tag{2.7}$$

or for the one point probability

$$\boxed{\partial_t P(n,t) = \sum_m \left[w(n|m)P(m,t) - w(m|n)P(n,t)\right]} \tag{2.8}$$

The Master equation can be seem as an gain-loose equation for the probability of each state n. Indeed the first term represents a gain due to the transitions from other states m, while the second one is a loosing term due to transitions from n to other states m. The initial condition is $P(n, t = 0) = P_0(n)$.

2.0.1 Birth-death (or one-step) processes

Suppose we can classify the states following a given order. In this way we have that the neighbouring states of n are the $n-1$ and $n+1$ states. We further suppose that only transitions between neghbouring states are allowed:

$$w(n|m) = 0 \qquad \forall m \neq n \pm 1. \tag{2.9}$$

If we write $w(n|n+1) = w^+(n-1)$ and $w(n|n-1) = w^-(n-1)$ we have

$$\boxed{\frac{\partial P(n,t)}{\partial t} = w^+(n-1)P(n-1,t) + w^-(n+1)P(n+1,t) - (w^+(n) + w^-(n))P(n,t)} \tag{2.10}$$

These kind of processes occur in several situations. Below are listed some of them.

1. Processes of recombination and generation of charged carriers
2. Growth of atoms on crystal surfaces
3. Birth and death of individuals
4. Chemical reactions

It is possible to distinguish 3 different classes of one-step processes

Linear processes The transitions $w^+(m)$ and $w^-(m)$ are linear functions of m

Non linear processes The transitions $w^+(m)$ and $w^-(m)$ are non linear functions of m

Random walks The transitions $w^+(m)$ and $w^-(m)$ are constants.

Poisson process

This is an example of one-step process of the random-walk type. One supposes that events occur indipendently as time goes on. The occurence probability is the same for any event. The process to be considered is the number of events $N(t)$ that have occured up to time t. A typical event could be, for example, the tunneling of an electron through a single barrier or the arrival of a person at a given queue; in this case $N(t)$ represents the length of the queue at time t. The process is characterized by

$$w^-(n) = 0, \quad w^+(n) = q, \quad P(n,0) = \delta_{n,0}. \tag{2.11}$$

and the master equation simplfies to

$$\boxed{\frac{\partial P(n,t)}{\partial t} = q\left(P(n-1,t) - P(n,t)\right)} \tag{2.12}$$

Before going on with the investigation of this process let us first summarize briefly some of the techniques commonly used to manipulate, simplify or solve a master equation.

Manipulation of the master equation

Sometime it is not necessary to know the full probability $P(n,t)$ but it would be enough to look at the time dependence of some its moments, in particular the mean and the variance of the process. For these moments the evolution equation can be simpler and more prone to be analytically solved. Since the mean is defined as

$$\langle n(t)\rangle = \sum_n P(n,t) \tag{2.13}$$

by multiplying the master equation

$$\frac{\partial P(n,t)}{\partial t} = w^+(n-1)P(n-1,t) - w^+(n)P(n,t) + w^+(n+1)P(n+1,t) - w^-(n)P(n,t) \tag{2.14}$$

by n and summing over n one gets

$$\frac{d}{dt}\langle n(t)\rangle = \sum_n nw^+(n-1)P(n-1,t) - \sum_n nw^+(n)P(n,t) + \sum_n nw^-(n+1)P(n+1,t) - \sum_n w^-(n)P(n,t) \tag{2.15}$$

If we now change the index name $n \to n+1$ in the sum

$$\sum_n nw^+(n-1)P(n-1,t) \tag{2.16}$$

becomes

$$\sum_n (n+1)w^+(n)P(n,t). \tag{2.17}$$

The same argument will bring the term

$$\sum_n nw^-(n+1)P(n+1,t) \tag{2.18}$$

into

$$\sum_n (n-1)w^-(n)P(n,t). \tag{2.19}$$

This finally gives

$$\boxed{\frac{d}{dt}\langle n(t)\rangle = \sum_n \left(w^+(n) - w^-(n)\right) P(n,t),} \tag{2.20}$$

which can also be written as

$$\boxed{\frac{d}{dt}\langle n(t)\rangle = \langle w^+(n) - w^-(n)\rangle.} \tag{2.21}$$

In order to find the evolution equation for the variance we should first compute the equation for the second moment

$$\langle n^2(t)\rangle = \sum_n n^2 P(n,t). \tag{2.22}$$

By following the same steps considered for the mean we obtain the differential equation

$$\frac{d}{dt}\langle n^2(t)\rangle = 2\langle n\left(w^+(n) - w^-(n)\right)\rangle + \langle w^+(n) + w^-(n)\rangle. \tag{2.23}$$

Finally, from the definition of the variance $V(n) = \langle n^2(t)\rangle - \langle n(t)\rangle^2$, we have

$$\frac{dV}{dt} = \frac{d}{dt}\langle n^2(t)\rangle - 2\langle n(t)\rangle \frac{d}{dt}\langle n^(t)\rangle \tag{2.24}$$

and inserting the expressions for $\frac{d}{dt}\langle n^2(t)\rangle$ and $\frac{d}{dt}\langle n^(t)\rangle$, we obtain

$$\boxed{2\langle (n - \langle n\rangle)\left(w^+(n) - w^-(n)\right)\rangle + \langle w^+(n) - w^-(n)\rangle.} \tag{2.25}$$

More generally, given an arbitrary function $f(n)$ one can write

$$\frac{d}{dt}\langle f(n)\rangle = \langle (f(n+1)-f(n))w^{+}(n)\rangle - \langle (f(n)-f(n-1))w^{-}(n)\rangle. \tag{2.26}$$

By considering the special case $f(n) = z^n$ its average

$$G(z,t) \equiv \langle f(n)\rangle = \sum_n z^n P(n,t) \tag{2.27}$$

its called the generating function of the process with probability $P(n,t)$. Indeed by knowing the derivatives of $G(z,t)$ one can get the moments of $P(n,t)$. For example

$$\langle n(t)\rangle = \left.\frac{\partial G(z,t)}{\partial z}\right|_{z=1}; \qquad \langle n^2(t)\rangle = \left.\frac{\partial^2 G(z,t)}{\partial z^2}\right|_{z=1} + \left.\frac{\partial G(z,t)}{\partial z}\right|_{z=1}. \tag{2.28}$$

It is interesting to notice that if $z = e^{is}$, $\phi(s,t) = G(e^{is},t)$ and

$$P(n,t) = \frac{1}{2\pi}\int_0^{2\pi} \phi(s,t)e^{-ins}ds. \tag{2.29}$$

Moreover, since the expression

$$\sum_n z^n P(n,t) \tag{2.30}$$

is formally a Taylor expansion of $G(z,t)$ around $z=0$ one has

$$P(n,t) = \frac{1}{n!}\left.\frac{\partial^n G(z,t)}{\partial z^n}\right|_{z=0} \tag{2.31}$$

Note that if n assumes negative values $G(z,t)$ can be written as a Laurent expansion.

Poisson process

Let us try to solve the occurence of events problem by using the approaches described above. The time evolution for this problem follows the differential equation

$$\frac{\partial P(n,t)}{\partial t} = w^{+}(n-1)P(n-1,t) - w^{+}(n)P(n,t) \tag{2.32}$$

with $w^{+}(m) = q$ forall m. Hence, for the mean we have

$$\frac{d}{dt}\langle n(t)\rangle = \sum_n w^{+}(n)P(n,t) = \langle q\rangle = q. \tag{2.33}$$

Solving this equation with the intial condition $n(t=0)=0$ gives

$$\langle n(t)\rangle = qt. \tag{2.34}$$

The equation for the second moment simplifies to

$$\frac{d}{dt}\langle n^2\rangle = 2q\langle n\rangle + q \tag{2.35}$$

and since $\langle n\rangle = qt$ we have

$$\frac{d}{dt}\langle n^2\rangle = 2q^2t + q. \tag{2.36}$$

By solving this equation with intial condition $\langle n^2(0)\rangle = 0$ we have

$$\langle n^2(t)\rangle = (qt)^2 + qt. \tag{2.37}$$

Finally, for the variance we get

$$V(t) = \langle n^2 \rangle - \langle n \rangle^2 = qt = \langle n \rangle. \tag{2.38}$$

We can now try to solve the full problem by looking at the time evolution for the generating function $G(z,t)$. From the equation of a generic $f(n)$ we have

$$\frac{d}{dt}\langle z^n \rangle = \langle (z^{n+1} - z^n) q \rangle = q(z-1)\langle z^n \rangle \tag{2.39}$$

giving

$$\boxed{\frac{\partial G(z,t)}{\partial t} = q(z-1)G(z,t).} \tag{2.40}$$

This is an equation of the form $y' = Ay$ whose solution is formally given by

$$G(z,t) = A(z)\exp\left[(z-1)qt\right] \tag{2.41}$$

Since $n(t=0) = 0$, $P(n,0) = \delta_{n,0}$ giving $G(z,0) = 1$. This condition is satisfied for $A(z) = 1$ forall z giving

$$\boxed{G(z,t) = \exp\left[(z-1)qt\right]} \tag{2.42}$$

On the other hand it is easy to see that, denoting $y = e^{qt}$,

$$\left.\frac{\partial^m y^z}{\partial z^m}\right|_{z=0} = (\log y)^m = (qt)^m \tag{2.43}$$

giving the final result

$$\boxed{P(n,t) = \frac{1}{n!}\left.\frac{\partial^n G}{\partial z^n}\right|_{z=0} = e^{-qt}\frac{(qt)^n}{n!}} \tag{2.44}$$

that is the Poisson probability distribution.

Radiation decay

Suppose to have a radioactive material and let $N(t)$ be the number of active nuclei at time $t > 0$. $P(n,t)$ is then the probability that at time t there are still n nuclei. If we denote by γ the decay probabiity per unit time for a single nucleus we have, for small Δt

$$\begin{aligned} p(n, t+\Delta t | n', t) &= 0 \qquad n > n' \\ &= n'\gamma\Delta \qquad n = n'-1 \\ &= O(\Delta^2) \qquad n < n'-1. \end{aligned} \tag{2.45}$$

In other words

$$\boxed{w(n'|n) = \gamma n' \delta_{n,n'-1}} \tag{2.46}$$

and the master equation of the process is

$$\frac{\partial P(n,t)}{\partial t} = \gamma(n+1)P(n+1,t) - \gamma n P(n,t). \tag{2.47}$$

giving $w^-(m) = \gamma m$ and $w^+(m) = 0$. For the mean we then have

$$\frac{d}{dt}\langle n(t) \rangle = -\gamma \langle n(t) \rangle \tag{2.48}$$

whose solution for the initial condition $\langle n(t=0) \rangle = N_0$ is

$$\boxed{\langle n(t) \rangle = N_0 e^{-\gamma t}.} \tag{2.49}$$

For the generating function we have

$$\boxed{\frac{\partial}{\partial t}G(z,t) = -\gamma(z-1)\frac{\partial}{\partial z}G(z,t)} \tag{2.50}$$

with initial condition

$$\boxed{G(z,0) = \sum_n z^n P(n,0) = \sum_n z^n \delta_{n,N_0} = z^{N_0}} \tag{2.51}$$

It is easy to show that the above equation is satisfied by any real function $G(z,t) = G((z-1)e^{-\gamma t}+1)$. By taking into account the initial condition we finally have

$$G(z,t) = e^{-N_0\gamma t}\sum_{n=0}^{N_0}\binom{N_0}{n} z^{N_0-n}\left(e^{\gamma t}-1\right)^n \tag{2.52}$$

giving

$$\boxed{P(n,t) = e^{-gammaN_0 t}\binom{N_0}{n}\left(e^{\gamma t}-1\right)^n.} \tag{2.53}$$

By multiplying both sides of the equation by z^n and summin over n we get an equation for the generating function

$$\frac{\partial G(z,t)}{\partial t} = \gamma\left[\sum_{n=0}^{\infty}(n+1)z^n P(n+1,t) - \sum_{n=0}^{\infty} nz^n P(n,t)\right] = -\gamma(z-1)\frac{\partial G(z,t)}{\partial z} \tag{2.54}$$

with initial condition $G(z,0) = \sum_{n=0}^{\infty} z^n P(n,0) = z^{N_0}$ since $P(n,0) = \delta_{n,N_0}$. The above equation is satisfied by any real function

$$G(z,t) = G(log(z-1) - \gamma t). \tag{2.55}$$

On the other hand

$$G(z,0) = z^{N_0} = \left[e^{log(z-1)}+1\right]^{N_0} \tag{2.56}$$

and, for any finite value of t we have

$$\begin{aligned} G(z,t) = \left[e^{log(z-1)-\gamma t}+1\right]^{N_0} \\ &= e^{-\gamma N_0 t}\left[z-1+e^{\gamma t}\right]^{N_0} \\ &= e^{-\gamma N_0 t}\sum_{n=0}^{N_0}\binom{N_0}{n} z^{N_0-n}\left(e^{\gamma t}-1\right)^n \end{aligned} \tag{2.57}$$

2.1 Stationary solutions of the master equation: Detailed balance

The master equation is fully determined once are given the transition rates $w(n|n')$. To compute the full solution $P(n,t)$ of the markov process $n(t)$ could be in general a very difficult task to achieve. Fortunately sometimes it is sufficient to look just at the stationary solutions $P_s(n)$. These are defined by

$$\frac{\partial P_s(n)}{\partial t} = 0 \tag{2.58}$$

and from the master equation we have the relation

$$\boxed{\sum_{n'\in\Omega}\left(P_s(n')w(n|n') - P_s(n)w(n'|n)\right) = 0} \tag{2.59}$$

The stationary solution is usually reached by the system in the long time limit and if the system is in contact with a thermal bath of fixed temperature T the stationary solution should coincide with the equilibrium canonical ensemble distribution $P_e(n)$. A way to satisfy condition (2.59) is by assuming that the relation holds term by term, i.e.

$$\boxed{P_s(n')w(n|n') - P_s(n)w(n'|n) = 0, \qquad \forall n, n'} \tag{2.60}$$

Eq. (2.60) is the so called *detailed balance* condition. It is a stronger (local) condition than (2.59) (integral) since it holds for each pair of states n, n' taken individually. For the special case in which the stationary solution coincides with the canonical equilibrium distribution $P_e(n) = \frac{1}{Z} d_n e^{-\beta E_n}$ with d_n being the degeneration of the energy level E_n, the detailed balance condition becomes

$$\boxed{d_{n'} e^{-\beta E_{n'}} w(n|n') = d_n e^{-\beta E_n} w(n'|n)} \tag{2.61}$$

or

$$\boxed{\frac{w(n'|n)}{w(n|n')} = \frac{d_{n'}}{d_n} e^{-\beta(E_{n'} - E_n)}.} \tag{2.62}$$

A simple appication of the detailed balance condition is related to the Monte Carlo method, a numerical stochastic procedure to sample states at equilibrium.

Monte Carlo method

The underlying idea of a Monte Carlo methos consists in building up a discrete (in time and space) markov process (markov chain) whose dynamics will sample, in the large t limit, random states whose statistic follow a given, preassigned, distribution $\pi(n)$. In statistical mechanics this distribution coincides with the equilibrium (canonical, microcanonical or grancanonical) distribution of the system. Suppose the system is at equilibrium with a thermal bath of temperature T. The equilibrium distribution is then given by $P_e(n) = \frac{1}{Z} e^{-\beta E_n}$ where, for simplcity, we have assumed $d_n = 1$. The detailed balance condition (2.62) becomes

$$\boxed{\frac{w(n'|n)}{w(n|n')} = \frac{P_e(n')}{P_e(n)} = e^{-\beta(E_{n'} - E_n)}.} \tag{2.63}$$

This condition can be satisfied by a large set of function of the ratio $P_e(n')/P_e(n)$. Indeed if we consider a function $F(x)$ such that

$$F\left(\frac{1}{x}\right) = \frac{1}{x} F(x), \tag{2.64}$$

assuming

$$F\left(\frac{P_e(n')}{P_e(n)}\right) = w(n'|n), \tag{2.65}$$

the detailed balance turns out to be automatically satisfied. Indeed

$$\frac{w(n'|n)}{w(n|n')} = \frac{F\left(\frac{P_e(n')}{P_e(n)}\right)}{F\left(\frac{P_e(n)}{P_e(n')}\right)} = \frac{P_e(n')}{P_e(n)} \frac{F\left(\frac{P_e(n)}{P_e(n')}\right)}{F\left(\frac{P_e(n)}{P_e(n')}\right)} = \frac{P_e(n')}{P_e(n)}. \tag{2.66}$$

As one can see the choice of F is quite arbitrary. The two most common choices are

$$F(x) = \min(x, 1), \qquad x > 0, \qquad \text{Metropolis} \tag{2.67}$$

and

$$F(x) = \frac{x}{1+x}, \qquad \text{Heat bath.} \tag{2.68}$$

Exercises

1. Consider a chemical reaction $A \leftrightarrow B$ with reaction reates k and k' respectively for the reaction $A \to B$ and $A \leftarrow B$. Consider the process $n(t) = n_B(t) \in \mathbb{N}$ where n_B is the number of the species B. We suppose to be able to maintain the number of the spacies A, n_A, to a constant value n_A (for example by a flux of such particles that compensates the evetual loos of them during the reaction). We can than assume $w^+(m) = kn_A$ and $w^-(m) = k'm$ to be respectvely tha rate of gain of the species B and the rate of decrease for the molecule B. The master equation is then

$$\frac{\partial}{\partial t} P(n,t) = kn_A P(n-1,t) + k'(n+1)P(n+1,t) - (kn_A + k'n)P(n,t). \tag{2.69}$$

Find the time evolution of the mean $\langle n(t) \rangle$ and of the variance $V(t)$.

2. Consider a population of individuals. Each individual has a probability per unit time d of dying and there is a probability per unit time b for an individual to enter in the population. It is easy to show that the corresponding master equation is given by

$$\frac{\partial P(n,t)}{\partial t} = d(n+1)P(n+1,t) + bP(n-1,t) - (dn+b)P(n,t). \tag{2.70}$$

(A) Starting from the above equation solve the corresponding problem for the mean $\langle n(t) \rangle$ and the generating function $G(z,t)$.

(B) Find the probability distribution $P(n,t)$ in the limit $t \to \infty$.

3: Asymmetric Randow walk with continuous time Let $n(t)$ the position of a particle on a 1d $\mathbb{Z}$ lattice. If we denote by α and β the uniform probability to go respectively to the right and to the left of position n, the master equation governing the time evolution of the one-point probability distribution is given by

$$\frac{\partial P(n,t)}{\partial t} = \beta P(n+1,t) + \alpha P(n-1,t) - (\alpha+\beta)P(n,t). \tag{2.71}$$

(A) Starting from the above equation solve the corresponding problem for the mean $\langle n(t) \rangle$ and the variance $V(n)$.

(B) Solve the corresponding problem for the generating function $G(z,t)$