Stochastic Processes and Diffusion Equation, Forward and Backward.

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1 Introduction.

One of the most powefull tool to invetigate stochastic processes is through the diffusion equation for the probabiliy density $p(x,t)$

$$\frac{\partial p}{\partial t}=\frac{\partial ap}{\partial x}+\frac{\partial^2 bp}{\partial x^2}$$

This equation is called the *forward* one. Very soon, the student also encounters the *backward* diffusion equation :

$$\frac{\partial p}{\partial t}=-a\frac{\partial p}{\partial x}+b\frac{\partial^2 p}{\partial x^2}$$

which is equivalent to the forward one, and is very useful to compute first passage times and absorption to boundaries probabilities. These two equations have however a profound assymetry : in the forward one, the drift and diffusion terms $a(x)$and $b(x)$ are part of the derivations, whether in the backward one, they are *out* of it.

In the following, we will revisit the derivation of the diffusion equation from a microscopic perspective and investigate the origin of this assymetry. ()

2 Kolmogorov equations (forward and backward).

Let us call $P(n, n_0, t)$ the probability of being in state n at time t, knowing that we have been at n_0 at time 0. This probability is the sum of all trajectories probabilities $K(n, n_0, t)$, beginning at $(0, n_0)$ and finishing at (t, n) (Fig.2.1left). . Of course, computing the weight of a given path is not easy. However, we can state the trajectory probabilities when the duration dt is infinitesimal. Let us for the moment concentrate on transitions between neighboring states (Fig.2.1right):

$$\begin{aligned} K(n \to n+1, dt) &= W^+(n)dt \\ K(n \to n-1, dt) &= W^-(n)dt \\ K(n \to n, dt) &= 1 - \left(W^+(n) - W^-(n)\right) dt \\ K(n \to n+k) &= 0 \text{ if } |k| > 1 \end{aligned} \tag{2.1}$$

knowing the infinitesimal rates, we can relate probabilities for two close times t and $t + dt$: go from n_0 to a state m during t, and from

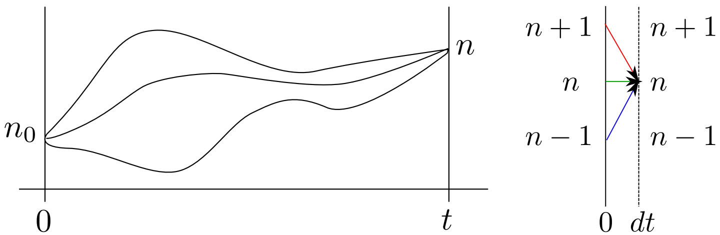

Fig. 2.1: left : $P(n, n_0, t) = \sum_{path} K(n, n_0, t)$; right : infinitesimal paths of equation (2.1).

this state, transfer into the state n during dt(Fig.2.2).

$$\begin{aligned} P(n,n_0,t+dt) &= P(n+1,n_0,t)W^-(n+1)dt \\ &+ P(n,n_0,t)\left(1-\left(W^+(n)-W^-(n)\right)dt\right) \\ &+ P(n-1,n_0,t)W^+(n-1)dt \end{aligned}$$

Now, it is trivial to develop the left hand side

$$P(n,n_0,t+dt)=P(n,n_0,t)+\frac{\partial P(n,n0,t)}{\partial t}dt$$

And deduce the differential equations governing the probabilities :

$$\begin{aligned} \frac{\partial P(n,n_0,t)}{\partial t} &= W^+(n-1)P(n-1,n_0)-W^+(n)P(n,n_0) \quad (2.2) \\ &+ W^-(n+1)P(n+1,n_0)-W^-(n)P(n,n_0) \end{aligned}$$

This is a nice system of first order differential equation, which we could formally write

$$\frac{d\vec{P}_t}{dt}=\bar{A}\vec{P}_t$$

where the matrix $\bar{A}$ is tridiagonal. It is called a *forward* equation, because we did the decomposition trick near the end point.

It is not hard to guess the backward equation : instead of decomposing near the end point, we'll do it near the starting point(Fig. 2.3) and write :

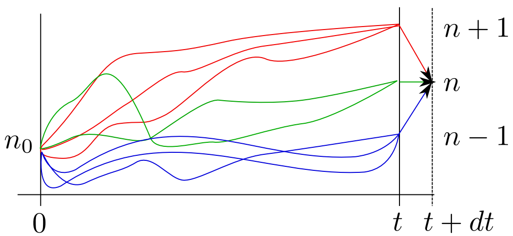

Fig. 2.2: Decomposition of the travel near the end state.

$$
\begin{aligned}
P(n, n_0, t+dt) &= P(n, n_0+1, t)W^+(n_0)dt \\
&+ P(n, n_0, t)\left(1 - \left(W^+(n_0) - W^-(n_0)\right) dt\right) \\
&+ P(n, n_0-1, t)W^-(n_0)dt
\end{aligned}
$$

Again, developping the left hand side, we find

$$
\begin{aligned}
\frac{\partial P(n, n_0, t)}{\partial t} &= W^+(n_0)\left(P(n, n_0+1, t) - P(n, n_0, t)\right) \\
&+ W^-(n_0)\left(P(n, n_0-1, t) - P(n, n_0, t)\right)
\end{aligned}
$$

We see here appearing the assymetry between the forward and backward equation in the way the transition rates are displayed in the equations. This assymetric behaviour is due to the fundamental assumption that time has a direction, and therefore n_0 is the emmiting end, whether n is the receiving end. Note that to further illustrate this assymetry, we have just flipped figure 2.2 to get figure 2.3, but the direction of time has not changed.

3 Diffusion equation.

Let us now suppose that the number of discrete states N is very large. Instead of tracking the states by the discrete variable n, we will introduce the continuous variable $x = n/N$. We also introduce the probability densities $p(x, x_0, t)dxdx_0 = P(n, n_0, t)$ where we have

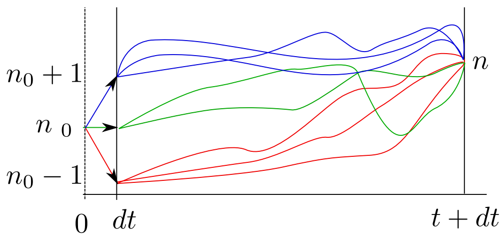

Fig. 2.3: Decomposition of the travel near the start state.

introduced $dx = 1/N$. This passage to continuum allows us to use standard tools of calculus. The rhs of first line of equation 2.2 for example reads

$$w^+(x-dx)p(x-dx,x_0,t) - w^+(x)p(x,x_0,t)$$

developping such expressions in powers of dx up to the second order, we get the forward diffusion equation :

$$\frac{\partial p(x,x_0,t)}{\partial t} = -\frac{\partial a(x)p(x,x_0,t)}{\partial x} + \frac{\partial b(x)p(x,x_0,t)}{\partial x^2}$$

where

$$\begin{aligned} a(x) &= \frac{1}{N}\left(w^+(x) - w^-(x)\right) \\ b(x) &= \frac{1}{2N^2}\left(w^+(x) + w^-(x)\right) \end{aligned}$$

$a(x)$ is called the drift term, $b(x)$ the diffusion coefficient. By applying the same procedure to the backward Kolmogorov equation, we get

$$\frac{\partial p(x,x_0,t)}{\partial t} = a(x)\frac{\partial p(x,x_0,t)}{\partial x_0} + b(x)\frac{\partial p(x,x_0,t)}{\partial x_0^2}$$

Of course, the same assymetry we had observed appears here between the forward and backward equations.

4 Generalisation.

In the above sections, we only considered transitions between neighbouring states $n \to n \pm 1$. We don't have to make such restrictions. Let us consider transitions from states n to $n+i$ with rate $W(n,i)$. Then, the same decomposition near the end point will bring us the general Kolmogorov equation

$$\frac{\partial P(n,n_0,t)}{\partial t} = \sum_i \left(W(n+i,i)P(n+i,n_0,t) - W(n,i)P(n,n_0,t)\right)$$

Taking the conitnuum limit $x = n/N$, $P(n, n_0, t)$ is replaced by $p(x, x_0, t)$ and $W(n-i, i)$ by $w(x-y, y)$, where $w(x-y, y)dy = W(n-i, i)$ Developing to the first order in $y = idy = i/N$, the term inside the rhs sum becomes

$$\sum_i \frac{\partial}{\partial x} y\, w(x, y) dy\, p(x, x_0, t)$$

and exchanging the summation over i and derivation over x :

$$\frac{\partial}{\partial x} p(x, x_0, t) \sum_i y\, w(x, y) dy$$

Here we recognize the term inside the sum which is the average of $w(x, y)$, taken at a fix x, which we will denote again by $a(x)$:

$$a(x) = \langle y \rangle_x = \int_I y w(x, y) dy$$

which is the average jump size from state x. The development to the second order will give us a term of the form

$$b(x) = \int_I y^2 w(x, y) dy = \left\langle y^2 \right\rangle_x$$

which is the second moment of the jumps originating at x.

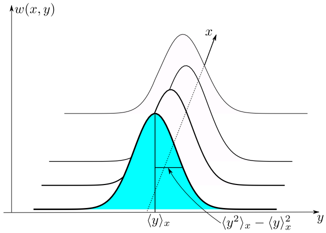

Fig. 4.1: Drift and diffusion coefficients for the general process, given jump rates $w(x, y)$.