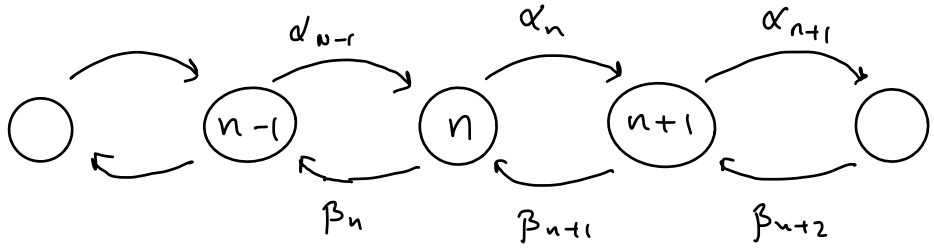
Lecture 5 – One-step processes

To practice a little bit master equations, we now look at particular type of stochastic processes that give rise to master equations we can systematically solve.

One-step processes are continous time Markov processes with range on the integers with transition probabilities only between adjacent sites. If α_n and β_n linear function of n, not both constant, the process is called linear



or

$$T_{m,n} = \begin{cases} \alpha_n \delta_{m,n+1} + \beta_n \delta_{m,n-1} & n \neq m \\ -(\alpha_n + \beta_n) & n = m \end{cases}$$

The Poisson process

$\beta_n = 0$; $\alpha_n = \lambda$ $\quad P_n(0) = \delta_{n,0}$

Master equation:

$$\frac{dP_n}{dt} = \lambda(P_{n-1} - P_n) \qquad n > 0$$

$$\frac{dP_0}{dt} = -\lambda P_0 \quad \Rightarrow \quad P_0(t) = e^{-\lambda t}$$

This gives

$$\frac{dP_1}{dt} = \lambda e^{-\lambda t} - \lambda P_1 \quad \Rightarrow \quad P_1(t) = \lambda t e^{-\lambda t}$$

Let's make the Ansatz $\quad P_n(t) = A_n(t) e^{-\lambda t}$

$$\frac{dP_n}{dt} = \frac{dA_n}{dt} e^{-\lambda t} - A_n(t) \lambda e^{-\lambda t} = \lambda (A_{n-1} - A_n) e^{-\lambda t}$$

or $\quad \frac{dA_n}{dt} = \lambda A_{n-1}$

By iteration we now have

$$A_0 = 1$$

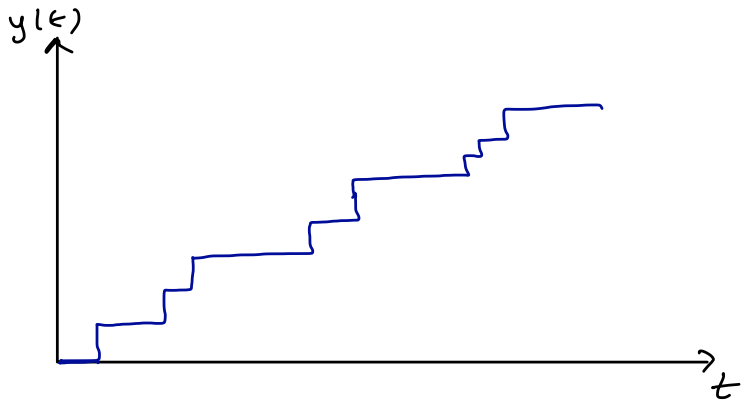
$$A_1 = \lambda t$$

$$\frac{dA_2}{dt} = \lambda A_1 = \lambda^2 t \quad \Rightarrow \quad A_2 = \frac{\lambda^2}{2} t^2$$

$$\cdots \quad A_n = \frac{\lambda^n}{n!} t^n \,, \quad \text{check} \quad \frac{dA_n}{dt} = \frac{\lambda^n}{(n-1)!} t^{n-1} = \lambda A_{n-1}$$

$$\Rightarrow \boxed{P_n(t) = \frac{(\lambda t)^n}{n!} e^{-\lambda t}}$$

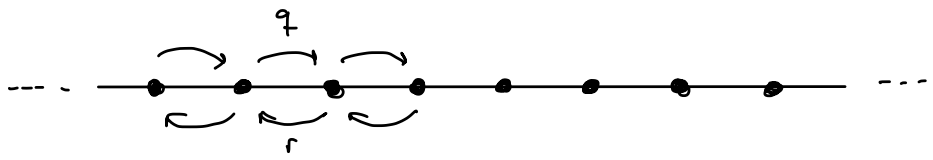
The Poisson process Y is defined as the number of steps taken between 0 and t. A sample function $y(t)$ looks like this:



Each step of same height but time of step randomly distributed.

Note: Compare this with the current plot in the last lecture.

Random walk



$$\frac{dP_n}{dt} = q P_{n-1} + r P_{n+1} - (q+r) P_n \qquad P_n(0) = \delta_{n,0}$$

$$\frac{d}{dt}\langle n \rangle = \frac{d}{dt}\sum_n n P_n = \sum_n n\left(q P_{n-1} + r P_{n+1} - (q+r) P_n\right)$$

$$= \sum_n \left(q(n+1) + r(n-1) - (q+r) n \right) P_n$$

$$= (q-r) \sum_n P_n = q - r$$

$\langle n \rangle(0) = 0$

$$\Rightarrow \quad \langle n \rangle(t) = (q-r)\,t$$ drift

Take from now on $q = r$.

Solve the master equation with Fourier transform

$$P_n = \frac{1}{2\pi}\int_0^{2\pi} \hat{P}_k\, e^{ikn}\, dk \quad , \quad \hat{P}_k = \sum_n P_n e^{-ikn}$$

$$\frac{d\hat{P}_k}{dt} = q \sum_n e^{-ikn}\left(P_{n-1} + P_{n+1} - 2P_n \right)$$

$$= q \sum_n e^{-ikn}\left(e^{ik} + e^{-ik} - 2 \right) P_n$$

$$= 2q\,(\cos k - 1)\,\hat{P}_k$$

$$\Rightarrow \quad \hat{P}_k(t) = e^{-2q(1-\cos k)t}$$ since $\hat{P}_k(0) = \sum_n \delta_{n,0} e^{-ikn} = 1$

Therefore

$$P_n(t) = \frac{1}{2\pi}\int_0^{2\pi} dk\; e^{-2qt(1-\cos k) + ikn} = e^{-2qt} I_n(2qt)$$

↑ modified Bessel function

Compare with the solution of the diffusion equation

$$\hat{P}_{diff}(k) = e^{-Dk^2 t}$$

Diffusion valid on large length scales, or small k.

$$2(1-\cos k) \simeq k^2 + \cdots$$

Approximately diffusive with $D = q$

We can further calculate

$$\langle n^2(t) \rangle = \sum_n n^2 P_n = -\frac{\partial^2}{\partial k^2} \sum_n P_n e^{-ikn} \Big|_{k=0}$$

$$= -\frac{\partial^2}{\partial k^2} \hat{P}_k \Big|_{k=0} = -\frac{\partial^2}{\partial k^2} e^{-2qt(1-\cos k)} \Big|_{k=0}$$

$$= \frac{\partial}{\partial k} 2qt \sin k \, e^{-2qt(1-\cos k)} \Big|_{k=0}$$

$$= 2qt$$

Some Probability theory

There are some general methods to solve for the probability distributions of linear one-step processes. We will demonstrate one of these below by study of decay processes and chemical reactions. But first we need some general probability theory.

Assume we have a random variable X defined on an interval I. Then, as usual

$$P(x) = \langle \delta(x - X) \rangle$$

$$\langle X \rangle = \int_I dx \, x P(x) \quad \text{etc.}$$

The characteristic function of the variable X is defined as

$$G(k) = \langle e^{ikX} \rangle = \int_I dx \, e^{ikx} P(x) \; ; \quad G(0) = 1$$

$G(k)$ is also the moment generating function since

$$G(k) = \sum_{m=0}^{\infty} \frac{(ik)^m}{m!} \langle x^m \rangle$$

By knowing $G(k)$ we can obtain the moments by taking derivatives

$$\frac{1}{i^n} \frac{\partial^n G}{\partial k^n} \bigg|_{k=0} = \langle x^n \rangle$$

The cumulant generating function is defined by $\ln G(k)$, with the cumulants being obtained by the Taylor expansion

$$\ln G(k) = \sum_{m=0}^{\infty} \frac{(ik)^m}{m!} \langle\langle x^m \rangle\rangle$$

The cumulants are then

$$\langle\langle x^n \rangle\rangle = \frac{1}{(i)^n} \frac{\partial^n \log G}{\partial k^n}\bigg|_{k=0}$$

The first few terms are:

$$\langle\langle x \rangle\rangle = \frac{1}{i}\frac{\partial \ln G}{\partial k} = \frac{1}{i}\frac{1}{G}\frac{\partial G}{\partial k}\bigg|_{k=0} = \langle x \rangle$$

$$\langle\langle x^2 \rangle\rangle = \frac{1}{(i)^2}\frac{\partial^2 \ln G}{\partial k^2} = \frac{1}{i^2}\frac{\partial}{\partial k}\left(\frac{1}{G}\frac{\partial G}{\partial k}\right) = \frac{1}{i^2}\left(\frac{-1}{G^2}\left(\frac{\partial G}{\partial k}\right)^2 + \frac{1}{G}\frac{\partial^2 G}{\partial k^2}\right)$$

$$= \langle x^2 \rangle - \langle x \rangle^2 = \sigma^2$$

etc.

Note: For some processes higher cumulants may not exist and the derivative is then only well defined up to the same n as number of moments that exist.

Q: Does this expansion remind you of other expansions you have met in your studies? Maybe in field theory and many-body theory.

For stochastic processes that take values only on the integers, it is sometimes convenient to use the probability generating function

$$F(z) = \langle z^x \rangle = \sum_n z^n P_n$$

which also generates moments by derivatives

$$F(z)\big|_{z=1} = 1$$

$$\frac{\partial F}{\partial z}\bigg|_{z=1} = \sum_n n P_n = \langle n \rangle$$

$$\frac{\partial^2 F}{\partial z^2}\bigg|_{z=1} = \sum_n n(n-1) P_n = \langle n^2 \rangle - \langle n \rangle \quad \text{etc.}$$

Radioactive decay

Assume we start with N radioactive nuclei.

Probability of decay in time $[t, t+dt]$ is $\gamma N\, dt$

Master equation

$$\frac{dP_n}{dt} = \sum_{n' \neq n} \left(W_{nn'} P_{n'} - W_{n'n} P_n \right)$$

$$= \gamma(n+1) P_{n+1} - \gamma n P_n$$

Let's calculate the probability generating function:

$$\frac{\partial F(z,t)}{\partial t} = \frac{d}{dt} \sum_{n=0}^{\infty} z^n P_n = \sum_{n=0}^{\infty} z^n \frac{dP_n}{dt}$$

$$= \gamma \sum_{n=0}^{\infty} z^n \left[(n+1) P_{n+1} - n P_n \right]$$

$$= \gamma \sum_{n=0}^{\infty} \left(\frac{\partial}{\partial z} z^{n+1} P_{n+1} - z \frac{\partial}{\partial z} z^n P_n \right)$$

$$= \gamma \frac{\partial}{\partial z} \sum_{n=1}^{\infty} z^n P_n - \gamma z \frac{\partial}{\partial z} \sum_{n=0}^{\infty} z^n P_n$$

$$= \gamma (1-z) \frac{\partial F}{\partial z}$$

Note: we can extend the summation range in the first term to start from $n=0$ since the term $z^0 P_0$ is independent of z.

We have now converted the master equation into the partial differential equation

$$\boxed{\frac{\partial F}{\partial t} - \gamma(1-z) \frac{\partial F}{\partial z} = 0}$$

How do we solve such equations?

We can use the method of characteristics. I describe this method later in these notes, but let's just use it here to solve this example.

Now, imagine first that F was independent of z, t. Then (z, t, F) would span a three dimensional manifold. Our equation for F defines a 2 dimensional submanifold in this space, which can be characterized by a set of integral curves parameterized by the real parameter s, such that

$$\begin{aligned} z &= z(s) \\ t &= t(s) \\ F &= F(z(s), t(s)) \end{aligned}$$

Then

$$\frac{dF}{ds} = \frac{dz}{ds}\frac{\partial F}{\partial z} + \frac{dt}{ds}\frac{\partial F}{\partial t} = 0$$

if

$$\frac{dz}{ds} = -\gamma(1-z) \quad \text{and} \quad \frac{dt}{ds} = 1$$

We now have three ordinary differential equations to solve.

First $\frac{dt}{ds} = 1 \Rightarrow t = t_0 + s$ We can choose our parameterization such that $t_0 = 0$

$$\int_{z_0}^{z} \frac{dz'}{1-z} = -\gamma \int_0^s ds' \Rightarrow -\ln\frac{1-z}{1-z_0} = -\gamma s$$

or

$$1 - z = (1-z_0)e^{\gamma s}$$

Last equation tells us that $F(z(s), t(s)) = \text{constant} = F(z_0, 0)$

But our initial condition at $t=0$ are

$$P_n(0) = \delta_{N,N} \Rightarrow F(z_0, 0) = \sum_n z_0^n P_n = z_0^N$$

Now, using $s=t$ we then have

$$\boxed{F(z,t) = \left[1 - (1-z)e^{-\gamma t}\right]^N}$$

With this we get

$$\langle n(t) \rangle = \left.\frac{\partial F}{\partial z}\right|_{z=1} = N e^{-\gamma t} \to 0 \text{ as } t \to \infty$$

That is

$$P_0 \to 1 \quad \text{and} \quad P_n \to 0 \text{ for } n > 0$$

$n = 0$ is called an absorbing state

$n > 0$ are transient states.

By Taylor expanding the probability generating function, we further get

$$F(z,t) = \left[(1-e^{-\gamma t}) + z e^{-\gamma t}\right]^N$$

$$= \sum_{n=0}^{N} \binom{N}{n} (1-e^{-\gamma t})^{N-n} z^n e^{-\gamma n t}$$

$$= \sum_{n} z^n P_n(t)$$

$$\Rightarrow \quad P_n(t) = \begin{cases} \binom{N}{n} (1-e^{-\gamma t})^{N-n} e^{-\gamma n t} & 0 \le n \le N \\ 0 & n > N \end{cases}$$

Here I follow D. Arovas lecture notes.

We want to solve a partial differential equation of the form

$$a_1(\vec{x},F)\frac{\partial F}{\partial x_1} + a_2(\vec{x},F)\frac{\partial F}{\partial x_2} + \cdots + a_N(\vec{x},F)\frac{\partial F}{\partial x_N} = b(\vec{x},F) \qquad (\#)$$

where $\vec{x} = (x_1, x_2, \ldots, x_N)$ ($\vec{x} = (z,t)$ in the decay example) and $a_i(\vec{x},t)$ and $b(\vec{x},F)$ are functions of $\vec{x}$ and F, but not of derivatives of F. Such equations are called "quasilinear". A solution $F(\vec{x})$ of (#) defines an N dimensional manifold in $N+1$ dimensional space (with coordinates $(\vec{x},F)$). This manifold can be characterized by a set of integral curves, or characteristic curves $x_j(s)$ parameterized by the real variable s, and defined by

$$\frac{dx_j}{ds} = a_j(x, F(x)) \qquad (*)$$

The variation of F with s is given by

$$\frac{dF}{ds} = \sum_j \frac{\partial F}{\partial x_j}\frac{dx_j}{ds} = \vec{\nabla}_x F \cdot \vec{a} = b(\vec{x},F) \qquad (**)$$

This means we have replaced the original partial differential equation with a set of $N+1$ ordinary differential equations. This needs to be supplemented by initial conditions

$$g(\vec{x},F)\big|_{s=0} = 0$$

Chemical reaction

$$A \underset{b}{\overset{a}{\rightleftharpoons}} B$$

Total sum of A and B molecules $= N$

$N_A = n$, $N_B = N - n$

Transition probability $A \to B \sim a N_a = an$

$B \to A \sim b N_b = b(N-n)$

Master equation:

$$\frac{dP_n}{dt} = a(n+1) P_{n+1} + b(N-(n-1)) P_{n-1} - (an + b(N-n)) P_n$$

That is:

$$\frac{\partial F}{\partial t} = \sum_n a(n+1) z^n P_{n+1} + b(N-n+1) z^n P_{n-1} - (an + b(N-n)) z^n P_n$$

$$= (a + bz)(1-z) \frac{\partial F}{\partial z} - bN(1-z) F$$

↑ Ex: verify this

Taking $n(0) = N$, i.e., only A molecules at $t = 0$ this has solution:

$$F(z,t) = \sum_{n=0}^{N} \binom{N}{n} \frac{(r - r e^{-(a+b)t})^{N-n} (1 + r e^{-(a+b)t})^n}{(1+r)^N} z^n$$

where $r = a/b$

Ex: Derive this result