Lecture 26

08.05.2019

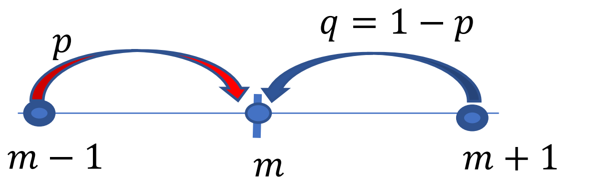
Master equations for Gaussian and Poisson stochastic processes

What is a master equation?

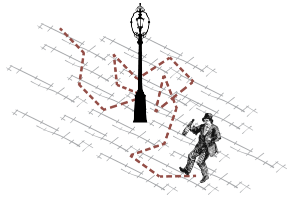
- Describes the time evolution of the probability distribution function for a stochastic process. Also called the rate equation

  - Gaussian process – Random walker, Diffusion equation

  - Poisson equation – Rate equation, Poisson distribution



Random walker



- At $N + 1$, we have two options:
  - RW takes a left jump $m + 1 \to m$
  - RW takes a right jump $m - 1 \to m$

Particle stochastic dynamics

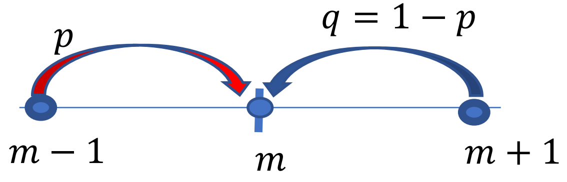
$$\mathrm{m}_{\mathrm{n+1}} = \mathrm{m}_{\mathrm{n}} + \Delta x_n, \quad \Delta \mathrm{x}_{\mathrm{n}} = \begin{cases} +1, \text{with probability p} \\ -1, \text{with probability } q \end{cases}$$

Master equation for a random walker (RW)

Probability density that a RW is at position m at time $t + \Delta t$ depends only on the probability density at the previous time t and the jump probability per unit step (no memory).

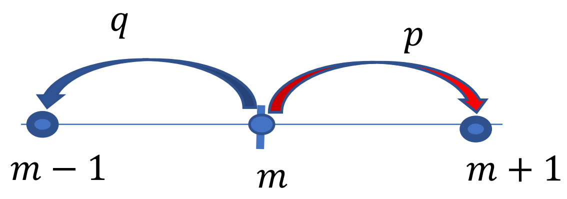
This means that the probability $\mathrm{P}(\mathrm{m}, t + \Delta t)$ that the RW is at position m at time $t + \Delta t$ depends on the probabilities at the previous times step t as:

i) If nothing happens at position m, then the probability does not change equals $\mathrm{P}(\mathrm{m}, t)$



ii) If the RW was at $m - 1$ and moves to the right or if jumps to the left from $m + 1$, then we have a contribution

$$pP(m-1, t) + qP(m+1, t)$$



iii) If it was at m and moves either right or left, then the change in probability is proportional to

$$-pP(m, t) - qP(m1, t) = -P(m, t)$$

Collecting all three possibilities, we can link the probabilities between successive timesteps as

$$P\,(m, t + \Delta t) = P(m, t) + pP(m-1, t) + qP(m+1, t) - P(m, t)$$

Hence the master equation is

$$\boldsymbol{P\,(m, t + \Delta t) = pP(m-1, t) + qP(m+1, t)}$$

Master equation

By Taylor expansion around t and rearranging terms, we obtain:

$$\frac{\partial P(m,t)}{\partial t} = \frac{p}{\Delta t}[P(m-1,t) - P(m,t)] + \frac{q}{\Delta t}[P(m+1,t) - P(m,t)]$$

Transition rates (hoping rates) for the right and left jumps

$$\frac{p}{\Delta t} \equiv w_{m\leftarrow m-1} = w_{m+1\leftarrow m}$$

$$\frac{q}{\Delta t} \equiv w_{m\leftarrow m+1} = w_{m-1\leftarrow m}$$

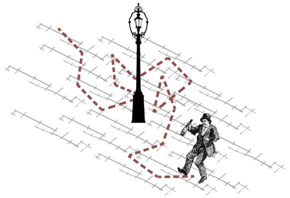
$$\frac{\partial}{\partial t}P(m,t) = w_{m\leftarrow m+1}P(m+1,t) + w_{m\leftarrow m-1}P(m-1,t) - w_{m-1\leftarrow m}P(m,t) - w_{m+1\leftarrow m}P(m,t)$$

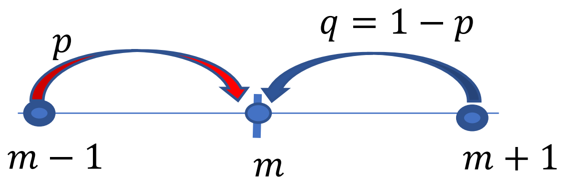
$$\frac{\partial P(m,t)}{\partial t} = \sum_n [w_{m\leftarrow n}P(n,t) - w_{n\leftarrow m}P(m,t)]$$

Where $w_{m\leftarrow n}$ are the transition rates from state n to state m, satisfying that

$$\sum_m w_{m\leftarrow n} = 1, for\ all\ n$$

Diffusion equation





For continuous space and time, the master equation for the probability density becomes the diffusion equation

$$\frac{\partial P(m,t)}{\partial t} = \frac{p}{\Delta t}[P(m-1,t) - P(m,t)] + \frac{q}{\Delta t}[P(m+1,t) - P(m,t)] \qquad (1)$$

We introduce $x = m\Delta x$ as the RW position along the continuous line. In the limit of $\Delta x \to 0$, we Taylor expand around x

$$P(x \pm \Delta x, t) - P(x,t) \approx \pm \Delta x \frac{\partial P}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 P}{\partial x^2}$$

Hence Eq. (1) becomes

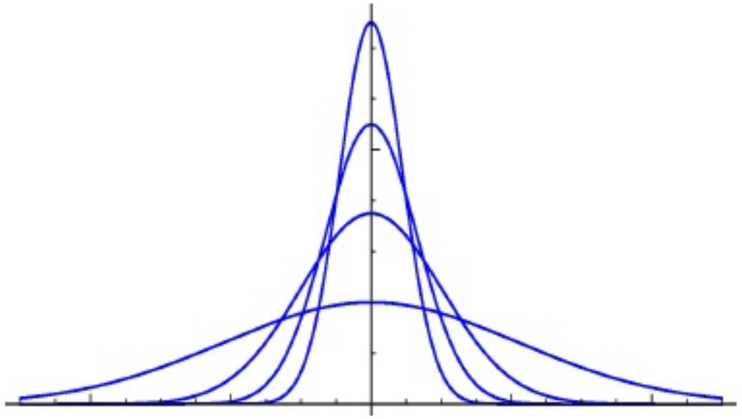
$$\frac{\partial P(x,t)}{\partial t} = -v \frac{\partial P(x,t)}{\partial x} + D \frac{\partial^2 P(x,t)}{\partial x^2}$$

$v = (p - q)\frac{\Delta x}{\Delta t}$ is the drift velocity for a biased RW

$D = \frac{\Delta x^2}{2\Delta t}$ is the diffusion coefficient of the RW determined by the microscopic variables (stepsize and time interval).

Diffusion equation in 1D: $v = 0$

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}, \text{ with initial condition } P(x,t) = \delta(x) \qquad (1)$$



Can be solved by Fourier transform $\hat{P}(k,t) = \int dk\, e^{ikx} P(x,t) \rightarrow \hat{P}(k,0) = 1$. *Apply FT to Eq. (1)*

$$\frac{d\hat{P}(k,t)}{dt} = -Dk^2\hat{P}(k,t) \rightarrow \hat{P}(k,t) = \hat{P}(k,0)e^{-Dk^2t}$$

By Inverse FT

$$P(x,t) = \frac{1}{2\pi}\int dk\, e^{-ikx}\hat{P}(k,t)$$

Gaussian probability distribution function

$$P(x,t) = \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}$$

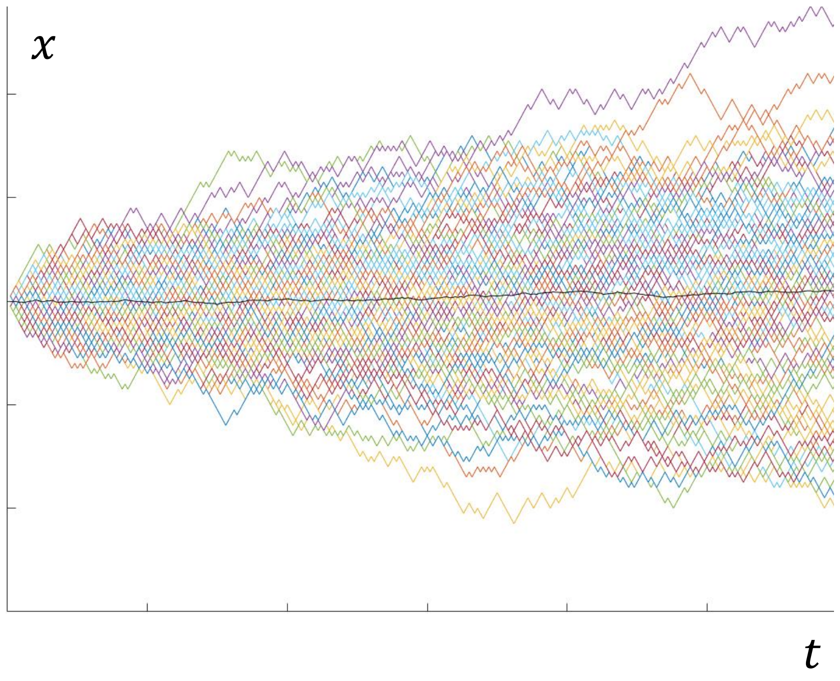
Gaussian PDF

$$\boldsymbol{P(x,t) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}}$$

Has two parameters: mean $\boldsymbol{\mu}$ and standard deviation $\boldsymbol{\sigma}$

Diffusion equation: mean dislacement

$$\frac{\partial P(x,t)}{\partial t} = D\,\frac{\partial^2 P(x,t)}{\partial x^2}$$



Average displacement is calculated as the first moment of the PDF

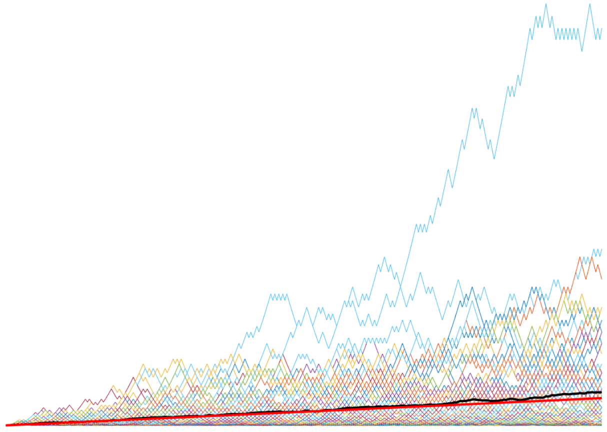
$$\mu = \langle x\rangle(t) = \int dx\; x\; P(x,t)$$

The evolution of the average displacement can be determined from the diffusion equation as

$$\frac{d}{dt}\langle x\rangle = \int dx\; x\,\frac{\partial P(x,t)}{\partial t} = D\int dx\; x\,\frac{\partial^2 P(x,t)}{\partial x^2} = 0$$

$$\mu(t) = \langle x\rangle(0) = 0$$

Diffusion equation: normal dispersion law



$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}$$

Mean square displacement can be calculated from the second moment

$$\sigma^2(t) = \langle x^2\rangle(t) = \int dx\, x^2\, P(x,t)$$

The evolution of the mean square displacement follows from the diffusion equation as

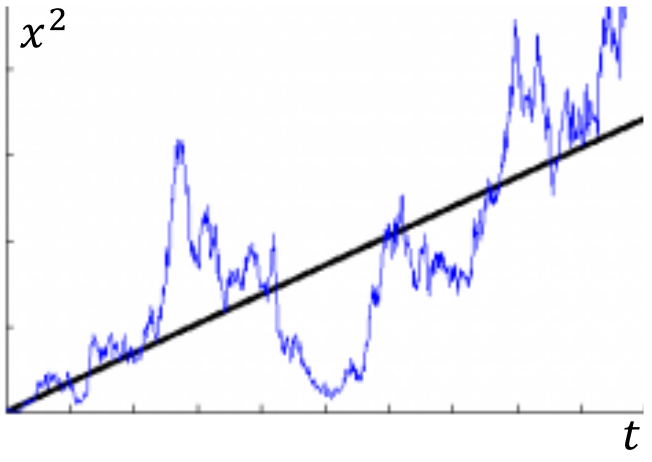
$$\frac{d}{dt}\langle x^2\rangle = \int dx\, x^2 \frac{\partial P(x,t)}{\partial t} = D\int dx\, x^2 \frac{\partial^2 P(x,t)}{\partial x^2}$$

After integration by parts

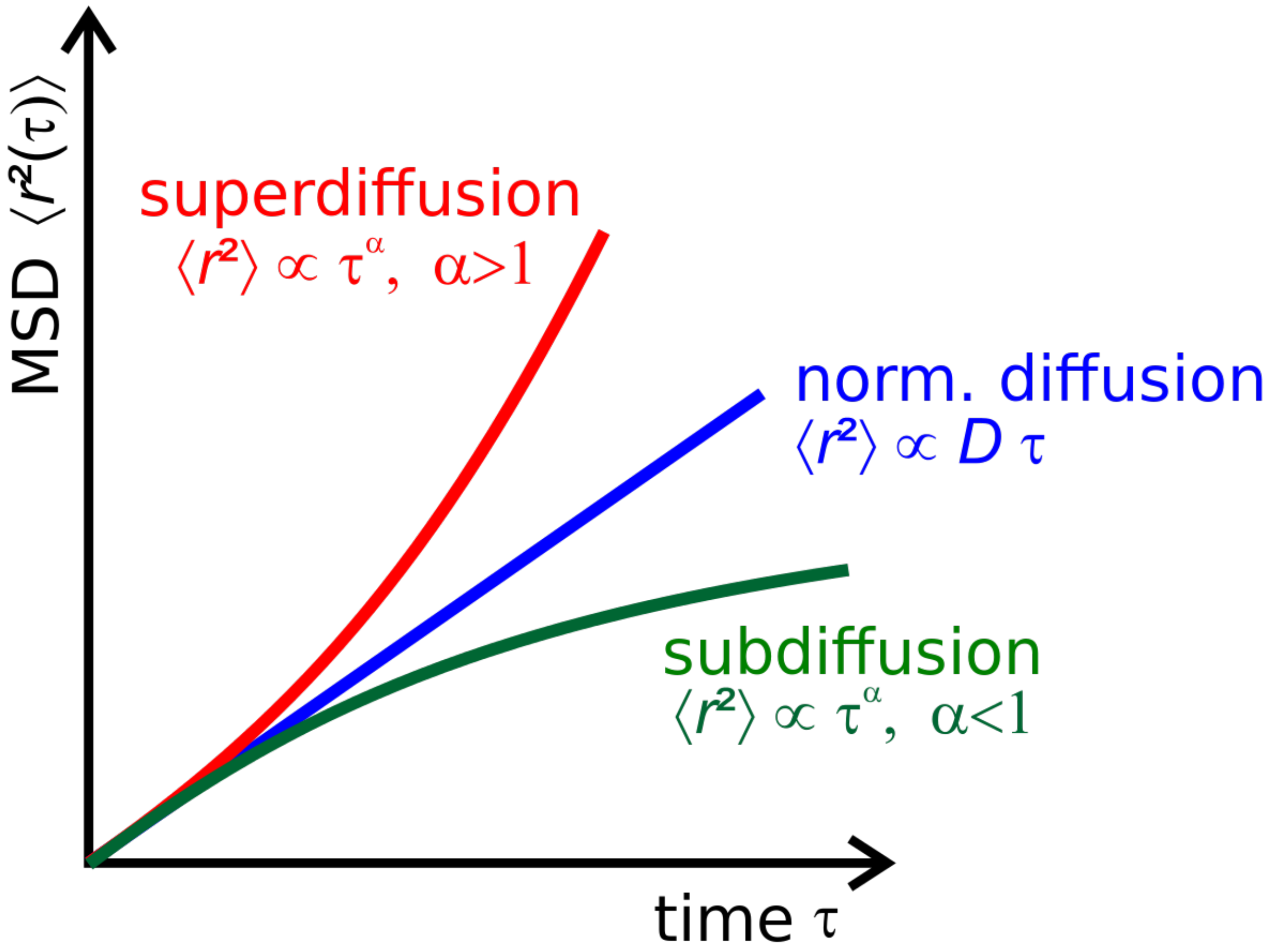
$$\frac{d}{dt}\langle x^2\rangle = -2D\int dx\, x\frac{\partial P(x,t)}{\partial x} = 2D\int dx\, P(x,t)$$

Using the normalization condition

$$\frac{d}{dt}\langle x^2\rangle = 2D \rightarrow \langle x^2\rangle(t) = 2Dt$$



Dispersion law



Poisson stochastic process

Describes discrete and independent random events that occur at a fixed rate, λ

Two important examples of such Poisson processes: **radioactive decay** and **death process in population dynamics**

Radioactive decay example:

Caesium-137 is a radioactive isotope of caesium which is formed by the nuclear fission of uranium- 235 and other fissionable isotopes in nuclear reactors and nuclear weapons. It has a half-life of 27 years (it takes 27 years for half of the radioactive nuclei to disintegrate)

Survival probability for one nucleus: $\boldsymbol{p_t = e^{-\lambda t}}$. The decay rate λ is estimated from the half-life time

$$\frac{1}{2} = e^{-\lambda\times 27} \rightarrow \lambda = \frac{\ln 2}{27} yr^{-1} = 8.2\times 10^{-10} s^{-1}$$ *very small decay rate!*

However, consider a small sample of $1\mu g\ Cs^{137} \rightarrow N \approx 10^{15}$ nuclei. Then, the mean decay rate $N\lambda \approx 8.2\times 10^{5}\ decays/s$

What is the probability of having m out of N events with decaying nuclei?

Radioactive decay

Decay probability for one nucleus: $\boldsymbol{q_t = 1 - e^{-\lambda t}}$

The probability of having n out of N **decay** events is given by the **binomial distribution**

$$Q_t(m) = \frac{N!}{m!\,(N-m)!}(1-p_t)^m p_t^{N-m}$$

This is equivalent to the probability that $n = N - m$ nuclei **survived** the decay

$$P_t(n) = \frac{N!}{n!\,(N-n)!}p_t^n(1-p_t)^{N-n}$$

Poisson distribution

In the limit $\boldsymbol{N \to \infty, and\ p_t \to 0}$ with fixed $Np_t = \mu_t$, we have that the probability of n surviving nuclei can be written as

$$P_{\mu_t}(n) = \frac{\mu_t^n}{n!}\frac{N!}{(N-n)!}\frac{1}{N^n}\left(1-\frac{\mu_t}{N}\right)^{N-n}$$

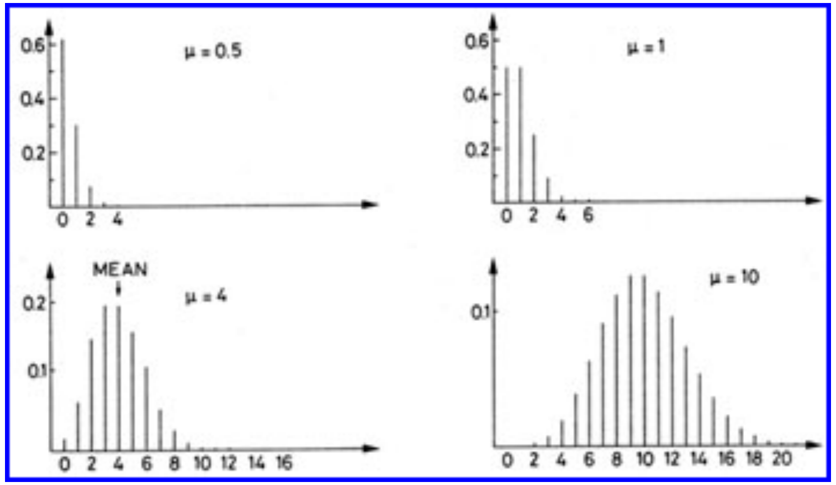
(Average) n surviving nuclei is small compared to the total number N

$$P_{\mu_t}(n) = \frac{{\mu_t}^n}{n!}\frac{N(N-1)\cdots(N-n)(N-n-1)\cdots 1}{(N-n)(N-n-1)\cdots 1}\frac{1}{N^n}e^{-\mu_t}$$

Poisson distribution

$$P_{\mu_t}(n) = \frac{{\mu_t}^n}{n!}e^{-\mu_t}, \quad Q_{\mu_t}(n) = \frac{{\mu_t}^{N-n}}{(N-n)!}e^{-\mu_t}$$

Poisson distribution



$$P_{\mu_t}(n) = \frac{\mu_t^n}{n!} e^{-\mu_t}$$

Normalization condition

$$\sum_n P_{\mu_t}(n) = \sum_n \frac{\mu_t^n}{n!} e^{-\mu_t} = 1$$

Average number of surviving nuclei $\langle n \rangle = Ne^{-\lambda t}$

$$\langle n \rangle = \sum_n n\, P_{\mu_t}(n) = e^{-\mu_t} \sum_n \frac{\mu_t^n}{n!} n = e^{-\mu_t} \left[\mu_t \frac{d}{d\mu_t} \right] e^{\mu_t} = \mu_t \rightarrow \langle n \rangle = \mu_t = Np_t$$

Mean-square number of surviving nuclei $\langle \Delta n^2 \rangle = Ne^{-\lambda t} = \langle n \rangle$

$$\langle n^2 \rangle = \sum_n n^2 P_{\mu_t}(n) = e^{-\mu_t} \sum_n \frac{\mu_t^n}{n!} n^2 = e^{-\mu_t} \left[\mu_t \frac{d}{d\mu_t} \right]^2 e^{\mu_t} = \mu_t^2 + \mu_t$$

$$\langle n^2 \rangle = \mu_t^2 + \mu_t \rightarrow \langle \Delta n^2 \rangle = \langle n^2 \rangle - \langle n \rangle^2 = \mu_t$$

Standard deviation: $\sqrt{\langle \Delta n^2 \rangle} = \sqrt{\langle n \rangle}$

(variance equal mean)→ Poisson fluctuations: $\frac{\sqrt{\langle \Delta n^2 \rangle}}{\langle n \rangle} = \frac{1}{\sqrt{\langle n \rangle}} \approx \frac{1}{\sqrt{N}}$

Master equation for Poisson process

Consider N radioactive nuclei at $t = 0$, such that $P(n, 0) = \delta_{n,N}$. Initially, all N nuclei survived the decay: $P(N, 0) = 1$ and $P(N-1,0) = P(N-2,0) = \cdots P(0,0) = 0$. However, as time goes by, we have a non-zero probability that only a fraction of the total number survived the decay at a given time. That fraction gets smaller and smaller, and evetually after sufficiently long time we expect no one surviving the decay $P(0, t \to \infty) = 1$.

At a time t between these two extremes, we expect that there is a finite probability $P(n, t)$ of having n out of N nuclei surviving the decay. We want to derive how this probability depends on the probability at the previous time.

Similarly to RW master equation, the probability $P(n, t)$ changes because of two possible scenarios:

i) Suppose that there were $(n+1)$ at t and that there is a nucleus (any of them!) will decay. The decay probability for a specific nucleus is $\mathrm{q}_{\Delta \mathrm{t}} = \left(1 - e^{-\lambda \Delta t}\right)$. But, any of the $(n+1)$ nuclei can decay, so the change that one of them will do that is larger and given by the binomial distribution $(n+1) q_{\Delta t} p_{\Delta t}^{n}$. The probability for $(n+1)$ survivers at t is $P(n+1, t)$, hence this scenario gives a contribution$(n+1) q_{\Delta t} p_{\Delta t}^{n} P(n+1, t)$.

ii) Suppose that there were (n) at t and a nucleus (any of them) will decay. The probability that one out of (n) will decay is the binomial distribution $n q_{\Delta t} p_{\Delta t}^{n-1}$. The probability for (n) survivers at t is $P(n, t)$, hence change in probability is proportional to $-\mathrm{n} \mathrm{q}_{\Delta \mathrm{t}} p_{\Delta t}^{n-1} P(n, t)$.

$$P(n, t + \Delta t) = P(n, t) + (n+1) q_{\Delta t} p_{\Delta t}^{n} P(n+1, t) - \mathrm{n} \mathrm{q}_{\Delta \mathrm{t}} p_{\Delta t}^{n-1} P(n, t)$$

Master equation for Poisson process

Consider N radioactive nuclei at $t = 0$, such that $P(n, 0) = \delta_{n,N}$. Initially, all N nuclei survived the decay: $P(N, 0) = 1$ and $P(N-1,0) = P(N-2,0) = \cdots P(0,0) = 0$. However, as time goes by, we have a non-zero probability that only a fraction of the total number survived the decay at a given time. That fraction gets smaller and smaller, and evetually after sufficiently long time we expect no one surviving the decay $P(0, t \to \infty) = 1$.

At a time t between these two extremes, we expect that there is a finite probability $P(n, t)$ of having n out of N nuclei surviving the decay. We want to derive how this probability depends on the probability at the previous time.

$$P(n, t + \Delta t) = P(n, t) + (n + 1) q_{\Delta t} p_{\Delta t}^{n} P(n + 1, t) - \mathrm{n} \mathrm{q}_{\Delta t} p_{\Delta t}^{n-1} P(n, t)$$

Taylor expanding around t:

$$\frac{\partial P(n,t)}{\partial t} = \frac{\left(1-e^{-\lambda \Delta t}\right) e^{-n\lambda \Delta t}}{\Delta t}(n + 1) P(n + 1, t) - \frac{\left(1-e^{-\lambda \Delta t}\right) e^{-(n-1)\lambda \Delta t}}{\Delta t} n P(n, t)$$

Taking the limit of $\Delta t \ll 1$

$$\frac{\partial P(n, t)}{\partial t} = \lambda(n + 1) P(n + 1, t) - \lambda n P(n, t), \qquad n = 1, \cdots N \qquad (1)$$

Where $\frac{q_{\Delta t}}{\Delta t} = \frac{1-e^{-\lambda \Delta t}}{\Delta t} \to \lambda$ is a fixed decaying rate.

Master equation: Generating function

We can solve the master equation for $P(n,t)$ by using the *generating function method*: We define the **generating function** as

$$G(s,t) = \sum_{n=0}^{N} s^n P(n,t), \qquad s < 1$$

Using together with Eq. (1), we derive the evolution equation for the generating function as

$$\frac{\partial G(s,t)}{\partial t} = \lambda \sum_{n}^{N} s^n [(n+1)P(n+1,t) - nP(n,t)]$$

$$\frac{\partial G}{\partial s} = \sum_{n=0}^{N} s^{n-1}\, nP(n,t) = \sum_{n=1}^{N} s^{n-1}\, nP(n,t) = \sum_{n=0}^{N} s^n\,(n+1)P(n+1,t)$$

$$\frac{\partial G(s,t)}{\partial t} = \lambda \left(\frac{\partial G}{\partial s} - s\frac{\partial G}{\partial s} \right)$$

Master equation: Generating function

$$\frac{\partial G(s,t)}{\partial t} = \lambda(1-s)\frac{\partial G}{\partial s}, \qquad G(s,t) = \sum_{n=0}^{N} s^n P(n,t), \qquad s < 1$$

Substitute $x = \ln(1-s)$

$$\frac{\partial G(s,t)}{\partial t} + \lambda\frac{\partial G}{\partial x} = 0 \to G(s,t) = g(x-\lambda t)$$

$g(x-\lambda t)$ arbitrary function determined from the initial condition

For $P_n(0) = \delta_{n,N} \to G(s,0) = s^N$, hence

$g(x) = s^N = (1-e^x)^N$ and in general $g(x-\lambda t) = \left(1-e^{x-\lambda t}\right)^N$

$$G(s,t) = \left(1-e^{x-\lambda t}\right)^N = \left[1-(1-s)e^{-\lambda t}\right]^N = \sum_{n=0}^{N} s^n \frac{N!}{n!\,(N-n)!} e^{-n\lambda t}\left(1-e^{-\lambda t}\right)^{N-n}$$

Probability of have n surving nuclei at time t is $P(n,t) = \frac{N!}{n!(N-n)!} p_t^n (1-p_t)^{N-n}, \; p_t = e^{-\lambda t}$

Master equation: Poisson process

Probability of have n surving nuclei at time t is Binomial Distribution

$$P(n,t) = \frac{N!}{n!\,(N-n)!} p_t^n (1-p_t)^{N-n}, \qquad p_t = e^{-\lambda t}$$

On long time limit and large sample, we recover as the limit distribibition the Poisson distribution

$$P(n,t) \to_{\substack{N\to\infty \\ p_t\to 0}} \frac{\mu_t^n}{n!} e^{-\mu_t}, \qquad \mu_t = N p_t$$

Master equation: moment evolution

$$\frac{\partial P(n,t)}{\partial t} = \lambda[(n+1)P(n+1,t) - nP(n,t)], \qquad n = 1, \cdots N$$

How does the mean number of surviving nuclei $\langle n \rangle$ change with time?

$$\frac{d\langle n \rangle}{dt} = \sum_{n=0} n \frac{\partial P(n,t)}{\partial t} = \lambda \sum_{n=0} [n(n+1)P(n+1,t) - n^2 P(n,t)]$$

$$\frac{d\langle n \rangle}{dt} = \lambda \sum_{n=0} [(n-1)nP(n,t) - n^2 P(n,t)] = -\lambda \langle n \rangle$$

$$\frac{d\langle n \rangle}{dt} = -\lambda \langle n \rangle \rightarrow \langle n \rangle = N e^{-\lambda t} = \mu_t$$

Master equation: moment evolution

$$\frac{\partial P(n,t)}{\partial t} = \lambda(n+1)P(n+1,t) - \lambda nP(n,t), \qquad n = 1, \cdots N$$

How does the mean-square number of surviving nuclei $\langle n^2 \rangle$ change with time?

$$\frac{d\langle n^2 \rangle}{dt} = \sum_{n=0} n^2 \frac{\partial P(n,t)}{\partial t} = \lambda \sum_{n=0} [n^2(n+1)P(n+1,t) - n^3 P(n,t)]$$

$$\frac{d\langle n^2 \rangle}{dt} = \lambda \sum_{n=0} [(n-1)^2 nP(n,t) - n^3 P(n,t)]$$

$$\frac{d\langle n^2 \rangle}{dt} = \lambda[\langle n \rangle - 2\langle n^2 \rangle]$$

Master equation: moment evolution

How does the mean-square number of surviving nuclei $\langle n^2\rangle$ change with time?

$$e^{2\lambda t}\frac{d\langle n^2\rangle}{dt} = e^{2\lambda t}\Gamma[\langle n\rangle - 2\langle n^2\rangle]$$

$$e^{2\lambda t}\frac{d\langle n^2\rangle}{dt} + 2\lambda e^{2\lambda t}\langle n^2\rangle = e^{2\lambda t}\Gamma\langle n\rangle \rightarrow \frac{d}{dt}\left[e^{2\lambda t}\langle n^2\rangle\right] = N\lambda e^{\lambda t}$$

$$e^{2\lambda t}\langle n^2\rangle - N^2 = N\,(e^{\lambda t} - 1)$$

$$\langle n^2\rangle = N^2 e^{-2\lambda t} + N\,(e^{-\lambda t} - e^{-2\lambda t})$$

Standard deviation in the fluctuations

$$\langle \Delta n^2\rangle = Ne^{-\lambda t}\left(1 - e^{-\lambda t}\right) = Np_t(1 - p_t) \rightarrow_{\substack{p_t\rightarrow 0\\ N\rightarrow\infty}} Np_t = \mu_t$$