13th January 2025 (Monday) →

Master equation →

$$\frac{\partial P(x,t)}{\partial t} = \int dx' \left[w(x|x') P(x',t) - w(x'|x) P(x,t) \right]$$

Transition probabilities

We often write,

$$w(x|x') = f(x-x'|x') = f(y|x-y)$$ → Convenient representation.

∴ On this change of variable,

$$\frac{\partial P(x,t)}{\partial t} = \int dy \left[f(y|x-y) P(x-y,t) - f(x-y|x) P(x,t) \right]$$

If $x-y$ is small enough, we can hope to Taylor expand.

We define,

$$R_n(x) = \int dy \; y^n f(y|x)$$ → Not quite a moment

and Taylor expand

$$\frac{\partial P(x,t)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial x^n} \left[R_n(x) P(x,t) \right]$$ □ Do it yourself

If this series truncates/terminates at $n=2$ (exactly)

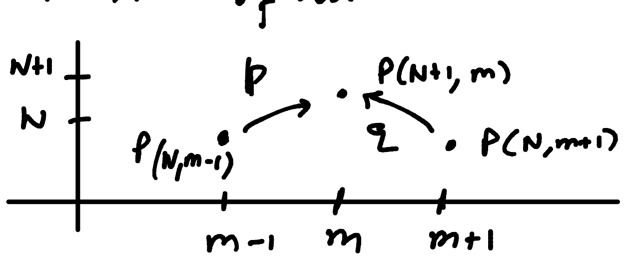
$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x} \left[R_1(x) P(x,t) \right] + \frac{1}{2} \frac{\partial}{\partial x^2} \left[R_2(x) P(x,t) \right]$$

(Fokker-Planck Eqn)

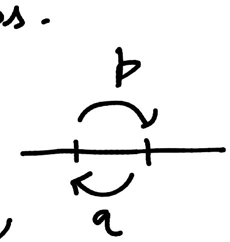
(*) Pawula's Theorem → If this series does not truncate at $n=2$, it does not terminate for any finite n.

Coming back to Random walk,
We reformulate in the language of master equation.

$P_N(m)$ = Prob of walker at m after N steps.



If,



$$\therefore P(N+1, m) = p\, P(N, m-1) + q\, P(N, m+1)$$

(For ease of calculation, we assume $p = q$ here (unbiased walker)) →

$$\Rightarrow P(N+1, m) = \frac{1}{2} \left[P(N, m-1) + P(N, m+1) \right]$$

$$\Rightarrow P(N+1,m) - P(N,m) = \frac{1}{2}\left[P(N,m-1) + P(N,m+1)\right] - P(N,m)$$

Now we assign finite changes of Δx to lattice steps, i.e,

$$X = m\Delta x$$

and time steps,

$$t = N\Delta t$$

$$\therefore \quad P(N+1,m) - P(N,m) = \Delta t \frac{\partial P}{\partial t} = \frac{1}{2}(\Delta x)^2 \frac{\partial^2 P}{\partial x^2}$$

$$\Rightarrow \boxed{\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2}} \quad \text{(Diffusion equation)}$$

☐ Do for general biased walker

Where, $D = \frac{(\Delta x)^2}{2(\Delta t)}$ → Diffusion constant.

How do we solve IVP of diffusion equation?

$$\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2}, \quad P(x,0) = \delta(x), \quad P(x,t) \to 0 \text{ as } x \to \pm\infty$$

The solution is given by,

$$P(x,t) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[\frac{-x^2}{2\sigma^2}\right] \longrightarrow \text{Normal distribution.}$$

$$\sigma^2 = 2Dt \longrightarrow \text{Thus, the distribution spreads out in time.}$$

☐ Do it manually.

The usual Normal distribution →

$$P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$

Now we show that in the continuum limit, the binomial distribution becomes the normal distribution.

$$P(m,N) = \frac{N!}{\left(\frac{N+m}{2}\right)!\left(\frac{N-m}{2}\right)!} p^{\left(\frac{N+m}{2}\right)} q^{\left(\frac{N-m}{2}\right)}$$

(*) We will now assume Stirling's formula (TBD in 1-2 classes from now)

Now,

$$\ln(P(m,N)) = \ln(N!) - \ln\left(\left(\frac{N+m}{2}\right)!\right) - \ln\left(\left(\frac{N-m}{2}\right)!\right) + \frac{N+m}{2}\ln p + \frac{N-m}{2}\ln q$$

Stirling's approx →

If N is large,

$$\ln(N!) \approx \left(N+\frac{1}{2}\right)\ln(N) - N + \frac{1}{2}\ln(2\pi) + O\left(\frac{1}{N}\right)$$

We put the approximation back in,

$$\therefore \ln(p(m,N)) = \left(N+\frac{1}{2}\right)\ln N - \left(\frac{N+m}{2}+\frac{1}{2}\right)\ln\left(\frac{N+m}{2}\right) - \left(\frac{N-m}{2}+\frac{1}{2}\right)\ln\left(\frac{N-m}{2}\right)$$
$$- N + \frac{N+m}{2} + \frac{N-m}{2} - \frac{1}{2}\ln(2\pi)$$
$$+ \frac{N+m}{2}\ln p + \frac{N-m}{2}\ln q$$

Note these substitutions, and calculate on your own.

$\delta_m = m - \langle m\rangle \rightarrow$ Deviation of m

$$m = \langle m\rangle + \delta_m$$
$$= N(p-q) + \delta_m$$

↳ As we derived

$$\therefore \frac{N+m}{2} = Np + \frac{\delta_m}{2} = Np\left[1+\frac{\delta_m}{2Np}\right]$$

$$\therefore \frac{N-m}{2} = Nq - \frac{\delta_m}{2} = Nq\left[1-\frac{\delta_m}{2Nq}\right]$$

If N is very large (as we have already assumed),

$$\ln(1\pm x) = \pm x - \frac{1}{2}x^2$$

(What? must have made a mistake here)

Solving with all this, we get,

$$P(m,n) = \frac{1}{\sqrt{2\pi\sigma_m^2}}\exp\left[-\frac{1}{2}\frac{(\delta m)^2}{\sigma_m^2}\right]$$

$$\sigma_m^2 = 4Npq$$

(*) ☐ Do this entire derivation manually.

We take the fourier transform of the probability distribution (for cumulants)

$$\tilde{p}(k) = \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(x-\mu)^2}{2\sigma^2} - ikx\right]$$

$$\Rightarrow \ln(\tilde{p}(k)) = \left[-ik\mu - \frac{k^2\sigma^2}{2}\right]$$
$$= \sum_{n=1}^{\infty}\frac{(-ik)^n}{n!}\langle x^n\rangle_c$$

Here, only $n=2,1$ survive $\rightarrow$ This is characteristic of the normal distribution.

$$\langle x\rangle_c = \langle x\rangle = \mu$$
$$\langle x^2\rangle_c = \langle x^2\rangle - \langle x\rangle^2 = \sigma^2$$
$$\langle x^n\rangle_c = 0 \quad \forall n > 2$$

Now, the Poisson distribution —

(iii) Birth – death process →

$$DNA\ [D] \xrightarrow[\text{transcription}]{K_t} mRNA\ [M] \xrightarrow[\text{degrades}]{K_d} \phi$$

$$\frac{d[m]}{dt} = K_t[D] - K_d[m]$$

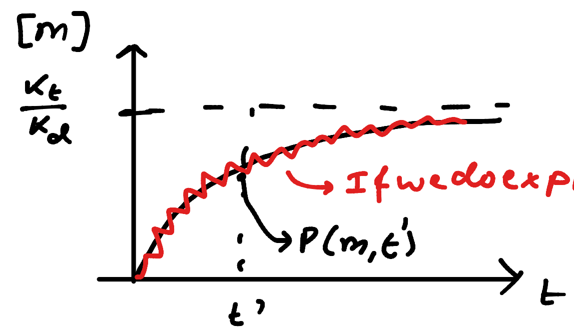
Let $[D] = 1$

Solving by I.F,

$$[m](t) = \frac{K_t - e^{-K_d t}}{K_d}$$

So, $t \to \infty$,

$$[m](t) = \frac{K_t}{K_d} \quad \longrightarrow$$



→ If we do expt. → So this motivates some randomness, stochastic process.

We formulate master-equation from this.

$$\frac{\partial P_m}{\partial t} = \underbrace{k_t P_{m-1} + K_d (m+1) P_{m+1}}_{\text{gain}} \underbrace{- K_t P_m - K_d m P_m}_{\text{Loss}}$$

Why? $(m+1)$ undergoes a decay, so now we have

Under steady state assumption, i.e. $\frac{\partial P_m}{\partial t} = 0$

$$(m+1)P_{m+1} = mP_m + \frac{K_t}{K_d}\left[P_m - P_{m-1}\right]$$

We define,

$$P_1 = \frac{K_t}{K_d} P_0$$ → No lower, as $m = -1$ is not sensible.

$$\Rightarrow P_2 = \frac{1}{2}\left(\frac{K_t}{K_d}\right)^2 P_0$$

$\vdots$

$$P_m = \frac{1}{m!}\left(\frac{K_t}{K_d}\right)^m P_0$$

↳ fixable by normalization.

We normalize by,

$$\sum_m P_m = 1 \Rightarrow P_0 = \exp\left[-\frac{K_t}{K_d}\right]$$

$$\therefore P_m = \frac{1}{m!}\left(\frac{K_t}{K_d}\right)^m \exp\left(-\frac{K_t}{K_d}\right)$$ → Poisson distribution.

Let us call, $\lambda = \frac{K_b}{K_d}$

$$\therefore \langle K \rangle = \sum_{K=0}^{\infty} \frac{\lambda^K}{K!} e^{-\lambda} \cdot K$$

$$= \lambda \cdot \sum_{K=1}^{\infty} \frac{\lambda^{K-1}}{(K-1)!} e^{-\lambda}$$

We may write it as, $K-1=n$,

$$= \lambda \sum_{n=0}^{\infty} \frac{\lambda^n e^{-\lambda}}{n!} = \lambda$$

☐ Do yourself

Also,

$$\langle K^2 \rangle = \sum_{K=0}^{\infty} \frac{\lambda^K}{K!} e^{-\lambda} \cdot K^2$$

$$= \sum_{K=0}^{\infty} \frac{\lambda^K}{K!} e^{-\lambda} \left[K(K-1) + K\right]$$

Some algebra

$$= \lambda^2 + \lambda$$

☐ Do

$$\therefore \sigma = \sqrt{\langle K^2 \rangle - \langle K \rangle^2} = \lambda$$

So, all the moments are going to be the same.

or, we find the discrete fourier transform.

$$\tilde{P}_\lambda(\tilde{K}) = \sum_{K=0}^{\sim} \frac{\lambda^K e^{-\lambda}}{K!} e^{-i\tilde{K}K}$$

$$= e^{-\lambda} \cdot \left[\sum_{K=0}^{\infty} \frac{(\lambda e^{-i\tilde{K}})^K}{K!}\right]$$

$$= e^{-\lambda} \cdot \exp\left[\lambda \exp\{-i\tilde{K}\}\right]$$

$$= \exp\left[\lambda \cdot \{\exp(-i\tilde{K}) - 1\}\right]$$

Now,

$$\ln(\tilde{P}_\lambda(\tilde{K})) = \lambda[\exp(-i\tilde{K}) - 1]$$

$$= \lambda \cdot \sum_{n=1}^{\infty} \frac{(-i\tilde{K})^n}{n!} \underset{\text{we equate to}}{=} \sum_{n=1}^{\infty} \frac{(-i\tilde{K})^n}{n!} \langle K^n \rangle_c$$

So, we see, all the cumulants $= \lambda$.

Thursday will be a tutorial — Problems will be given then.

15th January 2025 (Wednesday) →

- Probabilities of many random variables →

When does this happen? Many particles in N-dim space.

So,

$$S = \{-\infty < x_1, x_2, \dots, x_N < +\infty\} \rightarrow \text{Just positions, say}$$

or

$$\{v_1, v_2, \dots, v_N, q_1, q_2, \dots, q_N\} \rightarrow \text{Also velocities.}$$

Notation: $d^N x = \prod_{i=1}^{N} dx_i = \prod_{i=1}^{N} dv_i \prod_{i=1}^{N} dq_i$

Using this, $\int d^N x \, p(x) = 1$

What is this?

$p(x_1, x_2, \dots, x_N)$

When these are independent (Like in the case of ideal gas) and identical distributions,

$$p(x_1, \dots, x_N) = \prod_{i=1} p(x_i) \qquad \text{(iid R.V.)}$$

What is the probability of finding a particle at a particular location,

$$p'(\vec{q}) = \int \underbrace{p(\vec{v}, \vec{q})}_{\text{joint dist.}} d^3 v$$

Now, for conditionals,

$$p(\vec{v}, \vec{q}) = p(\vec{v} | \vec{q}) \, p(\vec{q})$$

Bayes' theorem,

$$p(\vec{v} | \vec{q}) = \frac{p(\vec{v}, \vec{q})}{p(q)}$$

→ joint

Conditional

Let $\{x_i : i = 1, \dots, N\}$ iid r.v. ⟶ Thus all of them drawn from same dist.

$$\therefore Y = \sum_{i=1}^{N} x_i \quad \text{(say)}$$

We want to find,

$$p(y) = ?$$

We write,

$$p(y) = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_N \, p(x_1, \ldots, x_n) \, \delta\left(y - \sum_{i=1}^{N} x_i\right)$$

Why? we only care about sets of $\{x_1, \ldots, x_n\}$ that add up to y.

Using iid,

$$p(y) = \int_{-\infty}^{\infty} p(x_1)\, dx_1 \int_{-\infty}^{\infty} p(x_2)\, dx_2 \cdots \int_{-\infty}^{\infty} p(x_n)\, dx_n \, \delta\left(y - \sum_{i=1}^{N} x_i\right)$$

We cannot integrate these → δ function has x_i dependence too.

We also define the characteristic function of $p(y)$ dist. (Fourier transform)

$$\phi_y(k) = \int_{-\infty}^{\infty} dy \exp[-iky] \, p(y)$$

Putting in prev expression for $p(y)$ here,

$$\phi_y(k) = \int_{-\infty}^{\infty} dy \exp[-iky] \left[\int_{-\infty}^{\infty} p(x_1)\, dx_1 \cdots \int_{-\infty}^{\infty} p(x_n)\, dx_n \, \delta\left(y - \sum_{i=1}^{N} x_i\right)\right]$$

Note, we may shift δ func to y integral, and thus replace y with $\sum_{i=1}^{N} x_i$ after integrating over y.

$$\Rightarrow \phi_y(k) = \int_{-\infty}^{\infty} p(x_1)\, dx_1 \cdots \int_{-\infty}^{\infty} p(x_n)\, dx_n \cdot \exp\left[-ik \sum_{i=1}^{N} x_i\right]$$

putting in each exp term & breaking up the sum

$$= \int_{-\infty}^{\infty} p(x_1) \exp[-ikx_1]\, dx_1 \cdots \int_{-\infty}^{\infty} p(x_n) \exp[-ikx_n]\, dx_n$$

$$= \phi_1(k)\, \phi_2(k) \cdots \phi_N(k)$$

Why? iid, each should have same characteristic.

$$= [\phi_X(k)]^N$$

Sometimes, we are not interested in $y = \sum_{i=1}^{N} x_i$, we are interested in,

$$y = \frac{1}{N} \sum_{i=1}^{N} x_i \quad , \quad k \to \frac{k}{N}$$

Thus,

$$\phi_y(k) = \left[\phi_x\left(\frac{k}{N}\right)\right]^N$$

By defn.

$$= \exp\left[N \ln\left\{\phi_x\left(\frac{k}{N}\right)\right\}\right] = \exp\left[N\left(\sum_{n=1}^{\infty} \frac{(-i\frac{k}{N})^n}{n!} \langle x^n\rangle_c\right)\right]$$

CGF form!

$$= \exp\left[\sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} \cdot \frac{\langle x^n\rangle}{N^{n-1}}\right]$$

Splitting up exp,

$$= \exp\left[-ik\langle x_c\rangle - \frac{k^2}{2!}\frac{\langle x^2\rangle}{N} + \underbrace{O\left(\frac{1}{N^2}\right)}_{}\right]$$

We ignore H.O. terms for large N.

$$= \exp\left[-ik\langle x\rangle_c - \frac{k^2}{2!}\frac{\langle x^2\rangle_c}{N}\right]$$

$\hookrightarrow$ Dist of a Gaussian / Normal

$$\therefore \phi_y(k) = \exp\left[-ik\langle x_c\rangle\right]$$

Central Limit Theorem

Say that a system has N particles / R.V. (Representative of size of system)

Now,

Observable $\sim O(N^0) \to P, T, \ldots$ (Intensive Thermo variables)

observable $\sim O(N^1) \to V, E, S, \ldots$ (Extensive Thermo variables)

$\circledast$ observable $\sim O(\exp(N)) \to$ # of configuration of system, etc

Say we want,

$$S = \sum_{i=1}^{N} \mathcal{E}_i = \sum_{i=1}^{N} \exp[N\phi_i]$$

Since this is an exp being summed, we have bounds,

$$0 \le \mathcal{E}_i \le \mathcal{E}_{max}$$

$\Rightarrow \quad 0 \le S \le N\mathcal{E}_{max} \to$ Note, S has a bound that is $O(N)$

$\Rightarrow$ S is extensive observable.

Say we define $\frac{\ln S}{N}$ as some new quantity.

$\therefore \quad 0 \le \frac{\ln S}{N} \le \frac{\ln \mathcal{E}_{max}}{N} + \frac{\ln N}{N}$

Now taking $\lim_{N\to\infty}$,

$\rightarrow \lim_{N\to\infty} \frac{\ln S}{N} \simeq \frac{\ln \mathcal{E}_{max}}{N} = \phi_{max}$

↳ why? $\mathcal{E}_{max} = \exp[N\phi_{max}]$

Now,

$I = \int dx \exp[N\phi(x)]$ (Partition function?)

Let us say,

$\phi(x) = \phi_{max}$ at $x = x_{max}$

Since it is maxima, $\phi'(x_{max}) = 0$

$$I = \int dx \exp\left[N\left\{\phi(x_{max}) - \frac{1}{2}|\phi''(x)|_{x_{max}}(x - x_{max})^2 + \dots\right]\right.$$

No autonomy for second derivative, apparently.

$$\therefore I \simeq \exp[N\phi(x_{max})] \cdot \underbrace{\int_{-\infty}^{\infty} dx \exp\left[-\frac{N}{2}|\phi''(x)|_{x_{max}}(x - x_{max})^2\right]}_{\text{Gaussian integral.}}$$

$$\rightarrow I \simeq \exp[N\phi(x_{max})]\sqrt{\frac{2\pi}{N|\phi''(x_{max})|}}$$

(Saddle point integration)

→ widely used in Physics.

→ We use this to prove Stirling's approx.

⊛ Tomorrow

16th January 2025 (Thursday) →

(TUTORIAL) →

① (Gaussian integral) →

$$\int_{-\infty}^{\infty} e^{-x^2/2}\, dx = \sqrt{2\pi} \quad (\text{Show})$$

We convert to polar to solve this.

$$\therefore I = \int_{-\infty}^{\infty} e^{-x^2/2}\, dx \Rightarrow I^2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-(x^2+y^2)/2}\, dx\, dy$$

We convert, $x^2+y^2 = r^2$ (plane polar)

$$\therefore r\cos\theta = x \Rightarrow dx = dr\cos\theta - r\sin\theta\, d\theta$$

$$\therefore r\sin\theta = y \Rightarrow dy = dr\sin\theta + r\cos\theta\, d\theta$$

$$\therefore I^2 = \int_0^{\infty}\int_0^{2\pi} e^{-r^2}(dr\cos\theta - r\sin\theta\, d\theta)(dr\sin\theta + r\cos\theta\, d\theta)$$

$$= \int_0^{\infty}\int_0^{2\pi} e^{-r^2}\Big(dr^2\cos\theta\sin\theta + r\,dr\,d\theta\cos^2\theta - r\,dr\,d\theta\sin^2\theta - r^2\sin\theta\cos\theta\, d\theta\, dr\Big)$$

$$\approx \int_0^{\infty}\int_0^{2\pi} e^{-r^2} r\, dr\, d\theta$$

Replace, $z = \frac{r^2}{2} \rightarrow dz = r\,dr$

$$I^2 = 2\pi\int_0^{\infty} e^{-z}\, dz = 2\pi$$

$$\therefore I = \sqrt{2\pi} \quad (\text{Shown})$$

② Show that the following PDF is markovian.

$$f(t) = \begin{cases} \lambda e^{-\lambda t}, & t \geq 0 \\ 0, & t < 0 \end{cases}$$

Soln: To be markovian, it is to be memoryless, i.e.,

$$P(t+s \mid t) = P(s)$$

Now, $P(t+s \mid t) = P(t)\, P(t+s, t)$ (Bayes)

In this notation, these are CDFs,

$$P(t \geq T+S \mid t \geq T) = P(t \geq S)$$

So, we are given PDF and we use, $P(t \geq T) = 1 - CDF(t)$

$$\therefore P(t \geq S) = 1 - \int_{-\infty}^{S} f(t)\,dt$$

$$= 1 - \int_{0}^{S} \lambda e^{-\lambda t}\,dt$$

$$= 1 + \left[e^{-\lambda t}\right]_0^S = 1 + \left(e^{-\lambda S} - 1\right)$$

$$= e^{-\lambda S}$$

$$P(t \geq T+S \mid t \geq T) = \frac{P(t \geq T+S,\ t \geq T)}{P(t \geq T)}$$

$$= \frac{P(t \geq T+S)}{P(t \geq T)} = \frac{e^{-\lambda(T+S)}}{e^{-\lambda T}}$$

$$= e^{-\lambda S}$$

$\therefore$ The distribution is markovian (exponential is only contd. dist that is markovian)

Change of variables →

PDF : $P(x) = 3(1-x)^2$

So, CDF →

$$CDF(x) = \int_{0}^{x} 3(1-t)^2\,dt$$

$$= 3 \cdot \frac{1}{(-1)} \cdot \left[\frac{(1-t)^3}{3}\right]_0^x$$

$$= \left[(1-t)^3\right]_x^0$$

$$= \left[1 - (1-x)^3\right]$$

Now, we change $y = (1-x)^3$, but the CDF should remain the same.

$$\therefore CDF(y) = 1 - y$$

$$\Rightarrow PDF(y) = \frac{d}{dy}\left(CDF(y)\right) = 1$$

* One can also just use the Jacobian, $PDF(y) = \left|\frac{dy}{dx}\right| PDF(x)$