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2 Fokker-Planck equation

This is the lecture note on Apr. 22, 2024 focusing on the random walks and Fokker-Planck equation.

2.1 Discrete time and discrete site random walk

We consider a particle on an infinite discrete chain with lattice constant Δx and the position of the site is represented as $n\Delta x$, ($n_{\min} < n < n_{\max}$). The time is also discretized with a finite period Δt and we discuss the position of the particle at discrete times $k\Delta t$, ($k = 0, 1, 2, \cdots$). The position of the particle at time $k\Delta t$ is defined by X_k. We assume the particle start from $X_0 = 0$ at $t = 0$.

Basic assumption is as follows: the displacement at k-th step ($k \geq 1$), $\Delta X_k \equiv X_k - X_{k-1}$, is a random variable taking $+\Delta x$ with a probability p and $-\Delta x$ with a probability q while the relation $p + q = 1$ holds. If the particle were at the edge of the system namely $X_k = n_{\min}\Delta x$ or $n_{\max}\Delta x$, the situation should be different and is considered in the last section. For the time being, we assume $n_{\min} = -\infty$ and $n_{\max} = \infty$. This is called **Markov process**, where ΔX_k are random variables constituting infinite set $\{\Delta X_1, \Delta X_2, \Delta X_3, \cdots\}$ are independent and identically distributed (i.i.d.). The position of the particle after k (≥ 1) steps is

$$X_k \equiv \sum_{j=1}^{k} \Delta X_j, \tag{1}$$

where $\{X_1, X_2, \cdots\}$ is also a set of random variables. This type of dynamics is called **discrete time and discrete site random walk**.

We evaluate the expectation value and the variance of ΔX_k:

$$\langle \Delta X_k \rangle = p(+\Delta x) + q(-\Delta x) = (p - q)\Delta x, \tag{2}$$

$$\langle (\Delta X_k)^2 \rangle = p(+\Delta x)^2 + q(-\Delta x)^2 = (\Delta x)^2,$$

$$\langle \delta(\Delta X_k)^2 \rangle = \langle (\Delta X_i)^2 \rangle - \langle \Delta X_i \rangle^2 = (\Delta x)^2 - (p - q)^2(\Delta x)^2 = 4pq(\Delta x)^2. \tag{3}$$

The "fluctuation" of the variable ΔX_k is $\sigma_p[\Delta X_k] \equiv \sqrt{\langle \delta(\Delta X_k)^2 \rangle} = 2\sqrt{pq}\Delta x$, which takes a maximum value when $p = q = 1/2$ and is zero when $p = 0$ or $p = 1$. While the expectation value $\langle \Delta X_k \rangle = (p - q)\Delta x$ is nonzero only for $p \neq q$.

Similarly, we evaluate the expectation value and variance of X_k:

$$\langle X_k \rangle = \langle \sum_{j=1}^{k} \Delta X_j \rangle = \sum_{j=1}^{k} \langle \Delta X_j \rangle = k(p - q)\Delta x, \tag{4}$$

$$\langle (X_k)^2 \rangle = \sum_{j=1}^{k} \langle (\Delta X_j)^2 \rangle + \sum_{j \neq \ell}^{k} \langle \Delta X_j \rangle \langle \Delta X_\ell \rangle,$$

$$\langle \delta(X_k)^2 \rangle = \langle (X_k)^2 \rangle - \langle X_k \rangle^2 = k(\Delta x)^2 + (k(k-1) - k^2)((p - q)\Delta x)^2 = 4pqk(\Delta x)^2. \tag{5}$$

When $p > q$, the average position of the particle moves to the right with a constant "speed" $\frac{\langle X_k \rangle - \langle X_{k-1} \rangle}{k\Delta t - (k-1)\Delta t} = (p-q)\Delta x/\Delta t$. Similarly for $p < q$, the average position moves to the left with a constant speed $(q-p)\Delta x/\Delta t$. The "fluctuation" of the variable X_i is $\sigma_p[X_k] \equiv \sqrt{\langle \delta(\Delta X_k)^2 \rangle} = 2\sqrt{pqk}\Delta x$. Therefore, when $p \neq q$, the ratio $\sigma_p[X_k]/\langle X_k \rangle = \frac{2}{p-q}\sqrt{\frac{pq}{k}}$ becomes smaller for larger k, which is **the law of larger number**.

2.2 Probability distribution function

We will consider the probability distribution of the particle position after k (≥ 0) steps, $W(x, k)$, with $X_k = x$. This probability distribution function needs to satisfy following relations:

$$W(x, k) \geq 0, \qquad \sum_{n=n_{\min}}^{n_{\max}} W(n\Delta x, k) = 1 \quad \forall k. \tag{6}$$

Obviously, the initial condition of the distribution function is

$$W(x, 0) = \begin{cases} 1, & x = 0 \\ 0, & x \neq 0 \end{cases} \tag{7}$$

Let us consider the case that there are r steps to the right and $k - r$ steps to the left within the i steps ($0 \leq r \leq k$). The total displacement is $x = r(+\Delta x) + (k - r)(-\Delta x) = (2r - k)\Delta x$, which results in

$$r = \frac{1}{2}\left(k + \frac{x}{\Delta x}\right), \qquad k - r = \frac{1}{2}\left(k - \frac{x}{\Delta x}\right). \tag{8}$$

Clearly, the position of the particle after k steps is in the range $-k\Delta x \leq x \leq k\Delta x$.

The probability of r steps to the right and $k - r$ steps to the left is $p^r q^{i-r}$, whose number of occurences is given by a combination ${}_kC_r = k!/(r!(k - r)!)$. Therefore, the probability distribution function is

$$W(x, k) = {}_kC_r p^r q^{k-r}. \tag{9}$$

We would like to consider the relation between the function $W(x, k - 1)$ and $W(x, k)$. The particle locating at x at i-th step was resulted from two possibilities. One is that the particle was at $x - \Delta x$ at $k - 1$-th step and jump to the right and the other is that the particle was at $x + \Delta x$ at $k - 1$-th step and jump to the left. Hence, the probability distribution at k-th step is

$$W(x, k) = pW(x - \Delta x, k - 1) + qW(x + \Delta x, k - 1). \tag{10}$$

This difference equation can be solved for $k \geq 1$ with the initial condition Eq. (7).

2.3 Continuum limit and Fokker-Planck equation

In order to make a connection with the Brownian motion discussed in the previous lecture, we take the continuum limit, $\Delta t \to 0$ and $\Delta t \to 0$ and consider the position of the particle at time $t = k\Delta t$, $X(t)$. Using the results of Eq. (4), we have

$$\langle X(t) \rangle = \langle X_k \rangle = \frac{t}{\Delta t}(p - q)\Delta x, \tag{11}$$

$$\langle \delta(X(t))^2 \rangle = \frac{t}{\Delta t} 4pq(\Delta x)^2. \tag{12}$$

We note that both of the expectation value and its variance linearly grow with time t. First, we require the variance is finite and the ratio appearing in it is

$$\frac{(\Delta x)^2}{\Delta t} = \text{finite} \equiv 2D, \tag{13}$$

where we introduced a positive constant D. Moreover, for $p \neq q$, the expectation value $\langle X(t) \rangle$ is also finite, namely, $p - q \propto \Delta x$. In particular, we choose the proportional constant as follows:

$$p - q = -\frac{v}{2D}\Delta x, \tag{14}$$

introducing a new constant v, which could be a positive or negative value. From the relation $p + q = 1$, we have

$$p = \frac{1}{2} - \frac{v}{4D}\Delta x, \qquad q = \frac{1}{2} + \frac{v}{4D}\Delta x. \tag{15}$$

Using these assumptions, we have the expectation value and variance of the position of the particle at time t as

$$\langle X(t)\rangle = \frac{t}{\Delta t}\frac{-v}{2D}(\Delta x)^2 = -vt, \tag{16}$$

$$\langle \delta(X(t))^2\rangle = \frac{t}{\Delta t}4\left\{\frac{1}{4}-\left(\frac{v}{4D}\Delta x\right)^2\right\}(\Delta x)^2 \to 2Dt, \tag{17}$$

where in the last we took the limit $\Delta x \to 0$. The first relation shows that the average velocity of the particle is $-v$. Assuming we have applied a constant external force to the particle in a fluid $F_{\text{ext}} = -f$, the total force to the field (in average) is $F_{\text{total}} = -f + \zeta v$, where ζ is the friction coefficient of the fluid. We expect the particle acquire a steady state of a velocity $-v$, that satisfies $f = \zeta v$.

The difference equation (10) is rewritten as

$$W(x,t) = pW(x-\Delta x, t-\Delta t) + qW(x+\Delta x, t-\Delta t), \tag{18}$$

and the initial condition reads $W(x,0) = \delta(x)$, where $\delta(x)$ is Dirac's delft function. Assuming the function $W(x,t)$ in the continuum limit is differentiable with x and t, by Taylor expansion

$$W(x\pm\Delta x, t-\Delta t) \sim W(x,t) - \frac{\partial W(x,t)}{\partial t}\Delta t \pm \frac{\partial W(x,t)}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 W(x,t)}{\partial x^2}(\Delta x)^2, \tag{19}$$

and hence the right-hand-side of Eq. (18) becomes

$$\text{r.h.s.} = W(x,t) - \frac{\partial W(x,t)}{\partial t}\Delta t + (q-p)\frac{\partial W(x,t)}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 W(x,t)}{\partial x^2}(\Delta x)^2. \tag{20}$$

Hence, after some manipulations we have

$$\frac{\partial W(x,t)}{\partial t} = v\frac{\partial W(x,t)}{\partial x} + D\frac{\partial^2 W(x,t)}{\partial x^2}, \tag{21}$$

which is a special example of the **Fokker-Planck equation**. When $v = 0$, this reduces to the diffusion equation, which was discussed in the previous lecture. Therefore, the parameter D can be identified with the **diffusion constant** of the particle. General solution of Eq. (21) for an infinite system is

$$W(x,t) = \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{(x+vt)^2}{4Dt}}, \tag{22}$$

(Check this !) which is a Gaussian distribution centered at $x = -vt$ and the variance $2Dt$. From this results, the system will never achieve a steady distribution and hence we could not expect an equilibrium.

2.4 Fokker-Planck equation in semi-infinite system

Let us consider a semi-infinite system where the particle can only move in the range $0 \leq x$ ($n_{\text{min}} = 0$ and $n_{\text{max}} = \infty$). In such system, an equilibrium state can be established from any initial conditions. Since the probability distribution does not change with time at equilibrium, $W(x,t) \to W_{\text{eq}}(x)$, we have

$$0 = v\frac{\partial W_{\text{eq}}(x)}{\partial x} + D\frac{\partial^2 W_{\text{eq}}(x)}{\partial x^2}, \tag{23}$$

which has a unique solution

$$W_{\text{eq}}(x) = W_0 e^{-\frac{v}{D}x}, \tag{24}$$

where a positive constant W_0 is determined by the normalization condition $\int_0^\infty dx W_{\text{eq}}(x) = 1$. Figure 1 shows the schematics of this distribution.

As discussed above, the velocity v is resulted from the external force $-f$ applying to the particle. The potential energy of this system is given by

$$E_{\text{p}} = fx. \tag{25}$$

The expectation value of the potential energy is

$$\langle E_{\rm p}\rangle = \langle fx\rangle = f\int_0^\infty dx\; xW_{\rm eq}(x) = f\frac{D}{v} = D\zeta, \tag{26}$$

and the average kinetic energy is zero (since the average position of the particle does not move). Using the equipartition theorem, the total energy of the particle is equal to $k_{\rm B}T$, and hence we have once again the relation

$$D = \frac{k_{\rm B}T}{\zeta}. \tag{27}$$

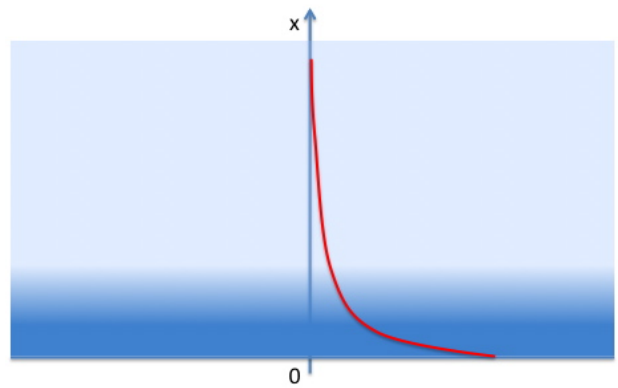

Figure 1: Equilibrium probability distribution $W_{\rm eq}(x)$ under an external force $-f$. This could be the distribution of the density of dusts (PM2.5, for example) as a function of altitude, assuming that the atmosphere is in thermal equilibrium with a constant temperature T.

2.5 Conclusions

We have discussed the random walk in discrete time and discrete sites and by taking the continuum limit, we obtain Fokker-Planck equation for the probability distribution function. By solving the equation under a finite force in a semi-infinite system, we obtain an equilibrium distribution and confirm the relation between the diffusion constant and the friction constant.