Diffusion and Random walks

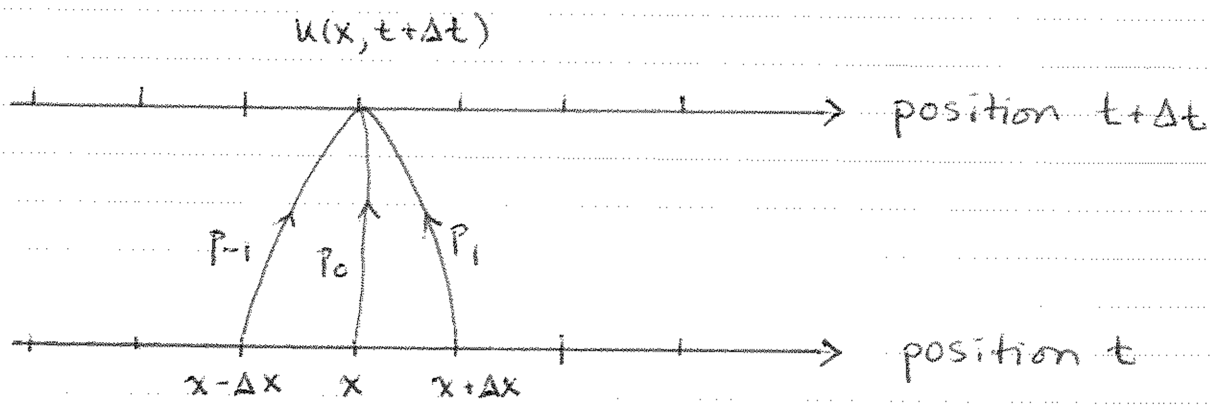
Diffusion can be viewed as the continuum limit of a discrete random walk process.

Let $X(t)$ be the random variable for the position of an organism and let $u(x,t)$ be probability density function.

$u(x,t)\Delta x$ = probability organism is located in the interval $(x, x+\Delta x)$ at time t

$$u(x,t)\Delta x = P(x < X(t) < x+\Delta x)$$

In a random walk one attributes probabilities to the organisms movement from time t to $t+\Delta t$.



Schematic illustrates a random walk where organism position at x, $t+\Delta t$ could have arisen from organism moving left or right Δx units with probabilties p_1, p_{-1} or remaining stationary with prob p_0.

For such a random walk (assuming independence)

$$u(x, t+\Delta t) = p_{-1}\, u(x-\Delta x, t) + p_0\, u(x, t) + p_1\, u(x+\Delta x, t)$$

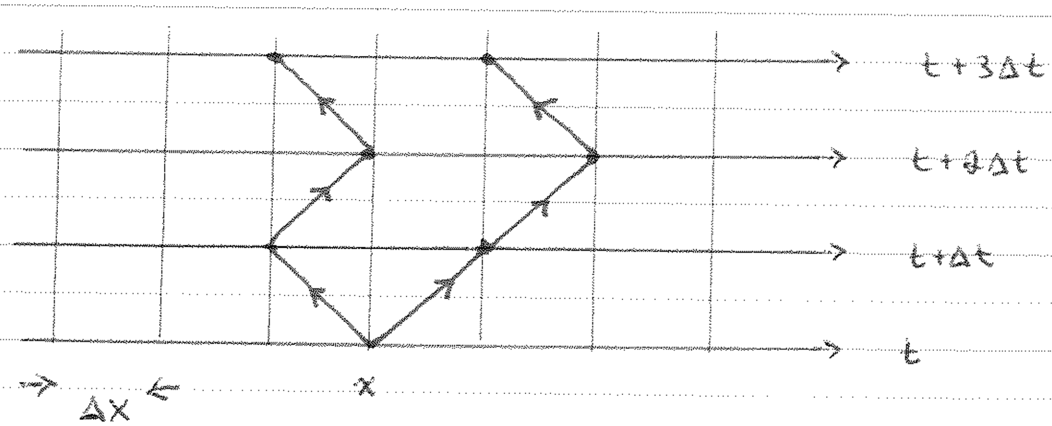
where

$$p_{-1} + p_0 + p_1 = 1$$

As a special case we consider $p = p = \frac{1}{2}$, $p_0 = 0$

$$(1) \quad u(x, t+\Delta t) = \frac{1}{2} u(x-\Delta x, t) + \frac{1}{2} u(x+\Delta x, t)$$

Here the organism moves left/right Δx units with equal probability and with certainty moves (doesn't stay a posit. x)



Shows two potential realizations for the random walk.

Continuum Limit ($\Delta x, \Delta t \to 0$)

$$(1) \qquad u(x, t+\Delta t) = \tfrac{1}{2} u(x-\Delta x, t) + \tfrac{1}{2} u(x+\Delta x, t)$$

Seek a PDE that $u(x,t)$ satisfies. Expand each term in a Taylor series about (x,t):

$$u(x, t+\Delta t) = u + u_t \Delta t + \tfrac{1}{2} u_{tt} \Delta t^2 + O(\Delta t^3)$$

$$u(x+\Delta x, t) = u + \quad \Delta x + \tfrac{1}{2} u_{xx} \Delta x^2 + O(\Delta x^3)$$

$$u(x-\Delta x, t) = u - u_x \Delta x + \tfrac{1}{2} u_{xx} \Delta x^2 + O(\Delta x^3)$$

After substituting these into the assumed rule (1) the u terms cancel:

$$(2) \qquad u_t \Delta t + \tfrac{1}{2} u_{tt} \Delta t^2 = \tfrac{1}{2} \Delta x^2 u_{xx} + \text{h.o.t.}$$

where h.o.t. denotes higher order terms. Dividing both sides by Δt and rearranging

$$(3) \qquad u_t = \underbrace{\left(\frac{\Delta x^2}{2 \Delta t}\right)}_{\text{fix constant}} u_{xx} - \tfrac{1}{2} u_{tt} \underbrace{\Delta t}_{\text{as } \Delta t \to 0} + \text{h.o.t}$$

and we arrive at the <u>diffusion eqn</u> for $u(x,t)$

$$(4) \qquad u_t = D \, u_{xx}$$

where

$$D = \frac{\Delta x^2}{2 \Delta t}$$

Earlier we showed that

$$(5) \qquad u(x,t) = \frac{1}{\sqrt{4\pi D t}}\, e^{-x^2/4Dt} \qquad x \in \mathbb{R},\ t>0$$

was a solution to the diffusion eqn (4). It is readily verified that

$$\int_{\mathbb{R}} u(x,t)\,dx = 1$$

so the fundamental solution in (5) is the probability density function for the random walk. Moreover,

$$P(a < X(t) < b) = \int_a^b u(x,t)\,dx$$

is the probability the organism is in (a,b) at time t.

<u>Connection to concentration</u>

If the "organism" in the preceding discussion is a molecule and Ω contains N such molecules which randomly move (independently) then

$$c(x,t) = N\,u(x,t) = \text{molecular (\#) concentrat.}$$

and $c(x,t)$ also satisfies a diffusion equation

$$c_t = D c_{xx}$$

More General Random Walks

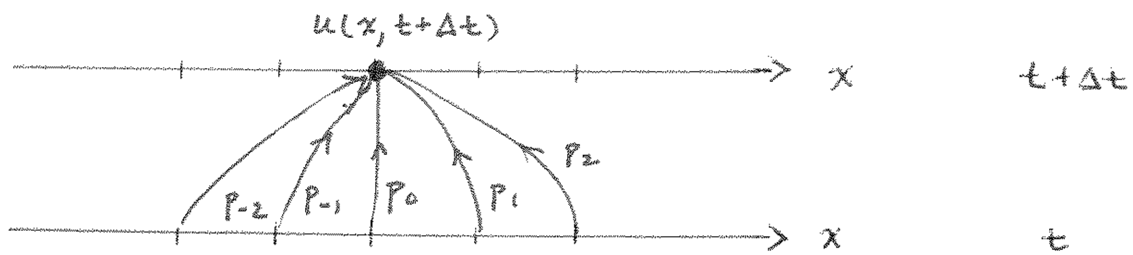
A more general rule for a particle random walk might be

$$(1) \qquad u(x, t+\Delta t) = \sum_{k=-N}^{k=N} p_k \, u(x+k\Delta x, t)$$

where p_k are transition probabilities and

$$\sum_{k=-N}^{N} p_k = 1$$

Below we illustrate such a rule for $N=2$



For instance

$p_2 \, u(x+2\Delta x, t)\,\Delta x$ = probability a particle in $(x+2\Delta x, x+3\Delta x)$ moves into $(x, x+\Delta x)$ at time $t+\Delta t$.

The most general (continuous) version of (1) is:

$$(2) \qquad u(x, t+\Delta t) = \int_{\mathbb{R}} p(\xi)\, u(x+\xi, t)\, d\xi$$

where $p(\xi)$ is a probability density function satisfying

$$(3) \qquad \int_{\mathbb{R}} p(\xi)\, d\xi = 1$$

If one approximates the integral in (2) as a Riemann sum the connection to (1) is made clear if $\xi_K = k\Delta\xi$, $p_K = p(\xi_K)\Delta\xi$.

Partial differential equations for $u(x,t)$ in the limit $\Delta t \to 0$ can be derived from (2). First expand the integrand as a Taylor series

$$u(x, t+\Delta t) = \int_{\mathbb{R}} p(\xi) \sum_{n=0}^{\infty} \frac{\xi^n}{n!} \frac{\partial^n u}{\partial x^n}(x,t)\, d\xi$$

$$(4) \qquad u(x, t+\Delta t) = \sum_{n=0}^{\infty} \left(\frac{1}{n!} \int_{\mathbb{R}} \xi^n p(\xi)\, d\xi \right) \frac{\partial^n u}{\partial x^n}(x,t)$$

Noting the $n=0$ term of (4) is

$$\underbrace{\int_{\mathbb{R}} p(\xi)\, d\xi}_{1}\; u(x,t) = u(x,t)$$

We obtain

$$(5) \qquad u(x,t+\Delta t) - u(x,t) = \sum_{n=1}^{\infty} \frac{1}{n!} \cdot m_n \frac{\partial^n u}{\partial x^n}$$

where the n^{th} moment m_n of $p(z)$ is

$$m_n \equiv \int_{\mathbb{R}} z^n p(z)\, dz$$

Then (5) becomes

$$\frac{u(x,t+\Delta t) - u(x,t)}{\Delta t} = \sum_{n=1}^{\infty} D_n \frac{\partial^n u}{\partial x^n}(x,t)$$

where $D_n = m_n (\Delta t\, n!)^{-1}$. Letting $\Delta t \to 0$ we have

$$(6) \qquad \frac{\partial u}{\partial t} \cong D_1 \frac{\partial u}{\partial x} + D_2 \frac{\partial^2 u}{\partial x^2} + D_3 \frac{\partial^3 u}{\partial x^3} + \cdots$$

When one truncates the series we obtain what is referred to as a Fokker-Planck partial differential equation such as

$u_t = D_1 u_x + D_2 u_{xx}$ advection/diffusion

$u_t = D_1 u_{xx} + D_3 u_{xxx}$ 3rd order F-P eqn.

Lecture 8: The Continuum Limit

Scribe: E.A. van Nierop

(Division of Engineering and Applied Sciences, Harvard)

March 1^{st}, 2005

In the previous lecture, we used the saddle-point method to derive a uniformly valid asymptotic approximation for the position of the Bernoulli random walk after many steps. In the first part of this lecture, we discuss how this solution can be applied to derive the limiting distribution of percentile order statistics, which arises, for example, when interpreting test scores or pricing Internet bandwidth. This was a question on Problem Set 2, so the reader is referred to the solutions available online for a detailed discussion.
In the second part of the lecture, we begin our analysis of the continuum limit of a random walk. In the first lecture, we saw how the continuous diffusion equation could be derived from a discrete random walk. We then investigated the behaviour of the walker position $P_N(x)$ for large N and employed such methods as the Gram-Charlier expansion and the method of steepest descent to better understand what goes on in the 'tail' of the distribution $P_N(x)$. Today, we return to the first lecture, and find out how one can 'jump' from a discrete walk to a continuous one more formally.

1 Kramers-Moyall Expansion

Recall Bachelier's equation from Lecture #2. That is for a random walk with identical, indepently distributed (IID) steps, we have

$$P_{N+1}(x) = \int_{-\infty}^{\infty} p(x-x')P_N(x')dx', \tag{1}$$

which is also the simplest expression for a Markov chain (see lecture #2).

Proceeding formally to derive the continuum limit ($N \to \infty$), we introduce $\rho(x,t)$ as the continuum approximation of $P_N(x)$, i.e. $\rho(x, N\tau) = P_N(x)$ where τ is the time between steps. Note that $\rho(x,t)$ is defined such that it is differentiable in x, t. We now seek a PDE for $\rho(x,t)$ (where $t \gg \tau$), and if $\sigma^2 = \langle x^2 \rangle = \int x^2 \rho(x) dx$, we consider also $\langle x_N^2 \rangle \sim \sigma^2 N$, such that $P_N(x)$ varies on length scales $L \gg \sigma$.

This implies that as $N \to \infty$, $p(x-x')$ is "localized" for $|x-x'| = O(\sigma)$ while $P_N(x') \sim \rho(x', N\tau)$ varies slowly at this scale. Hence, we Taylor expand $P_N(x')$ in Bachelier's equation: (replacing $x' = x - y$)

$$
\begin{aligned}
P_{N+1}(x) &= \int_{-\infty}^{\infty} p(y)P_N(x-y)dy, && (2)\\
&= \int_{-\infty}^{\infty} p(y)\sum_{n=0}^{\infty}\frac{(-y)^n}{n!}\frac{d^nP_N(x)}{dx^n}, && (3)\\
&= \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}m_n\frac{d^nP_N(x)}{dx^n}, && (4)\\
&= P_N(x)+\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}m_n\frac{d^nP_N(x)}{dx^n}, && (5)
\end{aligned}
$$

where the moments, m_n, are defined as usual ($m_n = \int x^n p(x)dx$) and they are assumed to *exist*. Note that in the last step we use $m_0 = 1$ which is always true. Bringing $P_N(x)$ to the other side and dividing by τ gives

$$\frac{P_{N+1}(x)-P_N(x)}{\tau} = \sum_{n=1}^{\infty}(-1)^n D_n \frac{d^nP_N(x)}{dx^n}, \qquad (6)$$

where $D_n = \frac{m_n}{n!\tau}$. Note that the left-hand-side now strongly resembles a time derivative of $P_N(x)$. Following through with that thought, and introducing $\rho(x,t)$ into the equations we get:

$$
\begin{aligned}
\frac{\partial\rho}{\partial t} &\approx \sum_{n=1}^{\infty}(-1)^n D_n\frac{\partial^n\rho}{\partial x^n} && (7)\\
&= -D_1\frac{\partial\rho}{\partial x}+D_2\frac{\partial^2\rho}{\partial x^2}-D_3\frac{\partial^3\rho}{\partial x^3}+\dots && (8)
\end{aligned}
$$

Often, as in Risken's recommended book *The Fokker-Planck Equation*, Equation (8) is referred to as "Kramers-Moyall" expansion. However, this should not strictly be interpreted as an asymptotic expansion, since errors are introduced by the first-order continuous time derivative on the left hand side. Note that no terms have been 'thrown away' on the right hand side, yet all higher-order time derivatives on the left have disappeared. Also, we should have known something fishy was going on since eq.(8) uses the *moments* rather than the cumulants which we know from earlier lectures to be the more important parameters.

As we shall see, this form of the Kramers-Moyall expansion is really only valid at leading order in the limit of infinitessimal steps (discussed below and by Risken), where only the first two terms survive,

$$\frac{\partial\rho}{\partial t}+D_1\frac{\partial\rho}{\partial x} = D_2\frac{\partial^2\rho}{\partial x^2} \qquad (9)$$

which is a linear advection-diffusion equation, the simplest case of the "Fokker-Planck equation" (discussed later in the class).

2 Continuum Derivation of the Central Limit Theorem

We will now systematically correct the Kramers-Moyall expansion and study the scaling of its terms. We will focus on the long-time (or many step, $N \gg 1$) limit, where we will see that the PDF spreads out and varies slowly in time. Thus, we consider Taylor expansion of the smooth continuum interpolant, $\rho(x,t)$, satisfying $P_N(x) = \rho(x, N\tau)$, around $t = N\tau$:

$$\frac{P_{N+1}(x) - P_N(x)}{\tau} = \frac{\partial \rho}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} + \frac{\tau^2}{3!}\frac{\partial^3 \rho}{\partial t^3} + \dots \tag{10}$$

Combining this with eq.(8) yields a modified expansion with high order derivatives in both time and space:

$$\frac{\partial \rho}{\partial t} + \sum_{n=2}^{\infty} \frac{\partial^n \rho}{\partial t^n}\frac{\tau^{n-1}}{n!} = \sum_{n=1}^{\infty} (-1)^n D_n \frac{\partial^n \rho}{\partial x^n} \tag{11}$$

This is the complete (formal) partial differential equation (PDE) equivalent to Bachelier's equation.

Scaling analysis: To obtain and accurate asymptotic approximation for the limit $N \to \infty$, we non-dimensionalize our variables by choosing a some typical length-scale L, which will be self-consistently (and uniquely) defined later in the analysis. Thus, we define $\tilde{x} = x/L$, $T = N\tau$ and $\tilde{t} = t/T$, and $\tilde{\rho} = \rho/L$ and obtain dimensionless PDE:

$$\frac{1}{T}\frac{\partial \tilde{\rho}}{\partial \tilde{t}} + \sum_{n=2}^{\infty} \frac{1}{T^n}\frac{\tau^{n-1}}{n!}\frac{\partial^n \tilde{\rho}}{\partial \tilde{t}^n} \sim \sum_{n=1}^{\infty} (-1)^n \frac{D_n}{L^n}\frac{\partial^n \tilde{\rho}}{\partial \tilde{x}^n} \tag{12}$$

$$\frac{\partial \tilde{\rho}}{\partial \tilde{t}} + \sum_{n=2}^{\infty} \frac{1}{N^{n-1} n!}\frac{\partial^n \tilde{\rho}}{\partial \tilde{t}^n} \sim -\frac{D_1 N\tau}{L}\frac{\partial \tilde{\rho}}{\partial \tilde{x}} + \frac{D_2 N\tau}{L^2}\frac{\partial^2 \tilde{\rho}}{\partial \tilde{x}^2} - \frac{D_3 N\tau}{L^3}\frac{\partial^3 \tilde{\rho}}{\partial \tilde{x}^3} + \dots \tag{13}$$

$$= -\frac{m_1 N}{L}\frac{\partial \tilde{\rho}}{\partial \tilde{x}} + \frac{m_2 N}{2L^2}\frac{\partial^2 \tilde{\rho}}{\partial \tilde{x}^2} - \frac{m_3 N}{3! L^3}\frac{\partial^3 \tilde{\rho}}{\partial \tilde{x}^3} + \dots \tag{14}$$

$$\tag{15}$$

Now, we re-scale x to accommodate the 'drift' of the random walker using $\tilde{z} = \tilde{x} - \frac{m_1 N}{L}\tilde{t}$, where $m_1 N/L$ is the drift velocity. We also define $\tilde{\rho}(\tilde{x}, \tilde{t}) = \phi(\tilde{z}, \tilde{t})$, so that

$$\frac{\partial \tilde{\rho}}{\partial \tilde{t}} = \frac{\partial \phi}{\partial \tilde{t}} + \frac{\partial \phi}{\partial \tilde{z}}\frac{\partial \tilde{z}}{\partial \tilde{t}} = \frac{\partial \phi}{\partial \tilde{t}} - \frac{m_1 N}{L}\frac{\partial \phi}{\partial \tilde{z}} \tag{16}$$

$$\frac{\partial^2 \phi}{\partial \tilde{t}^2} = \frac{\partial^2 \phi}{\partial \tilde{t}^2} + 2\frac{\partial^2 \phi}{\partial \tilde{z}\partial \tilde{t}}\frac{\partial \tilde{z}}{\partial \tilde{t}} + \frac{\partial^2 \phi}{\partial \tilde{z}^2}\left(\frac{\partial \tilde{z}}{\partial \tilde{t}}\right)^2 \tag{17}$$

$$= \frac{\partial^2 \phi}{\partial \tilde{t}^2} - 2\frac{m_1 N}{L}\frac{\partial^2 \phi}{\partial \tilde{z}\partial \tilde{t}} + \left(\frac{m_1 N}{L}\right)^2\frac{\partial^2 \phi}{\partial \tilde{z}^2} \tag{18}$$

$$\frac{\partial^n \tilde{\rho}}{\partial \tilde{x}^n} = \frac{\partial^n \phi}{\partial \tilde{z}^n}. \tag{19}$$

$$\tag{20}$$

Hence, the modified Kramers-Moyall expansion becomes:

$$\frac{\partial \phi}{\partial \tilde{t}} - \frac{m_1 N}{L}\frac{\partial \phi}{\partial \tilde{z}} + \left[\frac{1}{2N}\frac{\partial^2 \phi}{\partial \tilde{t}^2} - \frac{m_1}{L}\frac{\partial^2 \phi}{\partial \tilde{t}\partial \tilde{z}} + \frac{m_1^2 N}{2L^2}\frac{\partial^2 \phi}{\partial \tilde{z}^2}\right] + \left[\frac{1}{3! N^2}\frac{\partial^3 \phi}{\partial \tilde{t}^3} + \dots\right] + \dots =$$
$$- \frac{m_1 N}{L}\frac{\partial \phi}{\partial \tilde{z}} + \frac{m_2 N}{2L^2}\frac{\partial^2 \phi}{\partial \tilde{z}^2} - \frac{m_3 N}{3! L^3}\frac{\partial^3 \phi}{\partial \tilde{z}^3} + \dots \tag{21}$$

Note that in this equation the first derivative $\partial\phi/\partial\tilde{z}$ drops out which of course [illegible] point of introducing $\tilde{z}$. Remember that a proper choice for L will ensure that $\phi(\tilde{z})$ exists, [illegible] up as $N \to \infty$ and integrates to 1. We now consider a dominant balance of eq.(21) noting that the first term on the left hand side *must* be included since ϕ is known to evolve in time. It is then consistent to keep terms of order N/L^2 on the right hand side. To demonstrate this, consider what would happen if we decided to make the dominant balance with terms of order $N/L^3 \ldots$ such that $L \sim N^{1/3}$ and terms of order $N/L^2 \sim N^{1/3}$ which blows up as $N \to \infty$. Thus, we are led to the first-order approximation as $N \to \infty$ and with $\tilde{z} = O(1)$:

$$\frac{\partial \phi}{\partial \tilde{t}} \sim \frac{(m_2 - m_1^2)N}{2L^2} \frac{\partial^2 \phi}{\partial \tilde{z}^2} \equiv \frac{1}{2} \frac{\partial^2 \phi}{\partial \tilde{z}^2}. \tag{22}$$

So we are naturally led to choose $L = \sigma\sqrt{N}$ where $\sigma^2 = m_2 - m_1^2$ is the variance as usual / expected. Specifically, L does not depend on m_2 which the unmodified Kramers-Moyall expansion claims. This is essentially a continuum proof of the Central Limit Theorem. After all, we know how to solve the diffusion equation given an initial peak distribution $\phi(\tilde{z}, 0) = \delta(\tilde{z})$, namely

$$\phi(\tilde{z}, \tilde{t}) = \frac{1}{\sqrt{2\pi \tilde{t}}} e^{-\frac{\tilde{z}^2}{2\tilde{t}}} \tag{23}$$

$$P_N(x) = \frac{1}{\sqrt{2\pi\sigma^2 N}} e^{-\frac{(x - m_1 N)^2}{2\sigma^2 N}}, \tag{24}$$

where the scaling has been put back into the final expression for $P_N(x)$ and $\tilde{t} = 1$, i.e. we are 'in' the central region. A note on the validity of the continuum limit ... continuum diffusion implies that there is a finite (albeit very small) probability of finding the random walker at some enormous distance from its' starting point for any time $t = 0 + \epsilon$.

In the next lecture, we will show that the higher-order terms in the PDE of the modified Kramers-Moyall expansion reproduce the Gram-Charlier expansion of the discrete PDF at all orders, showing that the continuum limit provides a systematic approximation of the "central region".