Lecture 9: Kramers-Moyall Cumulant Expansion

Scribe: Jacy Bird
(Division of Engineering and Applied Sciences, Harvard)

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In this lecture, we study the higher-order terms in the Kramers-Moyall expansion for the continuum approximation, which satisfies a PDE generalizing the diffusion equation, for the long-time limit for a random walk with IID steps with finite moments. We show that the coefficients in the PDE involve cumulants, not moments (as commonly asserted), if the solution at various orders is to produce a valid asympototic expansion. This is done by an iterative method, , justified *a posteriori* by a continuum derivation of the correct Gram-Charlier expansion, as the asymptotic expansion of the Green function for the PDE.

1 Continuum Approximation of the Position of a Random Walk

As we saw in previous lecture, we can rewrite the Bachelier Equation as a infinite-sum, partial differential equation (PDE). Provided that the random walk has IID steps with finite moments, we derived that

$$P_{N+1}(x) - P_N(x) = \sum_{n=1}^{\infty} \frac{(-1)^n m_n}{n!} \frac{\partial^n P_N}{\partial x^n}. \tag{1}$$

We now substitute $\rho(x, N\tau)$ for $P_N(x)$ (where τ represents the time-step) and divide both sides by τ to get

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

Although real stochastic processes are discrete random walks, we usually care about the long-time limit of many steps. Examples include Brownian motion (where large particles bounce around in a gas) or financial time series. Therefore in Equation 2, we will consider the limit of $\tau \to 0$, since we are interested in much longer time scales. As shown in the previous lecture, when dealing with discrete random walks, strictly speaking, the right thing to do is to consider times $t = N\tau$=constant with $N \to \infty$, focusing on the appropriate length scale, $L(t) \gg \sigma$, much larger than the standard deviation of the step size, σ. Here, we will get similar results by fixing x, t and letting $\tau, \sigma \to 0$ with $D_2 = \sigma^2/2\tau$ fixed.

Recall that $\rho_(x, t+\tau)$ can be expanded as $\rho_(x,t) + \tau \frac{\partial \rho}{\partial t} + \frac{1}{2}\tau^2 \frac{\partial^2 \rho}{\partial t^2} + \sum_{n=3}^{\infty} \frac{\tau^n}{n!} \frac{\partial^n \rho}{\partial t^n}$. Thus Equation 2 can rewritten as

$$\frac{\partial \rho}{\partial t} + \sum_{n=2}^{\infty} \frac{\tau^{n-1}}{n!} \frac{\partial^n \rho}{\partial t^n} = \sum_{n=1}^{\infty} \frac{(-1)^n m_n}{n!\tau} \frac{\partial^n \rho}{\partial x^n}. \tag{3}$$

In the last lecture it was showed that the leading order behavior of Equation 3 was

$$\frac{\partial \rho}{\partial t} \sim -\frac{m_1}{\tau}\frac{\partial \rho}{\partial x} + \frac{m_2}{2\tau}\frac{\partial^2 \rho}{\partial x^2} - \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} \tag{4}$$

In this lecture we are going to calculate higher order behavior, so the first step is to expand Equation 3 to higher order. We find that

$$\frac{\partial \rho}{\partial t} = -\frac{m_1}{\tau}\frac{\partial \rho}{\partial x} + \frac{m_2}{2\tau}\frac{\partial^2 \rho}{\partial x^2} - \frac{m_3}{3!\tau}\frac{\partial^3 \rho}{\partial x^3} - \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} - \frac{\tau^2}{3!}\frac{\partial^3 \rho}{\partial t^3} + O\left(\frac{\partial^4 \rho}{\partial x^4}, \frac{\partial^4 \rho}{\partial t^4}\right) \tag{5}$$

2 Recursive Substitution in the Kramers-Moyall Expansion

Our goal is to rewrite the RHS of Equation 5 so that the lower order terms only consist of derivatives with respect to x. To do this we will employ recursive substitution.

We begin by differentiating both sides of Equation 5 with respect to t and multiply by $\frac{\tau}{2}$, so that

$$\frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} = -\frac{m_1}{2}\frac{\partial}{\partial x}\frac{\partial \rho}{\partial t} + \frac{m_2}{4}\frac{\partial^2}{\partial x^2}\frac{\partial \rho}{\partial t} - \frac{\tau^2}{4}\frac{\partial^3 \rho}{\partial t^3} + O\left(\frac{\partial^4 \rho}{\partial x^4}, \frac{\partial^4 \rho}{\partial t^4}\right) \tag{6}$$

The next step is to substitute $\frac{\partial \rho}{\partial t}$ from Equation 5 into Equation 6 so that Equation 6 becomes

$$\begin{aligned}\frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} = \; & - \frac{m_1}{2}\frac{\partial}{\partial x}\left(-\frac{m_1}{\tau}\frac{\partial \rho}{\partial x} + \frac{m_2}{2\tau}\frac{\partial^2 \rho}{\partial x^2} - \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2}\cdots\right) + \frac{m_2}{4}\frac{\partial^2}{\partial x^2}\left(-\frac{m_1}{\tau}\frac{\partial \rho}{\partial x} + \frac{m_2}{2\tau}\frac{\partial^2 \rho}{\partial x^2} - \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2}\cdots\right) \\ & - \frac{m_3}{12}\frac{\partial^3}{\partial x^3}\left(-\frac{m_1}{\tau}\frac{\partial \rho}{\partial x} + \frac{m_2}{2\tau}\frac{\partial^2 \rho}{\partial x^2} - \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2}\cdots\right)\cdots - \frac{\tau^2}{4}\frac{\partial^3 \rho}{\partial t^3}\cdots\end{aligned} \tag{7}$$

Equation 7 can be simplified to

$$\frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} = \frac{m_1^2}{2\tau}\frac{\partial^2 \rho}{\partial x^2} - \frac{m_1 m_2}{4\tau}\frac{\partial^3 \rho}{\partial x^3} + \frac{m_1}{2}\frac{\partial}{\partial x}\left(\frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2}\right) - \frac{m_1 m_2}{4\tau}\frac{\partial^3 \rho}{\partial x^3} - \frac{\tau^2}{4}\frac{\partial^3 \rho}{\partial t^3} + O\left(\frac{\partial^4 \rho}{\partial x^4}, \frac{\partial^4 \rho}{\partial t^4}\right) \tag{8}$$

and even further reduced to

$$\frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} = \frac{m_1^2}{2\tau}\frac{\partial^2 \rho}{\partial x^2} - \frac{m_1 m_2}{2\tau}\frac{\partial^3 \rho}{\partial x^3} + \frac{m_1^3}{4\tau}\frac{\partial^3 \rho}{\partial x^3} - \frac{\tau^2}{4}\frac{\partial^3 \rho}{\partial t^3} + O\left(\frac{\partial^4 \rho}{\partial x^4}, \frac{\partial^4 \rho}{\partial t^4}\right). \tag{9}$$

by noting that

$$\frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} = \frac{m_1^2}{2\tau}\frac{\partial^2 \rho}{\partial x^2} + O\left(\frac{\partial^3 \rho}{\partial x^3}, \frac{\partial^4 \rho}{\partial t^4}\right). \tag{10}$$

What we are effectively doing is pushing the time derivatives to higher order while gaining more x derivatives.

We now repeat this process again. We apply the operator $\tau\frac{\partial}{\partial t}$ on Equation 9 to get

$$\tau^2\frac{\partial^3 \rho}{\partial t^3} = m_1^2\frac{\partial^2}{\partial x^2}\frac{\partial \rho}{\partial t} + O\left(\frac{\partial^4 \rho}{\partial x^4}, \frac{\partial^4 \rho}{\partial t^4}\right). \tag{11}$$

Then we substitute $\frac{\partial \rho}{\partial t}$ from Equation 5 into Equation 11 so that Equation 11 becomes

$$\tau^2\frac{\partial^3 \rho}{\partial t^3} = -\frac{m_1^3}{\tau}\frac{\partial^3 \rho}{\partial x^3} + O\left(\frac{\partial^4 \rho}{\partial x^4}, \frac{\partial^4 \rho}{\partial t^4}\right). \tag{12}$$

Substituting Equation 12 into Equation 9, we see that Equation 9 can be rewritten as

$$\frac{\tau}{2}\frac{\partial^2\rho}{\partial t^2} = \frac{m_1^2}{2\tau}\frac{\partial^2\rho}{\partial x^2} - \frac{m_1 m_2}{2\tau}\frac{\partial^3\rho}{\partial x^3} + \frac{m_1^3}{4\tau}\frac{\partial^3\rho}{\partial x^3} + \frac{m_1^3}{4\tau}\frac{\partial^3\rho}{\partial x^3} + O\left(\frac{\partial^4\rho}{\partial x^4}, \frac{\partial^4\rho}{\partial t^4}\right). \tag{13}$$

Finally the results from Equations 12 and 13 are substituted into Equation 5 to give

$$\frac{\partial\rho}{\partial t} = -\frac{m_1}{\tau}\frac{\partial\rho}{\partial x} + \frac{m_2}{2\tau}\frac{\partial^2\rho}{\partial x^2} - \frac{m_3}{6\tau}\frac{\partial^3\rho}{\partial x^3} - \left(\frac{m_1^2}{2\tau}\frac{\partial^2\rho}{\partial x^2} - \frac{m_1 m_2}{2\tau}\frac{\partial^3\rho}{\partial x^3} + \frac{m_1^3}{2\tau}\frac{\partial^3\rho}{\partial x^3}\right) + \frac{m_1^3}{6\tau}\frac{\partial^3\rho}{\partial x^3} + O\left(\frac{\partial^4\rho}{\partial x^4}, \frac{\partial^4\rho}{\partial t^4}\right) \tag{14}$$

Collecting terms, we see that

$$\frac{\partial\rho}{\partial t} = -\frac{m_1}{\tau}\frac{\partial\rho}{\partial x} + \frac{\left(m_2 - m_1^2\right)}{2\tau}\frac{\partial^2\rho}{\partial x^2} - \frac{\left(m_3 - 3m_1 m_2 + 2m_1^3\right)}{6\tau}\frac{\partial^3\rho}{\partial x^3} + O\left(\frac{\partial^4\rho}{\partial x^4}, \frac{\partial^4\rho}{\partial t^4}\right) \tag{15}$$

which is an equation that relates $\frac{\partial\rho}{\partial t}$ to lower order derivatives that are only with respect to x.

The combinations of moments in Equation 16 are thus more naturally expressed as cumulants leading to

$$\frac{\partial\rho}{\partial t} = -\frac{C_1}{\tau}\frac{\partial\rho}{\partial x} + \frac{C_2}{2\tau}\frac{\partial^2\rho}{\partial x^2} - \frac{C_3}{3!\tau}\frac{\partial^3\rho}{\partial x^3} + O\left(\frac{\partial^4\rho}{\partial x^4}, \frac{\partial^4\rho}{\partial t^4}\right). \tag{16}$$

As we notice the pattern, it seems the higher-order Kramers-Moyall coefficients from the previous lecture should be defined in terms of cumulants, not moments:

$$\tilde{D}_n = \frac{C_n}{n!\tau} \tag{17}$$

so that the continuum limit is properly described by the following PDE,

$$\frac{\partial\rho}{\partial t} = \sum_{n=1}^{\infty}(-1)^n \tilde{D}_n \frac{\partial^n\rho}{\partial x^n} \tag{18}$$

Unlike the usual Kramers-Moyall moment expansion (with $\tilde{D}_n$ replaced by $D_n = M_n/n!\tau$), this PDE, when truncated at various orders, provides a valid asymptotic approximation of the position of the random walk, as we now show.

3 Gram-Charlier Expansion for the Green Function

Claim:

$$\frac{\partial\rho}{\partial t} = \sum_{n=1}^{\infty}\frac{(-1)^n C_n}{n!\tau}\frac{\partial^n\rho}{\partial x^n} \tag{19}$$

where C_n is the n^{th} cumulant.

We are now going to solve Equation 19 for $\rho(x,0) = \delta(x)$, and demonstrate that $\rho(x,t)$ is the same Gram-Charlier expansion we derived before by more rigorous means. First we take the Fourier transform of 19 and get

$$\frac{\partial\hat{\rho}}{\partial t} = \left(\sum_{n=1}^{\infty}\frac{(-1)^n C_n (ik^n)}{n!\tau}\right)\hat{\rho}. \tag{20}$$

Solving the differential equation leads to

$$\hat{\rho}(k,t) = e^{\left(\sum_{n=1}^{\infty} \frac{(-i)^n C_n}{n!\tau} k^n\right) t}. \tag{21}$$

Next, we note that $t/\tau = N$ and $\rho(x, N\tau) = P_N(x)$:

$$\hat{P}_N(k) = e^{\left(\sum_{n=1}^{\infty} \frac{(-i)^n C_n}{n!\tau} k^n\right) N}. \tag{22}$$

By the definition of cumulants, the RHS of Equation 22 is equal to $\hat{p}(k)^N$. Therefore

$$\hat{P}_N(k) = \hat{p}(k)^N \tag{23}$$

which is the familiar Fourier transform of Bachelier's equation,

$$P_N(x) = p^{*N}(x) = P_{N-1} * p(x) \tag{24}$$

so we know we have a systematic asymptotic approximation of $P_N(x)$ from the solution to the modified Kramers-Moyall expansion PDE, Eq (19). As we saw in lectures 3 and 4, the cumulant expansion of $\hat{P}_N(k)$, upon inverse Fourier transform, produces the Gram-Charlier expansion of $P_N(x)$, valid in the central region.

We have seen that the Gram-Charlier expansion is obtained from the solution to the PRE (19) for a localized intitial condition, $\rho(x, 0) = \delta(x)$. Since the PDE is linear, this is the Green function, $G(x, t)$, (for an infinite space) from which a general solution is easily constructed for any initial condition, $\rho(x, t) = G(x, t) * \rho(x, 0)$.

A major advantage of the continuum approximation to the discrete random walk is that the PDE can be solved, to the desired order, in more complicated multi-dimensional geometries, where discrete methods, such as Fourier transform are not easily applied. It also provides simple analytical insights into the final position of the random walk, which do not depend on the details of the step distribution, beyond the low-order cumulants.