Asymptotics Inside the Central Region and the Continuum Limit

David Vener (Department of Mathematics)

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In this lecture, we continue our discussion of the Central Limit Theorem begun in Lecture #3 by calculating corrections to the Gaussian distribution in the "central region" via the Edgeworth expansion. We will discover that the central region can often be extended well beyond $x - N\mu = O\left(\sigma\sqrt{N}\right)$, depending on the cumulants of the underlying distribution function for the individual steps. We then switch gears to consider the continuum limit of the random walk and derive a partial differential equation for the time evolution of its probability distribution function. In later lectures, we will derive the relationship between this equation and the Edgeworth expansion.

1 Edgeworth and Gram-Charlier Expansions

Recall that in Lecture #3, we considered the probability distribution function (PDF) P_N of the position (X_N) of a random flier who takes identical, independently distributed steps, each of which with PDF $p(x)$, mean μ, and variance σ^2. We then definited the normalized position, Z_N, with PDF $\phi_N(z)$ by

$$Z_N = \frac{X_N - N\mu}{\sigma\sqrt{N}}.$$

Then from the asymptotic expansion $(k \to 0)$ for p's cumulant generating function,

$$\psi(k) = \log \hat{p}(k) \sim -\frac{\sigma^2 k^2}{2} - \frac{ic_3 k^3}{3!} + \frac{c_4 k^4}{4!} + \cdots ,$$

we found an asymptotic expansion (as $N \to \infty$) for ϕ_N.

$$\phi_N(z) \sim \int_{-\infty}^{\infty} e^{-i\omega z} e^{-\frac{\omega^2}{2}} e^{\frac{\lambda_3}{3!}\frac{(i\omega)^3}{\sqrt{N}} + \frac{\lambda_4}{4!}\frac{(i\omega)^4}{N} + \cdots} \frac{d\omega}{2\pi}, \tag{1}$$

where $\omega = \sigma\sqrt{N}k$ and the λ_n are the normalized cumulants of $p(x)$.

Note 1: In this lecture, we will assume that $|c_3|, |c_4| < \infty$. We will discuss cases where one or both of these cumulants do not exist in later lectures.

Since the main contribution to the integral in (1) occurs near $\omega = 0$, we can find an asymptotic expansion for small ω of the third exponential in the integrand. That is, as $N \to \infty$

$$\phi_N(z) \sim \int_{-\infty}^{\infty} e^{i\omega z} e^{-\frac{\omega^2}{2}} \left[1 + \frac{\lambda_3}{3!} \frac{(i\omega)^3}{\sqrt{N}} + \frac{\lambda_4}{4!} \frac{(i\omega)^4}{N} + \frac{1}{2}\left(\frac{\lambda_3}{3!}\right)^2 \frac{(i\omega)^6}{N} + O\left(\frac{\omega^5}{N\sqrt{N}}\right)\right] \frac{d\omega}{2\pi}. \tag{2}$$

Noticing that

$$\int_{-\infty}^{\infty} (i\omega)^n e^{-i\omega z} e^{-\frac{\omega^2}{2}} = (-1)^n \frac{d^n}{dz^n} \int_{-\infty}^{\infty} e^{-i\omega z} e^{-\frac{\omega^2}{2}}$$

allows us to rewrite (2) to read

$$\phi_N(z) \sim \frac{e^{-\frac{z^2}{2}}}{\sqrt{2\pi}} \left[1 + \frac{\lambda_3}{3!} \frac{1}{\sqrt{N}} H_3(z) + \frac{1}{N}\left\{\frac{\lambda_4}{4!} H_4(z) + \frac{1}{2}\left(\frac{\lambda_3}{3!}\right)^2 H_6(z)\right\} + O\left(\frac{z^5}{N\sqrt{N}}\right)\right], \tag{3}$$

where $H_n(z)$ is the n^{th} Hermite polynomial defined by

$$\frac{d^n}{dz^n} e^{-\frac{z^2}{2}} \equiv (-1)^n H_n(z)\, e^{-\frac{z^2}{2}}.$$

Note 2: The Hermite polynomials come up in many different places in mathematical physics, including, perhaps most prominently, in the eigenfunctions for the quantum harmonic oscillator. The first few Hermite polynomials are

$$\begin{aligned} H_1 &= z, \\ H_2 &= z^2 - 1, \\ H_3 &= z^3 - 3z, \\ H_4 &= z^4 - 6z + 3, \\ H_5 &= z^5 - 10z^3 + 15z, \\ H_6 &= z^6 - 15z^4 + 15z^2 - 15. \end{aligned}$$

Therefore, as $N \to \infty$ we can write Equation (3) as

$$\phi_N(z) \sim \frac{e^{-\frac{z^2}{2}}}{\sqrt{2\pi}} \left[1 + \frac{h_3(z)}{\sqrt{N}} + \frac{h_4(z)}{N} + \cdots\right], \tag{4}$$

where

$$h_3(z) = \frac{\lambda_3}{3!} H_3(z), \tag{5}$$

$$h_4(z) = \frac{\lambda_4}{4!} H_4(z) + \frac{1}{2}\left(\frac{\lambda_3}{3!}\right)^2 H_6(z). \tag{6}$$

Note 3: In 1 dimension, this general expansion related to the CLT is often called the 'Edgeworth expansion' in the mathematical literature. (See, e.g. W. Feller, *An Introduction to Probability*, Vol. 2.) In more dimensions when related to random flights, expansions of this type are sometimes called 'Gram-Charlier Expansions'. (See, e.g. B. Hughes, *Random Walks and Random Environments.*)

2 Berry-Eséen Theorem

Although we will not prove it, the Berry-Eséen Theorem is a general statement on how well the distribution of the random flier is modelled by the Gaussian distribution. Define the cumulative distribution functions Φ_0 and Φ_N by

$$\begin{aligned}\Phi_0(z) &= \int_{-\infty}^{z} e^{-\frac{z'^2}{2}} \frac{dz'}{\sqrt{2\pi}}, \\ \Phi_N(z) &= \int_{-\infty}^{z} \phi_N(z')\, dz'.\end{aligned}$$

Then, if $< \Delta X_n >= 0$, $< \Delta X_n^2 >= \sigma^2 < \infty$, and $< |\Delta X_n|^3 >= r_3 < \infty$, the Berry-Eseen theorem states

$$|\Phi_N(z) - \Phi_0(z)| \leq \frac{3r_3}{\sigma^{\frac{3}{2}}\sqrt{N}},$$

which, remarkably, is a uniform bound for all N and z.

3 Width of the Central Region

3.1 Case 1: $0 < |\lambda_3| < \infty$

We'd like to know more accurately the region on which the Gaussian is good approximation for the distribution for the random flier's position after N steps. The approximation breaks down when the largest correction term is of order 1. That is when

$$\frac{\lambda_3}{3!}\frac{H_3(z)}{\sqrt{N}} \sim 1. \tag{7}$$

Since $H_3(z)$ is a polynomial of degree three, Equation (7) is equivalent to

$$\frac{z^3\lambda_3}{6} \sim \sqrt{N}.$$

Therefore, the central region is defined by

$$z_c \sim \left(\frac{6}{\lambda_3}\right)^{\frac{1}{3}} N^{\frac{1}{6}},$$

i.e.

$$x_c - N\mu \sim \sigma \left(\frac{6}{\lambda_3}\right)^{\frac{1}{3}} N^{\frac{2}{3}}.$$

3.2 Case 2: $\lambda_3 = 0, 0 < |\lambda_4| < \infty$

Now the leading order correction is $O\left(\frac{h_4(z)}{N}\right)$. Since $\lambda_3 = 0$, $h_4(z) = \frac{\lambda_4}{4!} H_4(z)$ which is a degree four polynomial. Thus the central region is defined by

$$z_c \sim \left(\frac{24}{\lambda_4}\right)^{\frac{1}{4}} N^{\frac{1}{4}}.$$

In terms of the orginal random walk, the central region is therefore defined by

$$X_c - N\mu = \sigma \left(\frac{24}{\lambda_4}\right)^{\frac{1}{4}} N^{\frac{3}{4}}.$$

Note 4: If $\lambda_3 \neq 0$, the $H_6(z)$ goes "bad" where $\frac{z^6}{N} \sim 1$, i.e. when $z_c \sim N^{\frac{1}{6}}$ which makes the second correction go bad in the same limit as the first term. In fact, all of the corrections go 'bad' in the same region if $\lambda_3 \neq 0$.

4 The Continuum Limit

4.1 Kramers-Moyal Expansion

Recall the basic Bachelier Equation from Lecture #2. That is for a random walk with identical, indepently distributed steps, all of whose moments exist, we have

$$P_{N+1}(x) = \int_{-\infty}^{\infty} P_N(x-y)\, p(y)\, dy. \tag{8}$$

Since the scale of P_N is much larger than that of $p(x)$, we can expand $P_N(x-y)$ around x, to find

$$P_{N+1}(x) = \sum_{l=0}^{\infty} \frac{(-1)^l m_l}{l!} P_N^{(l)}(x), \tag{9}$$

where the moments, m_l, are defined as before ($m_l = \int y^l p(y)\, dy$). Since $m_0 = 1$ and $m_1 = \mu$, we can write

$$P_{N+1}(x) - P_N(x) = \sum_{l=1}^{\infty} \frac{(-1)^l m_l}{l!} P_N^{(l)}(x). \tag{10}$$

If we let τ be the time in between steps, define $t = N\tau$, and (formally) take the limit as $\tau \to 0$, and let $\rho(x,t)$ be a slowly varying continous time-dependent density which reproduces the correct density profile at discrete times, $\rho(x, N\tau) = P_N(x)$, then we have from Equation (10) that

$$\frac{\partial \rho}{\partial t}(x,t) \approx -D_1 \frac{\partial \rho}{\partial x} + D_2 \frac{\partial^2 \rho}{\partial x^2} - D_3 \frac{\partial^3 \rho}{\partial x^3} + \cdots, \tag{11}$$

where

$$D_n(\tau) = \frac{m_n}{n!\,\tau}. \tag{12}$$

Equation (11) is sometimes called the 'Kramers-Moyall Expansion,' although this should not strictly be interpreted as an asymptotic expansion, due errors introduced by the continuous time derivative on the left hand side. The approximation is really only valid at leading order in the continuum limit, where only the first two terms in the sum survive,

$$\frac{\partial \rho}{\partial t} + D_1 \frac{\partial \rho}{\partial x} = D_2 \frac{\partial^2 \rho}{\partial x^2} \tag{13}$$

(This is the advection-diffusion equation, as mentioned in lecture 1). In the homework, the Kramers-Moyall expansion is derived for the more general case of transition probabilities depending on space and time, where the analogous leading-order equation is the 'Fokker-Planck equation', although again the higher-order terms must be modified, as we now describe.

4.2 Modified Kramers-Moyall Expansion

To correct the Kramers-Moyall expansion, we shall use a Taylor expansion of $P(x, t+\tau)$ around t. That is

$$\frac{P_{N+1}(x) - P_N(x)}{\tau} = \frac{\partial \rho}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} + \frac{\tau^2}{3!}\frac{\partial^3 \rho}{\partial t^3} + \cdots, \tag{14}$$

which upon combining with Equation (10) and rearranging reveals that

$$\frac{\partial \rho}{\partial t} = -\frac{m_1}{\tau}\frac{\partial \rho}{\partial x} + \frac{m_2}{2\tau}\frac{\partial^2 \rho}{\partial x^2} - \frac{m_3}{3!\tau}\frac{\partial^3 \rho}{\partial x^3} + \cdots - \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} - \frac{\tau}{3!}\frac{\partial^3 \rho}{\partial t^3} + \cdots. \tag{15}$$

Now taking $\frac{\tau}{2}\frac{\partial}{\partial t}$ of both sides of Equation (13), we have

$$\frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} = -\frac{m_1}{2}\frac{\partial}{\partial x}\frac{\partial \rho}{\partial t} + \frac{m_2}{4}\frac{\partial^2 \rho}{\partial x^2}\frac{\partial \rho}{\partial t} - \frac{m_3}{12}\frac{\partial^3 \rho}{\partial x^3}\frac{\partial \rho}{\partial t} + \cdots - \frac{\tau^2}{4}\frac{\partial^3 \rho}{\partial t^2} - \frac{\tau^3}{6}\frac{\partial^4 \rho}{\partial t^4} + \cdots. \tag{16}$$

Next we substitute for $\frac{\partial \rho}{\partial t}$ from Equation (13) to find

$$\frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} = \frac{m_1^2}{2\tau}\frac{\partial^2 \rho}{\partial x^2} - \frac{m_1 m_2}{2\tau}\frac{\partial^3 \rho}{\partial x^3} + \cdots - \frac{\tau^2}{4}\frac{\partial^3 \rho}{\partial t^3} + \cdots. \tag{17}$$

Now substituting back into Equation (13), we have

$$\frac{\partial \rho}{\partial t} = -\frac{m_1}{\tau}\frac{\partial \rho}{\partial x} + \left(\frac{m_2 - m_1^2}{2\tau}\right)\frac{\partial^2 \rho}{\partial x^2} - \left(\frac{m_3 - 3m_1 m_2}{3!\tau}\right)\frac{\partial^3 \rho}{\partial x^3} + \cdots \tag{18}$$

If we now subtitute recursively for $\frac{\partial^3 \rho}{\partial t^3}$ in terms of higher order time and spacial dervatives and so on we arrive at the formal expansion

$$\frac{\partial \rho}{\partial t} \sim -\tilde{D}_1 \frac{\partial \rho}{\partial x} + \tilde{D}_2 \frac{\partial^2 \rho}{\partial x^2} - \tilde{D}_3 \frac{\partial^3 \rho}{\partial x^3} + \cdots, \tag{19}$$

where the modified expansion coefficients are,

$$\tilde{D}_l = \frac{c_l}{l!\,\tau}. \tag{20}$$

We have only checked the first three terms explcitly, but in the next class, we will see that this formal expansion is indeed correct (when the cumulants are finite), in the sense that the Green function for Eq. (19) (solution for the initial condition, $\rho(x,0) = \delta(x)$) taken to all orders *exactly* reproduces the true PDF, $P_N(x)$, at the discrete times, $t = N\tau$. Moreover, truncating the expansion yields a valid asymptotic series for the Green function, which will naturally turn out to be the Edgeworth expansion derived above, thus justifying our formal derivation *a posteriori*. Thus, the PDE, Eq. (19), truncated at several terms provides valid asymptotic approximations for arbitrary initial conditions (by linearity), although the approximations may suffer from the same problems as the Edgeworth expansion (e.g. very small negative values are possible in the tails of a localized distribution).

In summary, although the Kramers-Moyall expansion, Eq. (11), is usually written in terms of moments, m_l, of the random displacements, via the coefficients, D_l, a careful analysis of the limit of continuous time yields the modified expansion, Eq. (19), where *the moments are replaced by the cumulants*, c_l.