Trajectory-based (Langevin) approach to Brownian motion

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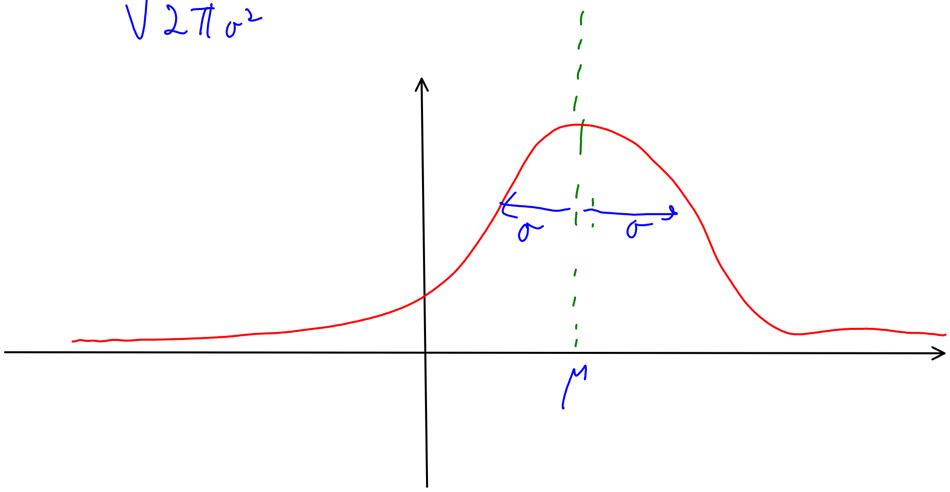
12:04 PM

No class or office hours Friday, January 30.

Third and most important example of random variable for this class:

Gaussian (normal) random variable

$$p_Z(z) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\frac{(z-\mu)^2}{\sigma^2}} \qquad \text{PDF}$$



$$\text{Parameters: } \mu = \mathbb{E} Z = \langle Z \rangle \qquad \text{mean}$$

$$\sigma = \sqrt{\mathbb{E}\left(Z - \langle Z \rangle\right)^2} \qquad \text{standard deviation}$$

The mean of a random variable gives the simplest quantitative statistic about it, namely its expected or average value.

The standard deviation of a random variable describes the next most important statistic, which is the typical amount by which a given realization of the random variable departs from its expected value.

The mean and standard deviation can be defined and meaningful for almost any random variable, but the interesting aspect abou t a Gaussian random variable is that it is completely described by the mean and standard deviation and one can define a Gaussian random va riable with arbitrary real mean values and positive standard deviations.

A collection of random variables $\{Z_n\}$

is said to be identically distributed when the random variables all have the same probability distribution (or PDF):

$$P_{Z_n}(B) = P_Z(B) \qquad \text{for all } n$$

$$p_{Z_n}(z) = p_Z(z)$$

The collection of random variables is said to be independent provided that:

$$P(Z_{n_1} \in B_1, Z_{n_2} \in B_2, \ldots, Z_{n_k} \in B_k)$$
$$= \prod_{j=1}^{k} P(Z_{n_j} \in B_j)$$

for any subcollection $\{n_1, n_2, \ldots, n_k\}$

Intuitively, independent random variables have the property that they do not influence each other (have no correlation). Mathematically, computing properties of collections of independent random variables can always be reduced to calculations involving one random variable at a time.

In our first simple random walk model for Brownian motion:

$$X_{n+1}(\omega) = X_n(\omega) + Z_n(\omega)$$

The fact that the Z_n are identically distributed means that the law of evolution of the Brownian particle does not change with time (doesn't get hotter or slow down, etc.) The fact that the Z_n are independent reflects the lack of memory (inertia) of the changes in position of the Brownian particle between successive observations.

So what PDF should the random variables Z_n have? To a large extent, it doesn't matter too much what we choose. It turns out that the behavior of the random walk, when we go to the continuous-time limit, will generally behave as if the probability distribution for the Z_n were Gaussian.

The reason is the Central Limit Theorem, which states that under some mild conditions, the sum of a large number of independent, identically distributed random variables has a Gaussian distribution. (The PDFs of the random variables being summed should not be too slowly decaying; see Lindeberg condition.)

Notice that: $$X_n(\omega) = X_0(\omega) + \sum_{j=1}^{n} Z_n(\omega)$$

For practical purposes, think of the random walk in the following way. Suppose that the time increment Δt is a value of time such that the random walk description (with independent, identically distributed observations) is valid to a good approximation.

For water molecules and objects on the nanometer scale,this means $\Delta t \gtrsim 10^{-12}$ s

For larger objects visible under the microscope (micron scale and larger), the necessary time increment will be larger, around $\Delta t \gtrsim 10^{-6}$ s

But typically, especially in the nineteenth century, the increments in time between actual observations is much larger than this time.

Observational time increment: $\Delta \tilde{t}$

We'll take $\Delta \tilde{t} = m \, \Delta t, \quad m \gg 1$

Define the observation time series:

$$\hat{X}_n = X_{mn}$$ (the random walk is observed only once every m steps)

$$\hat{X}_{n+1}(\omega) = \hat{X}_n(\omega) + \hat{Z}_n(\omega)$$

where $$\hat{Z}_n(\omega) = \underbrace{\sum_{j=0}^{m-1} Z_{nm+j}(\omega)}_{\text{sum of large \# of i.i.d. rv's} \sim \text{Gaussian}}$$

For this reason, we will proceed with the random walk model with a Gaussian PDF for the increments because this will emerge from a broad class of random walk models with arbitrary PDF for the increments if the random walk is observed at a coarse enough time scale. This actually has practical implications for molecular dynamics simulations, in that one can choose fairly arbitrary rules for how to generate the increments if one is observing the dynamics over a long time.

We now consider constructing a continuous-time description for the Brownian motion trajectory from this discrete-time model by taking a limit of small time increment. We will have to do this in a way that's similar to continuum theory for fluid mechanics, solid mechanics, etc.

$$\Delta t \ll \widehat{\Delta t} \ll \text{macro time scale}$$

Can we derive some sort of differential equation for this regime of typical physical interest where the time scales of experiments or simulations are well resolved enough that we want to use a continuous-time theory, but one which does not seek to describe very fine microscopic details.

Let's try and set up a differential equation:

$$\hat{X}_{n+1}(\omega) - \hat{X}_n(\omega) = \hat{Z}_n(\omega)$$

We would get an ordinary differential equation for this limit provided that the increment in the particle position scaled like:

$$\hat{Z}_n(\omega) \sim \widehat{\Delta t} \quad \times \quad \text{not true!}$$

To see why this isn't true, recall:

$$\hat{Z}_n(\omega) = \sum_{j=1}^{\widehat{\Delta t}/\Delta t} Z_{nm+j}$$

To see how this random variable scales with respect to the time increment, let's look at its fundamental statistical properties: $\widehat{\Delta t}/\Delta t$,, Mean: $\mathbb{E}\,\tilde{Z}_n(\omega) = \sum_{j=1} \mathbb{E}\, Z_{nm+j}$

$$\boxed{\mathbb{E}\left(\sum_{j=1}^{n} Y_j\right) = \sum_{j=1}^{n} \mathbb{E}\, Y_j}$$

We expect no bias in the increments of Brownian motion by symmetry.

$$\mathbb{E}\, Z_n = 0$$

$$\mathbb{E}\, \tilde{Z}_n = 0$$

Standard deviation?

Variance: $\mathrm{Var}\, \tilde{Z}_n = \sigma^2_{\tilde{Z}_n}$

$$\boxed{\mathrm{Var}\left(\sum_{j=1}^{n} Y_j\right) = \sum_{j=1}^{n} \mathrm{Var}\, Y_j \quad \text{provided the } \{Y_j\} \ \boxed{\text{independent.}}}$$

$$\mathrm{Var}\, \tilde{Z}_n = \mathrm{Var}\left(\sum_{j=0}^{m-1} Z_{nm+j}\right)$$

↑ independent

$$= \sum_{j=0}^{m-1} \mathrm{Var}\, Z_{nm+j} = \sum_{j=0}^{m-1} \mathrm{Var}\, Z$$

identically distributed

$$= m\, \mathrm{Var}\, Z = \frac{\widehat{\Delta t}}{\Delta t}\, \mathrm{Var}\, Z$$

$$\sigma_{\tilde{Z}_n} = \sqrt{\mathrm{Var}\, \tilde{Z}_n} = \sqrt{\frac{\widehat{\Delta t}}{\Delta t}}\; \sigma_Z$$

$$\sigma_{\tilde{Z}_n} \sim \sqrt{\widetilde{\Delta t}}$$

The "size" of a mean zero random variable is well-characterized by its standard deviation.

Moreover, since we argued that the $\tilde{Z}_n$ should have Gaussian distribution, we can write:

$$\tilde{Z}_n = c\sqrt{\widetilde{\Delta t}}\ \xi_n$$

where $\xi_n \sim N(0,1)$ (Gaussian (normal) distribution with mean zero and standard deviation 1)

are a sequence of independent standard Gaussian random variables.

$\sigma \xi_n + \mu$ will be a Gaussian random variable with mean μ and standard deviation σ

If we tried to derive an ordinary differential equation: $= \tilde{X}_n(\omega)$

$$\frac{\tilde{X}((n+1)\widetilde{\Delta t},\omega) - \tilde{X}(n\widetilde{\Delta t},\omega)}{\widetilde{\Delta t}} = \frac{\tilde{Z}_n(\omega)}{\widetilde{\Delta t}} = \frac{c\sqrt{\widetilde{\Delta t}}\ \xi_n}{\widetilde{\Delta t}}$$

$$= \frac{c\,\xi_n}{\sqrt{\widetilde{\Delta t}}}$$

The right hand side does not converge as $\widetilde{\Delta t} \to 0$

This helps to explain why the experimental attempts to measure the velocity of Brownian motion in the nineteenth century saw contradictions and problems! Basically the experiments were trying to measure the limit of the left hand side with small time increment but this equation shows that the result will always depend on the time increment used. It's like a inconsistent numerical scheme.

We therefore have to take a different approach to describing the equation for Brownian motion:

Einstein's simple but crucial insight was to describe the motion of the Brownian particle trajectory without referring to velocity. Later formulation of the continuous-time description (by Wiener, etc.) of the trajectory stays with this philosophy:

Stochastic differential equation:

$$d\tilde{X}(\tilde{t}) = c\, dW(\tilde{t})$$

in analogy to writing ordinary differnetial equation

$$\frac{dX}{dt} = f(X, t)$$

$$dX = f(X, t)\,dt$$

$$X(t+\Delta t) - X(t) \approx f(X(t), t)\,\Delta t$$

We just have to develop basic calculus rules for the Wiener process W(t).