BROWNIAN MOTION

Giulio Gallo

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1 Introduction

This little project aims to derive the equations describing the Brownian motion and then use numerical methods to solve a stochastic differential equation.

2 Brief Historical introduction

In 1827 Robert Brown observed that, when small pollen grains are suspended in water, they start to move erratically and irregularly. He proved that this motion was present in any suspension of fine, inorganic particles, therefore ruling out the hypothesis it could be biologically driven.
Brown himself was not able to provide a satisfactory explanation of this phenomenon. Only in 1905 Einstein solved the riddle, providing a simple yet effective explanation of the phenomenon. This pioneering work can be regarded as one of the first uses of stochastic models in physics. This work was also of capital importance because it finally proved that the atomic hypothesis correctly predicts natural behavior. Indeed, in a conference held in 1911 in Paris, Arrhenius said that, after the works of Einstein, Smoluchowski (who arrived at similar conclusions as Einstein), and Perrin (who proved experimentally the work of Einstein) the atomic hypothesis could no longer be questioned.
A similar derivation was done later by Langevin. His derivation can be more easily generalized, but it would still take 40 years to have a rigorous theory of stochastic differential equations, which Ito will carry out.

3 The diffusion equation

3.1 Einstein derivation

To solve the problem, Einstein made two hypotheses:

- The motion of the suspended pollen particles is caused by the frequent impact with water molecules
- This motion can be described in terms of probabilities of imbalances of statistically independent impacts

This implies that:

- each pollen particle executes a motion independent of all other particles
- the movement of the same pollen particle in different time intervals can be considered as independent, i.e., it exists a typical time τ such that, in two successive time intervals τ, the motion executed by the particle can be thought of as events which are independent to each other

Let's assume that we have n particles suspended in the liquid. In a time τ, some particles may move in the x direction by an amount Δ, which can be positive or negative. The number of particles which experience a shift between Δ and $\Delta + d\Delta$ is expressible in the form:

$$dn = n\Phi(\Delta)d\Delta \tag{1}$$

where $\Phi(\Delta)$ is a frequency distribution of the shifts Δ, which has to satisfy the following properties:

- $\int_{-\infty}^{\infty} \Phi(\Delta)\, d\Delta = 1$
- $\Phi(\Delta) = \Phi(-\Delta)$
- is different from zero only for small values of Δ

Let now $\nu = f(x,t)$ be the number of particles per unit of volume. We want to compute the distribution of particles at a time $t+\tau$. Considering that $f(x,t)dx$ will give us the number of particles in the plane perpendicular to the x-axis, then we have that the number of particles in such plane at the time $t+\tau$ will be equal to the sum of all the particles that were distant Δ from the plane, that moved a distance which is exactly equal to Δ. This sum must be done taking into account the frequency of occurrence of each Δ, expressed through the function $\Phi(\Delta)$:

$$f(x,t+\tau)dx = dx \int_{-\infty}^{\infty} f(x+\Delta,t)\Phi(\Delta)\, d\Delta \tag{2}$$

this equation is the Chapman-Kolmogorov equation: the probability for a particle of being at x at time $t+\tau$ is given by the sum of all possible pushes Δ from position $x+\Delta$ multiplied by the probability of being at $x+\Delta$ at time t. This is a result of the assumption that the process has no memory, that is to say, it is only necessary to know the position at time t to predict its position at time $t+\tau$.
Starting from this equation, we can Taylor expand for time and position:

- $f(x,t+\tau) = f(x,t) + \tau\frac{\partial f}{\partial t} + ...$
- $f(x+\Delta,t) = f(x,t) + \frac{\partial f(x,t)}{\partial x}\Delta + \frac{\partial^2 f(x,t)}{\partial x^2}\frac{\Delta^2}{2!} + ...$

that leads to:

$$f + \tau\frac{\partial f}{\partial t} = f\int_{-\infty}^{\infty}\Phi(\Delta)\, d\Delta + \frac{\partial f}{\partial x}\int_{-\infty}^{\infty}\Delta\Phi(\Delta)\, d\Delta + \frac{\partial^2 f}{\partial x^2}\int_{-\infty}^{\infty}\frac{\Delta^2}{2!}\Phi(\Delta)\, d\Delta \tag{3}$$

using the property 3.1, the first integral in the right-hand side of the equation is equal to one, using 3.1, the second integral is zero (odd function of a symmetry interval). By naming:

$$D = \frac{1}{\tau}\int_{-\infty}^{\infty}\frac{\Delta^2}{2!}\Phi(\Delta)\, d\Delta$$

we finally get:

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2} \tag{4}$$

which is the diffusion equation. This equation can be solved using Fourier transform. Indeed, in the Fourier space, $\frac{d^2 f}{dx^2} = -k^2\tilde{f}(k)$ and in doing the Fourier transform of both sides of the equation we get:

$$\frac{d\tilde{f}(k,t)}{dt} = -Dk^2\tilde{f}(k,t)$$

from which:

$$\tilde{f}(k,t) = e^{-Dk^2 t}\tilde{f}(k,0)$$

If we choose as the initial condition a gaussian packet (so a state that is very well restricted), knowing that the Fourier transform of a Gaussian is still a Gaussian, the final solution is therefore:

$$f(x,t) = \frac{n}{\sqrt{4\pi D}}\frac{e^{\frac{-x^2}{4Dt}}}{\sqrt{t}} \tag{5}$$

if we think of this equation as a function of only the x variable and t as a parameter, this is the equation of a Gaussian and its $\sigma^2 = 2Dt$. In this case, this value assumes particular importance, since it represents the mean square displacement $MSD(t)$ that the particle experiences in the x direction, or the square root of the arithmetic mean of the square of the displacement in the x-axis direction:

$$MSD(t) = \sqrt{\bar{x}^2} = \sqrt{2Dt} \tag{6}$$

3.2 Langevin's derivation

Langevin assumes that the particle only acts two forces:

- viscous drag: assuming the particle is a sphere of radius a immersed in a liquid with viscosity η, and assuming the formula for the drag is the same as for a macroscopic object, $F_a = -6\pi\eta a dx/dt$
- fluctuating force X: it represents the impact of molecules of the liquid on the particle; it must therefore be negative or positive with equal probability

from Newton's equation, we get:

$$m\frac{d^2x}{dx^2} = -6\pi\eta a\frac{dx}{dt} + X \tag{7}$$

this a stochastic differential equation, and the role of the random term is played by X. We say that X is a Gaussian white noise with null average (this translates the affirmation that it can be, with equal probability, negative or positive), and δ correlated in time

$$\langle X(t)X(t')\rangle = c\delta(t-t')$$

which translates the information that the process has no memory.
To solve this equation, we multiply each side by x, then using the fact that

$$\frac{d^2}{dt^2}(x^2) = 2\left[\left(\frac{dx}{dt}\right)^2 + x\frac{d^2x}{dt^2}\right]$$

and averaging, we get:

$$\frac{m}{2}\frac{d^2}{dt^2}\langle x^2\rangle - m\langle\left(\frac{dx}{dt}\right)^2\rangle = -3\pi\eta a\frac{d\langle x^2\rangle}{dt} + \langle Xx\rangle \tag{8}$$

We should make two comments on 8. Firstly, we exchanged the order of derivative and average in the first term because it is linear, but the same is not possible in the second term (which, indeed, is not linear). Secondly, this average can either be seen as a temporal integral mean, or as a spacial mean, where each point in space is weighted with 5.
From statistical mechanics, the mean kinetic energy of the Brownian particle at equilibrium should be:

$$\langle\frac{1}{2}mv^2\rangle = \frac{1}{2}k_BT$$

and rembering that $\frac{dx}{dt} = v$, we can further semplify the equation.
Moreover,

$$\langle xX\rangle = 0$$

this comes from the fact that every change Δ is independent of the preceding change, a thing that Langevin implicitly assumes in his derivation. X is an extremely irregular function and we think of it as being independent from x, so that the irregularities of x in time do not go in the same direction as that of X, giving their product to be different than zero. This is equal to the conditions imposed by Einstein.
All these considerations lead to:

$$\frac{m}{2}\frac{d^2}{dt^2}\langle x^2\rangle + 3\pi\eta a\frac{d\langle x^2\rangle}{dt} = k_BT \tag{9}$$

yielding the solution:

$$\frac{d\langle x^2\rangle}{dt} = \frac{k_BT}{3\pi\eta a} + Ae^{-6\pi\eta at/m} \tag{10}$$

with A a constant. Since we are interested in a long time, we can neglect the transient (that is to say, neglect the decaying exponential). We therefore have:

$$\langle x^2\rangle - \langle x_0^2\rangle = \frac{k_BT}{3\pi\eta a}t \tag{11}$$

where $\langle x_0^2\rangle$ is the arbitrary constant we get when solving the equation 10, and since x_0, the initial position of the particle, can be set to zero, $\langle x_0^2\rangle = 0$. Equation 11 corresponds to 6, provided that we call

$$D = k_BT/6\pi\eta a$$

By measuring the value of D, knowing that $k_B = R/N_a$, with R the constant of gas and N_a the Avogadro number, we can infer the number of molecules in the solution by measuring macroscopic parameters. If we go back to the way we derived this result, we see that we assumed two things: that the grain has to behave like a macroscopic object subjected to friction according to the Navier-Stokes equation, but, at the same, it has to behave like a microscopic object, since we used the theorem of equipartition of the energy. The Brownian motion, as was stated in the introduction, therefore provided an experimental way to show the existence of atoms, that definitely closed the disputes between physicists who believed in the atomic hypothesis and physicists and those who did not, like Ostwald and Mach.

4 Numerical methods to solve a stochastic differential equation

We want to integrate the stochastic differential equation

$$\dot{x}(t) = q(x) + g(x)\zeta(t) \tag{12}$$

where $\zeta(t)$ is a Gaussian white noise of mean zero and delta correlated in time, so has the same properties as X in the previous section.
The standard way to integrate the differential equation assumes that the function has certain regulaties, for example, to use the Euler method they need to be C^1. The function $\zeta(t)$ is very irregular (we can think of it as a series of Dirac's deltas spread all over the real axis); nevertheless, it can be integrated.
To build the algorithm, it is firstly needed to discretize the time $t = t_i = t_0 + ih$, with t_0 initial time and $i = 0, 1, 2, \ldots$, h integration time step. We want to write a recurrence relation in which we express $x(t_{i+1})$ as a function of $x(t_i)$. By integrating the equation between t_i and t_{i+1} we get:

$$x(t_{i+1}) = x(t_i) + \int_{t_i}^{t_{i+1}} q(x(s))\, ds + \int_{t_i}^{t_{i+1}} g(x(s))\zeta(s)\, ds \tag{13}$$

We can now Taylor expand q(x(s)) and g(x(s)) around the point $x = x(t_i)$.We are assuming that these function are smooth enough, but these hypothesis is not very restrictive since for most physical application they are. We obtain:

$$q(x(s)) = q(x(t_i)) + \frac{dq(x(t_i))}{dx}[x(s) - x(t_i)] + o[(x(s) - x(t_i))^2] + \ldots \tag{14}$$

$$g(x(s)) = g(x(t_i)) + \frac{dg(x(t_i))}{dx}[x(s) - x(t_i)] + o[(x(s) - x(t_i))^2] + \ldots \tag{15}$$

Substituting 15 and 14 into 13, we get:

$$\begin{aligned} x(t_{i+1}) = x(t_i) &+ \int_{t_i}^{t_{i+1}} q(x(t_i))\, ds + q'(x(t_i)) \int_{t_i}^{t_{i+1}} (x(s) - x(t_i))\, ds + ho[(x(s) - x(t_i))^2] \\ &+ g(x(t_i)) \int_{t_i}^{t_{i+1}} \zeta(s)\, ds + g'(x(t_i)) \int_{t_i}^{t_{i+1}} (x(s) - x(t_i))\zeta(s)\, ds + o(x(s) - x(t_i))^2 \int_{t_i}^{t_{i+1}} \zeta(s)\, ds \end{aligned} \tag{16}$$

Our goal is now to semplify this equation and evaluate the integrals.
The second term will simplify to:

$$\int_{t_i}^{t_{i+1}} q(x(t_i)) = q(x(t_i))h$$

the third, fourth and last term can be neglected (they are in higher order in h, and we will just consider terms up to order h).
We want to evaluate:

$$I = \int_{t_i}^{t_{i+1}} \zeta(s)\, ds$$

In order to do so, we will consider its square

$$I^2 = \int_{t_i}^{t_{i+1}} \zeta(s)\, ds \int_{t'_i}^{t'_{i+1}} \zeta(u)\, du$$

we need to use the properties of the $\zeta(s)$:

$$\langle w(t) \rangle = \int_{t_i}^{t_{i+1}} \langle \zeta(s) \rangle\, ds = 0 \tag{17}$$

$$\langle w(t)w(t') \rangle = \int_{t_i}^{t_{i+1}} \int_{t'_i}^{t'_{i+1}} \langle \zeta(s)\zeta(u) \rangle\, dsdu = \int_{t_i}^{t_{i+1}} \int_{t'_i}^{t'_{i+1}} \delta(s-u)\, dsdu \tag{18}$$

this second integral is different than zero only if the two intervals $[t_i, t_{i+1}]$ and $[t'_i, t'_{i+1}]$ overlap (assuming $t_i < t'_i$), and in this case integral reduces to

$$\int_{t_i}^{t_{i+1}} \int_{t'_i}^{t'_{i+1}} \delta(s-u)\, dsdu = t_i - t'_i + h$$

Since we will only consider discrete time, $t_i = ih$, $t'_i = t_j = jh$, so $\langle \zeta(t)\zeta(t') \rangle = h\delta_{ij}$. If we now introduce a set of independent variables u_i distributed according to a Gaussian of null mean and with variance 1:

$$\langle u_i \rangle = 0; \langle u_i u_j \rangle = \delta_{ij}$$

we can finally write that

$$I = \sqrt{h} u_i$$

We still have to calculate:

$$J = \int_{t_i}^{t_{i+1}} (x(s) - x(t_i))\zeta(s)\, ds$$

to evaluate this integral, we would need to know the value of x(s) in the time interval $[t_i, t_{i+1}]$, that is to say, we would need to know the answer to the problem we are trying to solve. In order to overcome this issue, we substitute $s = t_i$ into the equation 13:

$$x(s = t_i) = x(t_i) + g(x(t_i)) \int_{t_i}^{t_{i+1}} \zeta(s)\, ds + o(h) \tag{19}$$

and so we get:

$$J = g(x(t_i)) \int_{t_i}^{t_{i+1}} \int_{t_i}^{s} \zeta(s)\zeta(u)\, du\, ds + o(h) \int_{t_i}^{t_{i+1}} \zeta(s)\, ds$$

the second term in order $h^{\frac{3}{2}}$, so we can safely neglect it, the other can be calculated using Statonovich calculus and yields $\frac{hu_i^2}{2}$.
Putting all together into equation 116, we finally get:

$$x(t_{i+1}) = x(t_i) + hq(x(t_i)) + g(x(t_i))h^{\frac{1}{2}}u_i + \frac{1}{2}g(x(t_i))g'(x(t_i))hu_i^2 + o(h^{\frac{3}{2}}) \tag{20}$$

The function $q(x)$ represents the deterministic force acting on the pollen particle.
Processes where $g'(x) = 0$ have particular physical interest and are called additive processes. For an additive process:

$$x(t_{i+1}) = x(t_i) + hq(x(t_i)) + g(x(t_i))h^{\frac{1}{2}}u_i + o(h^{\frac{3}{2}}) \tag{21}$$

4.1 Free Brownian particle

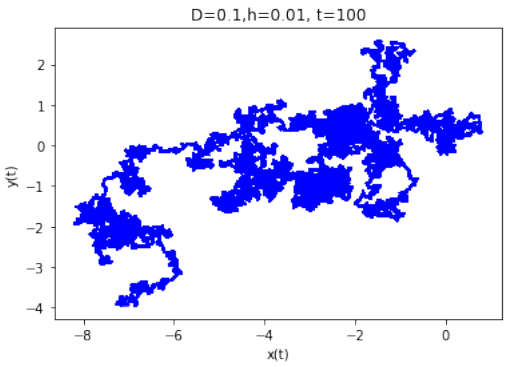
In this section we study the motion of a free Brownian particle, this means that $q(x) = 0$ and $g(x) = const.$ In particular, we choose $g(x) = \sqrt{2D}$.
The dynamics for this equation is

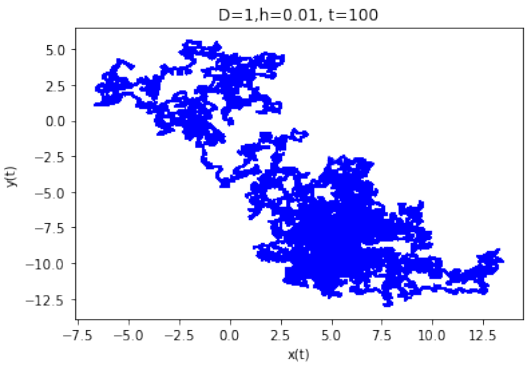
$$\dot{x}(t) = \sqrt{2D}\zeta(t) \tag{22}$$

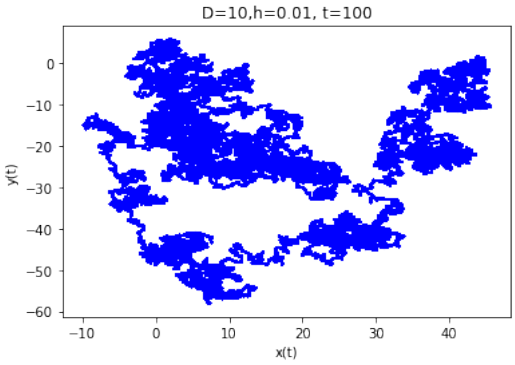
Following the same steps described in the previous section and simplifying equation 20:

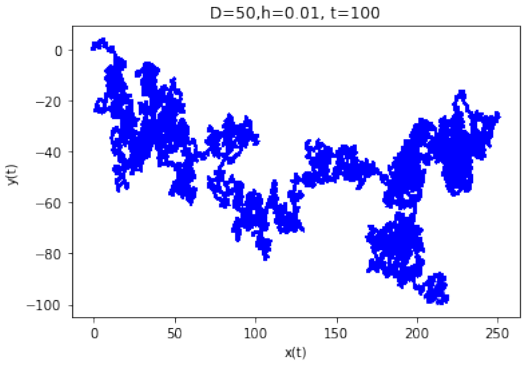
$$x(t_{i+1}) = x(t_i) + \sqrt{2Dh}u_i \tag{23}$$

If we plot the position $x(t)$ and $y(t)$ for different values of D, we get the following graphs:









From these graphs, it can be clearly seen the larger the value of D, the more the space explored by the walker.
We now want to show that the average displacement $MSD(t)^2 = 2Dt$ as stated in the previous section. To do so, we follow the following procedure:

- a value of t is fixed, and we choose one value of D, which will be changed later
- N walkers are made to walk a fixed number of steps (steps=t/h), and their positions are registered
- at the same temporal step, we calculate $msd(t) = \langle x(t)^2 \rangle - \langle x(t) \rangle^2$
- the preceding steps are repeated, but with a different value of D
- the line $y = 2Dt$ is plotted to show that the points follow the expected trend

The same procedure is followed also to show that σ^2 is linear in t.
We can finally report all the obtained graphs: