Brownian motion

Friday, January 16, 2009
12:09 PM

Office hours are Tuesdays and Fridays 4-5 PM, starting January 27.

No classes next week; next class is on January 27.

References: K, "Brownian Motion"

See also Nelson, Dynamical Theories of Brownian Motion

History:
- observations by Brown 1828
- controversy about cause through 1905
- statistical mechanics was under heavy development starting in the 1860s (Gibbs, Boltzmann), why wasn't this sufficient to explain Brownian motion?
  - the difficulty is that the velocity of the particles undergoing Brownian motion was difficult to measure -- different experimentalists get different numbers. People were beginning to settle on kinetic theory/statistical mechanics as being the explanation but they could not get quantitative agreement with experimental measurements.
- Einstein developed a quantitative theory that was validated a few years later by Perrin. He actually wasn't trying to study Brownian motion; he wanted to develop testable ways to assess the atomic hypothesis. Not only did Einstein explain Brownian motion, he developed a formula that could be used to compute Avogadro's number, counting how many molecules there are in a given amount of material. This is one of the fundamental contribution that settled the atomic hypothesis into the mainstream.
  - Einstein's methodology was "Eulerian": considering continuum densities and deterministic partial differential equations. Smoluchowski expanded Einstein's approach later.
  - Later, Langevin, Ornstein, and Uhlenbeck developed a complementary framework based on stochastic differential equations for the particle trajectory. This can be thought of as a "Lagrangian" approach. This gives equivalent results by different methods.

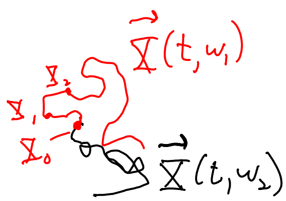
Both the Eulerian and Lagrangian points of view remain useful complementary tools.
- Lagrangian trajectory: stochastic differential equations
- Eulerian continuum density PDE: Fokker-Planck method and/or Kolmogorov equation method

We will start with the Lagrangian trajectory-based (Langeivn) approach first because I find it conceptually simpler.

We will start with the simplest diffusion model.

We will represent the trajectories of the particle as $\vec{X}(t,\omega)$

$$\underset{\text{position}}{\vec{X}}\,(\underset{\text{time}}{t},\ \underset{\text{realization (experiment)}}{\omega})$$



The randomness comes into the problem because we don't know which ω corresponds to a given experiment.

Let's proceed with developing a concrete probabilistic model to model Brownian motion in terms of a generalized random walk (not restricted to a spatial lattice).

To approach the problem, we will discretize time into epochs with spacing Δt

$$t_n = n \Delta t$$

$$\vec{X}_n(\omega) = \vec{X}(t_n, \omega)$$

For simplicity, let's start pretending that space is one-dimensional (ignore vectors for now).

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

The increments $Z_n(\omega)$ will be taken to be independent, identically distributed random variables.

Here we need to briefly discuss some basic probability concepts. For further reading:

- Gardiner, Ch. 2.1-2.5, 2.8
- Grigoriou, Ch.2 (overkill)
- Selections from my lectures notes (with Majda) from turbulent diffusion scanned online

probability distribution on state space $\mathbb{R}$

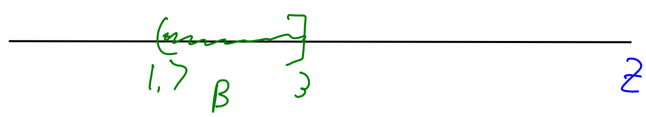
probability measure on Ω

First of all, we need to discuss the notion of probability distribution for a random variable:

$$P_{Z_n}(B) = P(Z_n \in B) = \text{Prob}(Z_n \in B)$$

This is an event in the sample space

for nice (Borel) subsets of $\mathbb{R}$



What this means is the following. The realizations ω live in some abstract sample space Ω. Every experiment or every outcome of a random variable corresponds to some point ω in this sample space -- the uncertainty is which ω corresponds to a given experiment. This uncertainty is quantified by a probability measure P which returns probabilities that a given experiment will fall in a prescribed nice subset A of this sample space. This generally has to be defined through a model which has the following restrictions:

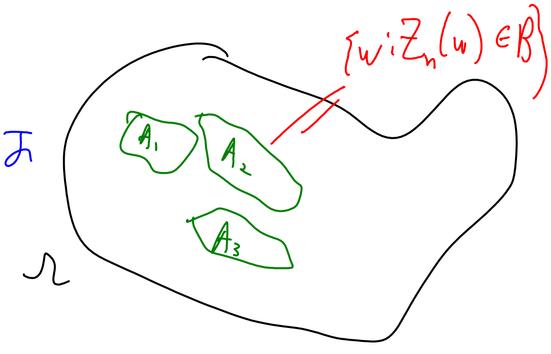
$$P(\Omega) = 1$$

$$P(A) \geq 0 \quad \text{for all } A \in \mathcal{F}$$

For disjoint (mutually exclusive) sets $\{A_j\}_{j=1}^{\infty}$

$$P\left(\bigcup_{j=1}^{\infty} A_j\right) = \sum_{j=1}^{\infty} P(A_j) \quad \text{for } A_j \in \mathcal{F}$$

countable union



$\mathcal{F}$ is σ-algebra of measurable sets (events)

The most concrete of these objects is the probability distribution of the random variable since it is defined on a concrete state space (here $\mathbb{R}$ or $\mathbb{R}^3$)

But the probability distribution is still a measure (real-valued function of sets), would be nice to work with ordinary functions instead. The most general way to do this for one-dimensional random variables is through the cumulative distribution function (CDF):

$$\text{CDF} \rightarrow \underbrace{F_{Z_n}}_{\text{deterministic function}}(z) = P(Z_n \le z)$$

One can show that this completely describes the probability distribution. We will actually primarily work with a related object, the probability density function (PDF), which is very useful for continuously distributed random variables.

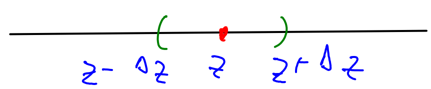
It is uniquely defined by the property that for any arbitrary nice (Borel) set B

$$P(Z_n \in B) = \int_B \underbrace{p_{Z_n}(z)}_{\text{PDF}}\, dz$$

$$F_{Z_n}(z) = \int_{-\infty}^{z} p_{Z_n}(z')\, dz'$$

A few technical comments: For the PDF to exist as an ordinary function, the random variable must be absolutely continuous. If the random variable has discrete components (atoms), then the PDF approach can still work if one is willing to work with Dirac delta functions. There is also a pathological case called singular continuous distributions which almost never are relevant for real-world investigations with the exception of propagation of waves through disordered material.

Another way to think of PDFs, perhaps more intuitively is by considering sets of the form $B = (z - \Delta z, z + \Delta z)$



$$P_{Z_n}(B) = P_{Z_n}(z - \Delta z, z + \Delta z) = P(|Z_n - z| < \Delta z)$$

$$= \int_{z-\Delta z}^{z+\Delta z} p_{Z_n}(z')\, dz'$$

$$= p_{Z_n}(z)\,(2\Delta z) + o(\Delta z)$$

$$p_{Z_n}(z) \approx \frac{P(|Z_n - z| < \Delta z)}{\ell(z-\Delta z, z+\Delta z)} \quad \text{for small } \Delta z$$

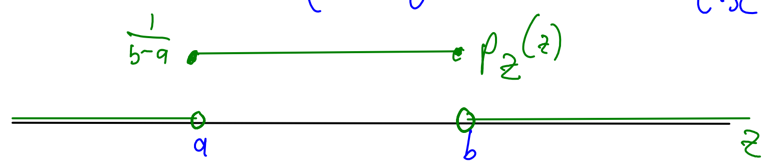
In higher dimensions, the same approximation works; one just divides by the appropriate volume measure of the neighborhood of the point z.

Examples of random variables and probability density functions

Uniform distribution:

$$Z \sim U[a,b]$$

$$p_Z(z) = \begin{cases} \frac{1}{b-a} & a \leq z \leq b \\ 0 & \text{else} \end{cases}$$

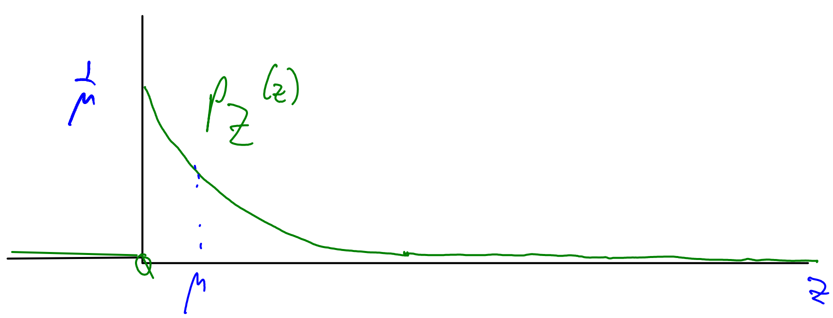


It doesn't matter how you define PDF's at points of discontinuity (but it does matter for the CDF!).

Exponential distribution:

$$p_Z(z) = \begin{cases} \frac{1}{\mu} e^{-z/\mu} & \text{for } z \geq 0 \\ 0 & \text{for } z < 0 \end{cases}$$

where μ is a constant positive real parameter



In fact μ is the mean or expected value of the exponential distribution.

$$\langle Z \rangle \doteq \mathbb{E} Z \equiv \int_{-\infty}^{\infty} z\, p_Z(z)\, dz$$