Laboratory no. 1: Simulation of Brownian motion

Aim

The aim of the laboratory is to acquaint with the Brownian motion phenomena and to create it's computer simulation using Monte Carlo algorithm. A numerical model will next be used for validation of the properties resulting from the theory.

Introduction

Brownian motion is the random motion of the particles suspended in the fluid (liquid or gas). This phenomena is named after the Scottish botanist Robert Brown who was living in the XIX century. In 1827 he was observing a pollen grains floating on the surface of the liquid using the microscope. He discovered that the particles are moving chaotically in different directions but he was not able to determine the mechanisms that caused this motion. Initially it was explained by a mysterious „life force" attributed to biological particles, but later on Brown demonstrated that the same effect occurs when inorganic particles are used. By the way he used a small crumbs of the famous Sphinx for that. Despite numerous attempts, scientific explanation for this phenomena appeared nearly 100 years later.

The Brownian motion theory was presented independently by two scientists, Albert Einstein in 1905 and Marian Smoluchowski in 1906. They explained in precise detail using different approaches, how the motion that Brown had observed was a result of the pollen being moved by individual water molecules This explanation of Brownian motion served as convincing evidence that atoms and molecules exist, and was further verified experimentally by Jean Perrin in 1908. Perrin was awarded the Nobel Prize in Physics in 1926 "for his work on the discontinuous structure of matter". Figure 1 illustrates an example of Brownian trajectory for a single particle in 2D.

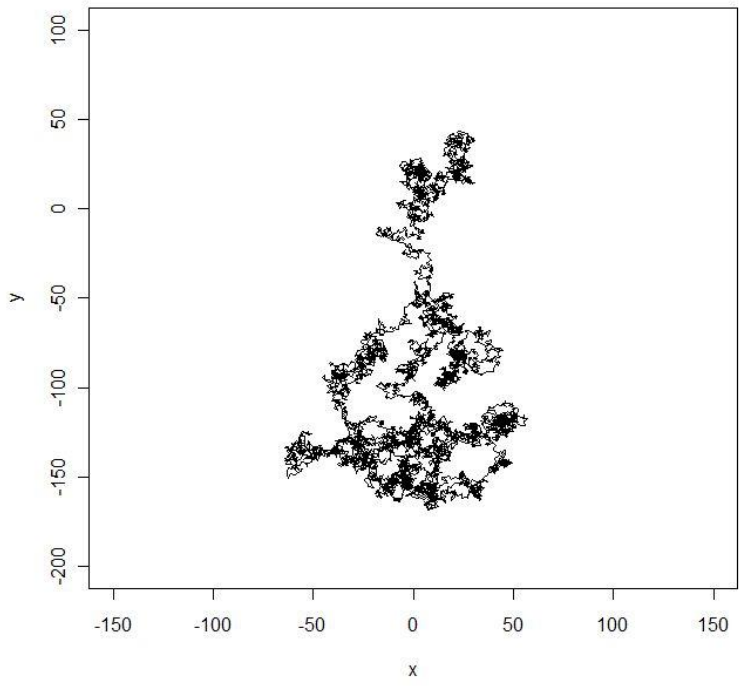

Figure 1 Picture of 2D Brownian trajectory for a single particle. Number of time steps N=1000

Brownian motion can be described in the same way as a random walk movements. A random walk is a stochastic or random process, consisting of a series of random steps. Particle position vector in n+1 time step is dependent on the position in n time step and random movement d, so after n time steps a particle position will be equal to:

$$x_n = x_{n-1} + d \qquad (1)$$

where:

d- random movement in the single time step

Thus, the position after N time steps is the sum of N random values. According to Central Limit Theorem (CLT) the sum of N independent random values tends toward a normal distribution of parameters $\mu=\langle x\rangle=0$, $\sigma^2=\langle x^2\rangle$ (commonly known as a *bell curve*) even if the original variables themselves are not normally distributed.

Mean square of displacement after N time steps is equal to:

$$\langle x_N^2 \rangle = \nu a^2 t \qquad (2)$$

where:

$a^2 = \langle d^2\rangle$ - mean square of a single movement
ν – average number of movements in a unit of time
t – time

Figure 2 shows the relationship (2) for a simulation of 1000 particles using Monte Carlo method.

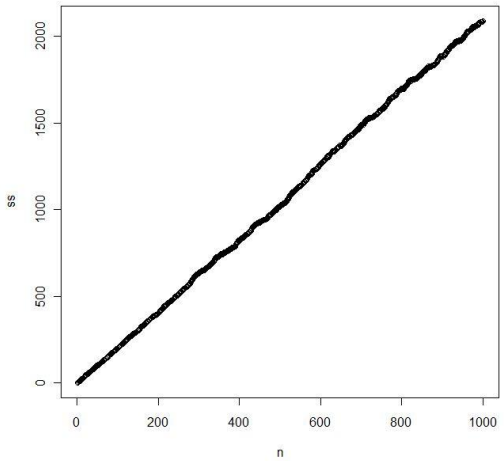

Figure 2 Relationship between mean square of displacement and time for the population of 1000 particles

Monte Carlo simulation

For the simulation we will use a pseudorandom number generator having normal probability distribution having parameters μ=0 i σ=1, however other probability density functions are also allowed (eg. one can make a coin toss and assign +1 for head and -1 for tail).

For 2D simulation a position of a particle (x,y) is calculated In the following way:

1. For the initial time step a position (x,y) is equal to [0 0]
2. Start of the time step loop

3. Draw of 2 pseudorandom numbers, first for dx and second for dy
4. Apply equation (1) for new x and y coordinates
5. Repeat point 3 and 4 assumed number of iterations

Laboratory outline

1. Writing the computer programme simulating Brownian motion In 2D using the methodology described above
2. Demonstration of the examples of single and multiply 2D trajectories
3. Validation of the relationship between mean square of displacement and time using model created in point 1 (at least several hundreds of particles simulation is required)
4. Demonstration of self-similarity property of brownian trajectories. Calculation od the autocorrelation function for selected trajectory
5. Demonstration of time evolution of particles density (number of particles per unit area) starting from the same point (at least several hundreds of particles simulation is required)
6. Conclusions

Computer programme can be written in any programming language or software environment. Recommended environment is MATLAB. Programme code supplemented with appropriate comments should be included as a part of a report prepared in pdf format and send to the tutor by email no later than one week after the laboratory. The report has to include at least points 1, 2 and 6 and optionally points 3-5 (to be decided by a tutor).