Modelling of Diffusion: Simple Anomalous Diffusion

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Introduction

In 1827, Scottish botanist Robert Brown noticed that particles in a liquid move chaotically in different directions. Later, this kind of motion was classified as *Normal Diffusion.* In the beginning of the 20th century, Albert Einstein showed that for long times mean squared displacement (MSD) of Brownian particles is proportional to time. $< x^2 > \propto t$. However, in some cases, we have deviation from this formula and have non-linear relationship: $< x^2 > \propto t^{\alpha}$. This kind of diffusion is called ***anomalous diffusion.*** Diffusion is a fundamental process observed across various disciplines such as: physics, biology and even finance. Due to its significance in various fields, it's important to classify some random processes and differ them from each other. This poster will provide a brief introduction into anomalous diffusion: key points will be mentioned and simulation results using Monte-Carlo method will be shown.

Normal Diffusion

Normal diffusion can be easily understood through the concept of random walk. In random walk, particles move in random directions, simulating the random thermal motion that drives diffusion. Albert Einstein found out that ***Mean Squared Displacement*** dependence over time is linear:

$$\langle x^2 \rangle \propto t$$

On the other hand, ***Mean Displacement*** is always zero:

$$\langle x \rangle = 0$$

Figure 1 shows the simulation of 2D random walk and on **Figure 2** we see Mean Squared Displacement dependence over time (on top) and Mean Displacement over time (on bottom).

Figure 1

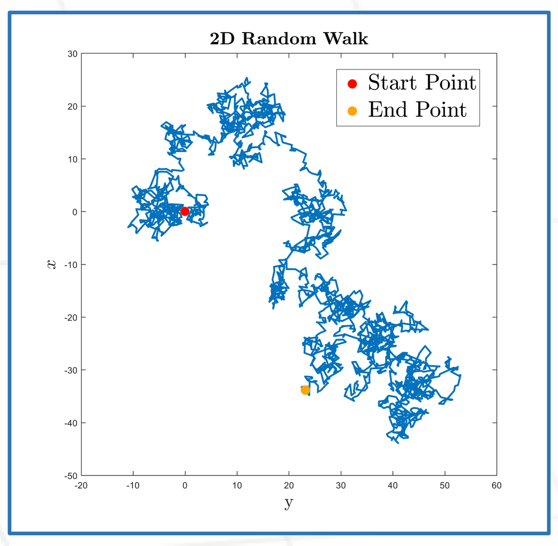
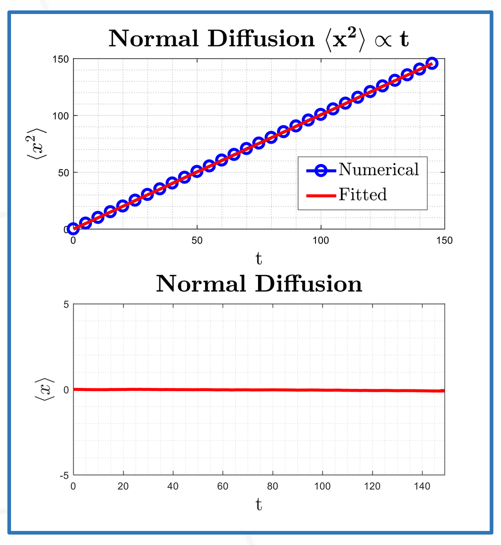


Figure 2



Superdiffusion

When some random process is influenced by the previous state of the system, we say that we have a diffusion with memory. Correlation with previous conditions causes anomalous diffusion. Here is a simple example of SUPERDIFFUSION:

Suppose, we have a particle that changes its velocity after every time interval τ and the change of velocity after each collision is: $\Delta v = \pm u$. We need to find ***Mean Squared Displacement*** dependence over time.

Velocity on **N**-th step: $V_N = \sum_{i=0}^{N} \Delta v_i$, then:

$$\Delta x_N = \tau v_N = \tau \sum_{i=0}^{N} \Delta v_i$$

So,

$$\Delta x_N = \tau[N\Delta v_0 + (N-1)\Delta v_1 + \cdots + \Delta v_n].$$

Of course: $\langle \Delta v \rangle = 0$

Velocity *changes* are not correlated, so: $\langle \Delta v_i \Delta v_k \rangle = 0$

So we have:

$$\langle \Delta x_N^2 \rangle = \tau^2 u^2 \sum_{k=0}^{N} (N-k)^2$$

We know that: $\sum_{m=0}^{N} m^2 = \frac{1}{3} N \left(N + \frac{1}{2}\right)(N+1) \approx \frac{1}{3} N^3$

Then we have: $\langle \Delta x^2 \rangle \approx \frac{1}{3} \tau^2 u^2 N^3$, Full time: $t = N\tau$

So we have our final equation will be:

$$\langle \Delta x^2 \rangle \approx \frac{1}{3} \tau^2 u^2 \left(\frac{t}{\tau}\right)^3 = \frac{u^2}{3\tau} t^3$$

We can rewrite the last equation as: $\boldsymbol{\langle \Delta x^2 \rangle \approx D t^3}$

Where $D \equiv \frac{u^2}{3\tau}$ is the Diffusion Coefficient.

Using Monte-Carlo method, we made a simulation of described random motion. Initial conditions:

$u = 2$, $\tau = 1$, $N = 100\,000$, $T = 300$; Where N is the number of particles.

Figure 3 shows the graphs of numerical, fitted and theoretical dependence.

After fitting, we calculated the diffusion coefficient and compared it with theoretical value:

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D Coefficient (Numerical): 1.33711
D Coefficient (Theoretical): 1.33333
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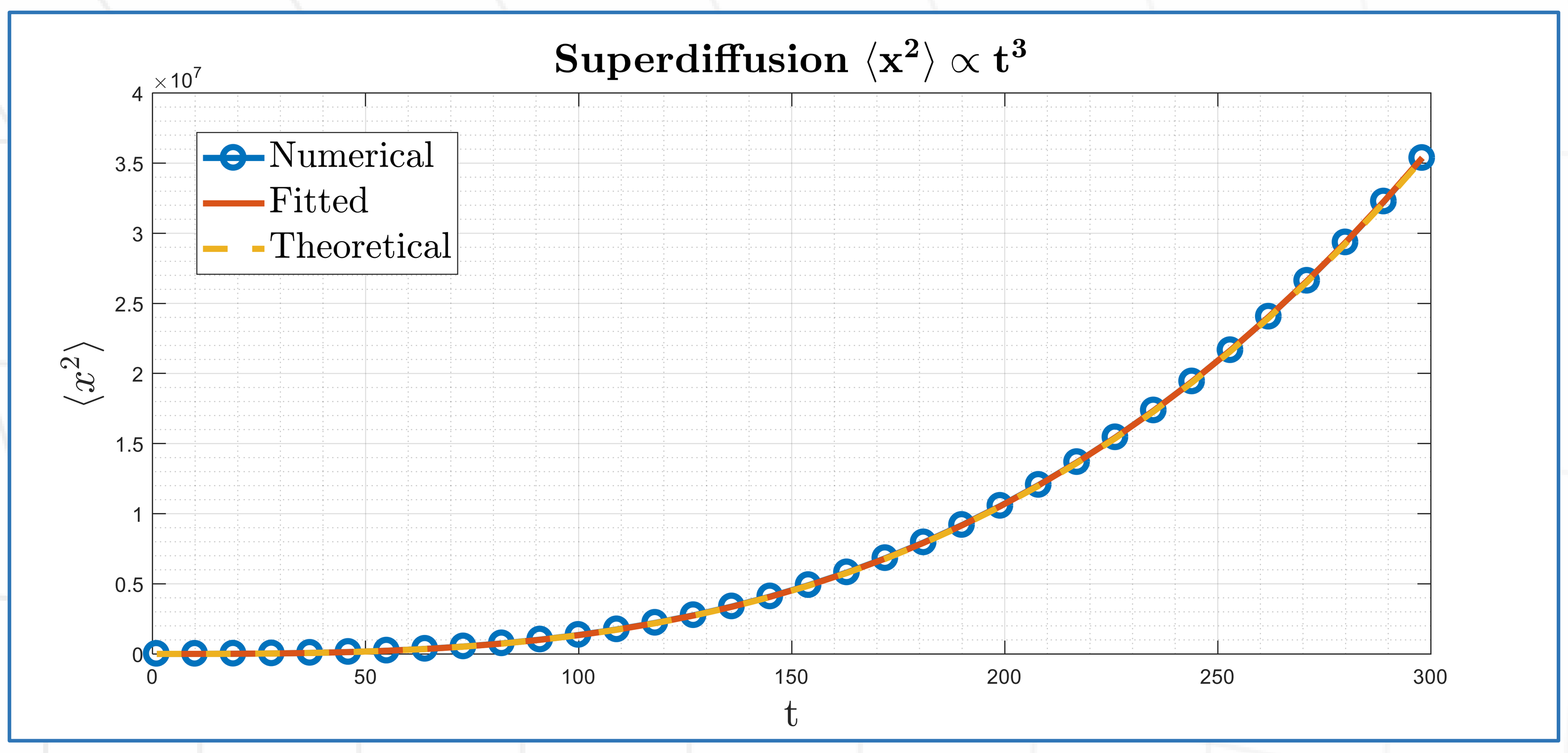
Figure 3



Subdiffusion

When ***Mean Squared Displacement*** dependence of time is $\langle x^2 \rangle \propto t^{\alpha}$, where $0 < \alpha < 1$ we have **SUBDIFFUSION**.

Suppose we have a photon which is scattering while entering an environment where scattering coefficient (μ_s) is not constant and depends on the position: $\mu_s = \mu_0 e^{\beta x}$. Photon moves randomly in every direction and its step size is also random. Normalized PDF for the step size is: $p(r) = \mu_s e^{-\mu_s r}$, from this PDF we get CDF: $F(r) = 1 - e^{-\mu_s r}$.

Using Monte-Carlo method and inverse transform sampling, we can generate random step sizes: $r = -\frac{1}{\mu} \ln(1 - \xi)$, where ξ is a random number from standard uniform distribution in the interval (0,1).

In this case, we get subdiffusion: particles spread slower than in normal diffusion.

MSD over time is nonlinear: $\langle x^2 \rangle \propto t^{\alpha}$.

To calculate α we used "logarithmic fitting":

$$\langle x^2 \rangle = D t^{\alpha}$$

$$\ln\langle x^2 \rangle = \alpha \cdot \ln t + \ln D$$

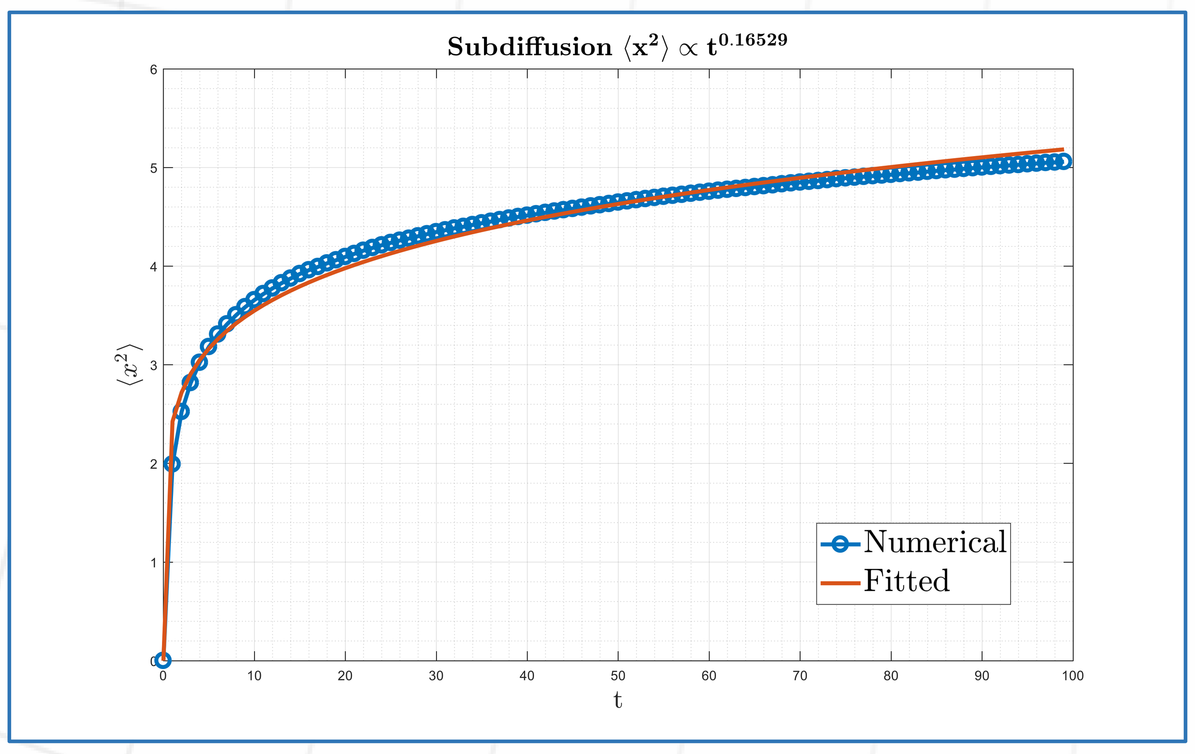
After taking natural logarithm from both sides, we used `polyfit` function to calculate D and α

Initial conditions:

$\mu_0 = 1$, $\beta = 3$, $N = 100\,000$, $T = 100$; Where N is the number of particles.

Figure 4 shows the comparison of numerical and fitted graphs.

Figure 4

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Coefficient:  D = 2.42563
alpha = 0.16529
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Conclusion

In conclusion, anomalous diffusion deviates from classical Brownian motion, exhibiting non-linear relationships between mean squared displacement (MSD) and time. Unlike normal diffusion, where MSD scales linearly with time, anomalous diffusion, however, exibits nonlinear relationship: $< x^2 > \propto t^{\alpha}$. It can be subdiffusive with $\alpha < 1$ or superdiffusive with $\alpha > 1$. Understanding these deviations is important for accurately describing diffusion in complex systems, such as biological tissues. This poster underlines the key points of anomalous diffusion and demonstrates the results of Monte-Carlo simulation.