Homework assignment 3
Due Date: 1st of December EOD
Course: Stochastic Methods in Mathematical Modelling
Instructor: Prof. Vladimir Palyulin
Teaching Assistant: Maria Larchenko

Problem 1. First-passage on a semi-infinite line (4 points)

An agent starts at coordinate x_0 and performs Brownian motion with a diffusion coefficient D on a semi-infinite interval $[0, \infty)$ with an absorbing boundary condition at $x = 0$.

1. Write down the Fokker-Planck equation for the PDF $p(x, t)$ of an agent position, initial and the boundary conditions. (1 point)
2. Solve the equation and find $p(x, t)$ analytically. (1 point)
3. Find the survival probability $S(t)$ of an agent as a function of time analytically. (1 point)
4. Run a number of simulations with parameters $x_0 = 1, D = 1$, gather statistics and compare your analytical solution for $S(t)$ with the numerical results. (1 point)

Problem 2. Active Brownian motion in two dimensions (2 points)
The simplified equations of motion for an active Brownian particle in two dimensions are given by following set of Langevin equations

$$\begin{cases} \dot{x} = v_0 \cos\theta, \\ \dot{y} = v_0 \sin\theta, \\ \dot{\theta} = \sqrt{2D_R}\eta(t), \end{cases}$$

where $\eta(t)$ is a Gaussian white noise.

1. Obtain analytical expressions for the first and the second order moments for x and y positions (i.e. $\langle x(t)\rangle$, $\langle y(t)\rangle$, $\langle x(t)^2\rangle$, $\langle y(t)^2\rangle$).
2. Compare your results with numerical simulations of the Langevin equations.
3. Find out the leading order behaviour at short $t \ll 1$ and long times $t \gg 1$.

Problem 3. Fractional derivatives (1 point)

Using the definition and the properties calculate analytically if possible and plot the corresponding Riemann-Liouville fractional derivatives ${}_0D_x^\alpha$ on the interval $[0, 2]$:

1. ${}_0D_x^\alpha x^3, \alpha = 0.25, 0.5, 0.75$
2. ${}_0D_x^\alpha \exp(x), \alpha = 0.25, 0.5, 0.75, 1$

Problem 4 (Subdiffusion and fractional differential equations, 3 points)
By definition the subdiffusion is a process with a mean-squared displacement sublinear in time i.e. $\langle \Delta x(t)^2\rangle \sim t^\alpha, \alpha < 1$. The subdiffusion in its simplest can be simulated within the so-called continous time random walk model (CTRW). A particle can jump to the right/left on the 1D lattice. For

simplicity let's assume that the jumps can occur only to the nearest neighbour site. If the waiting time before each jump is constant or the average of the waiting time distribution is finite the corresponding diffusion process will be Brownian.

The idea of subordination. Interestingly the trajectory as a sequence of visited nodes will be identical for the Brownian and the subdiffusive motion. Hence, one could simulate the subdiffusion by simulating the trajectory as a normal random walk and then drawing the waiting time at each jump from the heavy-tailed distribution.

1. Use this idea to write a program for modelling of subdiffusion on the infinite line by using discrete jump model. Assume that $U(x) = const$, i.e. the probability to jump to the left and to the right is 1/2. Now, the waiting time before every jump is drawn from a skewed alpha-stable distribution. If the alpha-stable distribution has a skewness parameter $\beta = 1$ then it only has positive values and the heavy tail with a power law decay $1/t^{1+\alpha}$.

   The values from α-stable distributions with $\beta = 1$ can be sampled, for instance, according to the equations

   $$\xi_\alpha = \frac{\sin(\alpha\Theta)}{(\sin\Theta)^{1/\alpha}} \left(\frac{\sin((1-\alpha)\Theta)}{W}\right)^{\frac{1-\alpha}{\alpha}}, \tag{1}$$

   here W is an exponential variable ($P(W > w) = e^{-w}, w \geq 0$), Θ is uniform on $[0, \pi]$ and the equation is applicable only for $0 < \alpha < 1$ (More details you could find in chambers1976.pdf).

2. Sample 100000 values from the distribution ξ_α for $\alpha = 0.25; 0.5; 0.75$ and plot the corresponding distribution histograms.

3. Plot a sample trajectory for $\alpha = 0.25$ as a function of time and compare it with the Brownian case (in the Brownian case all waiting times are identical).

4. Collect the data for program simulating the subdiffusion and plot the probability distribution functions (PDFs) at $t = 0.1, 1, 10, 100$ for stable exponent $\alpha = 0.25, 0.75$ (*Reminder.* For subdiffusion $\alpha < 1$.). Assume that the starting position $x_0 = 0$, i.e. $P(x, 0) = \delta(x)$.

5. Compare the PDFs of the subdiffusive motion with those of the Brownian motion at $t = 0.1, 1, 10, 100$.

6. Compute the mean-squared displacement $\langle \Delta x^2(t) \rangle$ as a function of t. Find the power-law exponent of this dependence. (Extra 1 point)

7. compare the results qualitatively with the analytical solution of the corresponding subdiffusive fractional Fokker-Planck equation elucidated in a theoretical detour below. The solution can be represented as a series,

   $$P(x,t) = \frac{1}{\sqrt{4\pi K_\alpha t^\alpha}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\Gamma(1-\alpha(n+1)/2)} \left(\frac{x^2}{K_\alpha t^\alpha}\right)^{n/2}. \tag{2}$$

   For numerics you are free to select any K_α (also note that the series converge for $|x| < 1$).

Theoretical detour. The time-fractional Fokker-Planck equation

One can derive the following expression for the subdiffusion called as fractional Fokker-Planck equation,

$$\frac{\partial P(x,t)}{\partial t} = {}_0 D_t^{1-\alpha} \left(\frac{\partial}{\partial x}\frac{U'(x)}{m\eta} + K_\alpha \frac{\partial^2}{\partial x^2}\right) P(x,t), \tag{3}$$

where ${}_0D_t^{1-\alpha}$ stands for the Riemann-Liouville fractional derivative, which is a non-local operator defined for $0 < \alpha < 1$ as

$$ {}_0D_t^{1-\alpha} P(x,t) = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t dt' \frac{P(x,t')}{(t-t')^{1-\alpha}} \tag{4}$$

and K_α is fractional diffusion coefficient which in this case has a dimension cm^2/sec^α. The Riemann-Liouville derivative has a very simple Laplace image,

$$\mathcal{L}\left\{ {}_0D_t^{-\alpha} P(x,t) \right\} = s^{-\alpha} P(x,s), \alpha \geq 0. \tag{5}$$

The solution of the equation 3 can be found analytically in terms of Fox H-functions and for $U(x) = 0$ and with initial condition $P(x,0) = \delta(x)$ it reads

$$P(x,t) = \frac{1}{\sqrt{4\pi K_\alpha t^\alpha}} H_{1,2}^{2,0} \left[\frac{x^2}{4K_\alpha t^\alpha} \middle| \begin{array}{l} (1-\alpha/2, \alpha) \\ (0,1), (1/2,1) \end{array} \right]. \tag{6}$$

The Fox H-functions are a general class of functions which generalise Meijer G-functions. Their properties are very convinient for some integration opertations and direct/inverse Laplace tranforms. An H-function value can be computed from series expansion. In the case of the solution (6) the expansion is Eq. 2.