NTNU **Institutt for fysikk**

Contact during the exam:
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Exam in TFY4275/FY8907 CLASSICAL TRANSPORT THEORY
Feb 14, 2014

Allowed help: Alternativ **D**
All written material

This problem set consists of 5 pages.

Due : *Mar 24, 2014*

This is the project work of the class. You are allowed during the course of the work to discuss the problems among yourself, take hints from each others, discuss solution strategies, and eventually to compare results. Moreover, for the numerical part, you may consult faculty members (including the class instructor). However, it is expected that what you hand in is your own work, and should not be a copy of someone else's work.

There are two possible options for the project as listed below. You shall choose one of them. I expect option 1, which is closer to "real-science", to be more challenging than option 2.

The problem set consists of a mix of analytic and numerical work. You are asked to work out, and hand in, the solutions to the problems presented below. In your suggested solutions, you should present enough details so that I easily can follow what you are doing. To pass, you are required to at least complete 2/3 of the project set (more or less correctly). For the numerical work you may use any programing language that you like. However, you are requested to hand in your code (electronically) in working order.

The work is due **Mar. 24, 2014**.

You are reminded that this project will not contribute toward the final grade of the class. However, the project is compulsory, so you need to pass it in order to be allowed to take the exam.

That is all. Good luck!

Project Option 1

Develop a code for simulating an Ornstein-Uhlenbeck process by using the Gillespie algorithm described in the following paper

D.T. Gillespie
Exact numerical simulation of the Ornstein-Uhlenbeck process and its integral,
Phys. Rev. E **54**, 2084 (1996).
`http://link.aps.org/doi/10.1103/PhysRevE.54.2084`,

Demonstrate explicitly that the simulated process indeed is an Ornstein-Uhlenbeck process. This can for instance be done by calculating the correlation function.

Project Option 2

Problem 1.

a) Define the characteristic function (moment generating function), $G_\xi(k)$, of a random variable ξ defined by the probability distribution $p(\xi)$.

b) How is the average $\langle e^\xi \rangle$ (ξ is a random variable) defined in terms of cummulants? Given the characteristic function, $G_\xi(k)$, what is then the cummulant generating function?

c) Argue why the characteristic function of a *Gaussian* random variable, ξ_G, is given by

$$G_{\xi_G}(k) = \exp\left(i\mu k - \frac{\sigma^2 k^2}{2}\right),$$

where μ and σ denote the mean and standard deviation, respectively. (Note: No full mathematical derivation is asked for).

d) What is the *main* difference between a random variable and a stochastic process? Give a real-life example of both of them.

e) Given a general stochastic process, what is needed to fully define it?

Problem 2. Random Walk

We consider the sum of N random variables ξ_i

$$x_N = \sum_{i=1}^{N} \xi_i,$$

where *all* the ξ_i's are *independent* and *identically* distributed (*i.e.* a random walk with steps ξ_i and position x_N at "time" $t = N$). The standard deviation of the (identical) steps (the random variables ξ_i) we denote by σ_ξ.

a) Formulate with words the Central Limit Theorem (CLT).

b) Use this to describe what the CLT predicts for the distribution of x_N, $p(x_N)$ when

i) $\sigma_\xi < \infty$?

ii) $\sigma_\xi = \infty$?

No mathematical details needed (if you do not like to do so....).

c) For the two cases mentioned above (*i* and *ii*), write down an expression for σ_{x_N}. When $\sigma_\xi < \infty$ express your answer in terms of σ_ξ and N.

d) What is the characteristic function of the random variable x_N given the $G_\xi(k)$? What is the distribution of x_2, denoted $p_2(x_2)$, expressed in terms of the distribution of ξ_i, $p(\xi)$.

e) Now let us set $\xi_i = N(0, \sigma)$ for all i's, *i.e.*, is Normally (Gaussian) distributed with zero mean and standard deviation $\sigma < \infty$. Show *mathematically* that your above statement for σ_{x_N} is correct.

Problem 3.
Exercise set no. 6.

Problem 4.
Exercise set no. 7.

Comment : You may find problem 7f somewhat challenging...

Problem 5.
The file http://web.phys.ntnu.no/˜ingves/Teaching/TFY4275/Data/time-series.tar.gz contains several time series, $x(t)$, recorded with uniform sampling interval, Δt, (and $t = 0$ defined arbitrarily).

In this problem, you are asked to determine which of them are results of (ordinary) diffusion.

a) Describe theoretically the method that you are planning to use for distinguishing a diffusion process from a non-diffusing one?

b) Now apply this method to the numerical data and determine which of the time series are diffusive processes.

Problem 6.
In this problem we will solve the diffusion equation numerically. Here, you will have to do some investigation by yourself to locate the adequate techniques suited for the task, since the numerical aspects have not been covered in the class.

You will have to discretized the diffusion equations, with a suitable time step, Δt, and space discretization interval, Δx. It should be noted that any choice for Δt and Δx may *not* give stable solutions. To figure out for which stable solution can be reached is part of your "research" involved in completing this problems (you are not required to prove your answer regarding stability).

a) Write a program that solves numerically the standard diffusion problem described by the equation

$$\partial_t C(x,t) = D\, \partial_x^2 C(x,t). \tag{1}$$

Here, $C(x,t)$, denotes the concentration (of something) at position x at time t, and $D > 0$ is a constant. The initial condition is assumed to be $C(x,0) = C_0\delta(x)$, and the boundary conditions are $C(\pm\infty, t) = 0$. Assume (for simplicity) that $D = 1m^2/s$ and $C_0 = 1$.

[**Hint** : Consider using the Crank-Nicholson scheme]

Compare your numerical result with the known analytic result ("the propagator").

b) We will now assume that the diffusion constant is spatially dependent

$$D(x) = \begin{cases} D_+ & x > 0 \\ D_- & x < 0 \end{cases}, \tag{2}$$

where $D_\pm > 0$ are constants.

Physically this situation corresponds, for instance, to the situation of heat conduction in a rod made out of two pieces of material of different heat conducting properties.

What is the relevant diffusion equation in this case? What is expected of the solution (again when $C(x,0) = C_0\delta(x)$)?

c) Solve the diffusion equation from subproblem b numerically by modifying the numerical scheme developed in subproblem a. Write down explicitly and *explain* the numerical scheme that you are implmenting (*i.e.* using). Assume that $D_- = 1m^2/s$ and $D_+ = 2m^2/s$. Plot the solutions for a representative selection of times.

d) Finally assume that the diffusion constant is given by

$$D(x) = 1 + \frac{\pi}{2} + \arctan\left(\frac{x - x_0}{\Delta}\right). \tag{3}$$

Explain what the significance of the parameters x_0 and Δ are? What happens to $D(x)$ in the limit $x_0 \to 0$ and $\Delta \to 0$.

e) Assuming the diffusion constant, Eq. (3), describe what is the relevant diffusion equation in this case? Solve this equation numerically for suitable choices of $x_0 \neq 0$ and $\Delta \neq 0$ assuming the same initial and boundary condition as above. Check your numerical solution in the limit $x_0 \to 0$ and $\Delta \to 0$.

Plot the solutions for a selection of times showing the concentration profile propagating over the diffusion constant "barrier" (using appropriate values, chosen by you, for $x_0 \neq 0$ and $\Delta \neq 0$).