20 March

Tell me in the chat window if there are
audio/video problems

Today: (Virtual) Computer Lab
20 Mar, 27 Mar, 24 Apr

Computer project
First part due date Fri 3 April

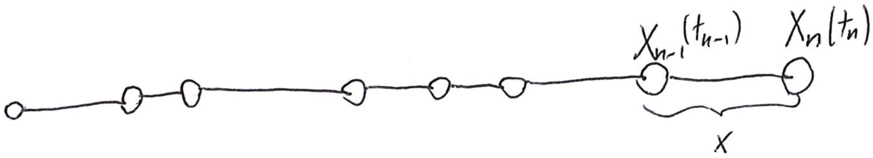
Final assessment being planned, not yet settled

Plan:

Review diffusion

Look at Exercises in Computer Project

Present demo of MATLAB (& python)



$$\text{CLT: } p(X_N) = \frac{1}{\sqrt{2\pi N\sigma^2}} \exp\left(-\frac{(X_N - N\mu)^2}{2N\sigma^2}\right)$$

7.1 Recap

We already encountered *diffusion* in section 2.4. It is widespread phenomenon and describes chemical spill as well as the tracking of a pedestrian. Its underlying assumptions are:

General conditions for Diffusion:

- If x_n is the position of the walker at time t_n, the position x_{n+1} only depends on x_n.
- The displacement $x := x_{n+1} - x_n$ is described by a stochastic process with probability distribution $p(x)$.

$$X_N = \sum_{i=1}^{N} x_i$$

We usually work with equally distributed time steps $t_n = \Delta t\, n$.

$$\Delta t = \frac{t_n}{n} = 1$$

Key observation for (normal) diffusion:

- The standard deviation for the 1-step process

$$\sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$$\mu = \langle x \rangle$$

$$\langle x^r \rangle = \int x^r p(x)\, dx$$

  exists and is finite.

- For a large number of steps N, the probability distribution $P(x_N)$ is Gaussian:

total walk length prob. distribution

$$P(x_N) = \frac{1}{\sqrt{2\pi\, t\, D^2}} \exp\left\{-\frac{(x_N - v_{\mathrm{dr}} t)^2}{2tD^2}\right\},$$

  where the drift velocity v_{dr} and the diffusion constant D are given by:

$$v_{\mathrm{dr}} = \langle x \rangle / \Delta t\,, \qquad D = \sigma_1 / \sqrt{\Delta t}\,.$$

- The difusion length is

$$\ell = \sqrt{\langle x_N^2 \rangle - \langle x_N \rangle^2} = D\sqrt{t}\,. \tag{75}$$

  This is the famous law of diffusion.

Total walk length: $N\mu = v_{dr}\, t = v_{dr}\,(\Delta t\, N) = v_{dr}\, N$

Total walk length variance: $N\sigma^2 = D^2 t$ diffusion coeff.

$$\sigma\sqrt{N} \propto \sqrt{t}$$

Statistical Physics 2019/20
MATH327
Kurt Langfeld

UNIVERSITY OF LIVERPOOL

COMPUTER PROJECT PART A

Student ID:

Marks: ____________ (of 50)

Instructions: Complete the three exercises below. Scan this sheet and your workings, and submit along with your code on VITAL. While the guidance below specifies some relevant MATLAB commands, you may use a different programming option if you prefer. This sheet contributes 4% to your overall mark for this module.

Due date: 3 April 2020, 17:00.

↗ reproducibility
Deterministic sequence from "seed"
are approximately uncorrelated

(Pseudo-)

Exercise 1: Random numbers

Initialise the random number generator. In MATLAB, this can be done using the command `rng(314156)`. Generate a sequence of n uniformly distributed random numbers $u_i \in [0, 1]$ with $i = 1, \cdots, n$ using the MATLAB command `rand`.

$p(u) = 1$
$0 \le u \le 1$

Complete the table below by estimating the average and the standard deviation σ as

$$\langle u \rangle \approx \frac{1}{n} \sum_{i=1}^{n} u_i,$$

$$\sigma \approx \sqrt{\frac{1}{n} \left(\sum_{i=1}^{n} u_i^2 \right) - \langle u \rangle^2}.$$

n	10	20	100	200	1000	100,000
$\langle u \rangle$						
σ						

[8 marks]

Calculate the exact average and standard deviation:

$$\langle u \rangle = \underline{\hspace{4cm}}, \qquad \sigma = \underline{\hspace{4cm}}.$$

[4 marks]

Exercise 2: Histogram

Initialise the random number generator, in MATLAB using `rng(314156)`.

If $u \in [0, 1]$ is a uniformly distributed random number (see Exercise 1), define the random number x by

$$x = \overbrace{\mathrm{asin}\,(2u - 1)}^{F(u)}\,, \qquad x \in [-\pi/2, \pi/2]\,,$$

where `asin` is MATLAB's arcsine command.

Generate an array X of 100,000 random numbers x. Plot the histogram of these random numbers using the MATLAB command `histogram`.

[10 marks]

Starting with the relation $p(u)\ du = p(x)\ dx$, calculate the probability distribution $p(x)$ of the random number x.

$$p(x) \ = \ \underline{\hspace{4cm}}.$$

Use this to calculate the exact average and standard deviation:

$$\langle x \rangle = \underline{\hspace{4cm}}, \qquad \sigma = \underline{\hspace{4cm}}.$$

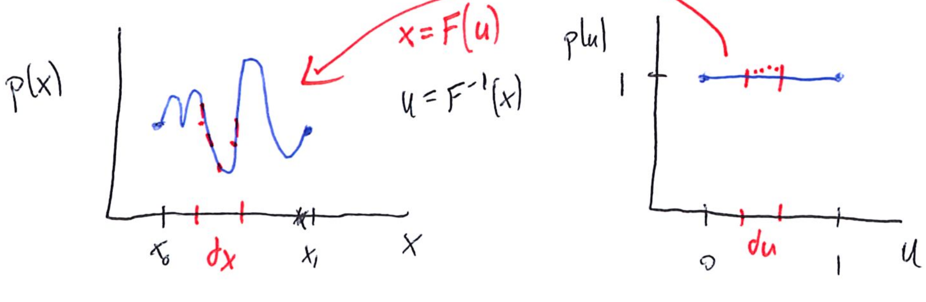
Does your histogram match these results?

[8 marks]

"Inverse transform sampling"

$$p(u)\, du = p(x)\, dx$$

$$p(x) = p(u) \frac{du}{dx} = p(u) \frac{d}{dx} (F^{-1}(x))$$



Exercise 3: Random walk

Iinitialise the random number generator, in MATLAB using `rng(314156)`.

CORE PROCESS: Start with $x_0 = 0$. For a given N, perform the iteration

$$x_k = x_{k-1} + x, \qquad k = 1, \cdots, N,$$

where x in each step is a random number with (see Exercise 2)

$$p(x) = \frac{1}{2}\cos(x), \qquad x \in [-\pi/2, \pi/2].$$

(a) Using the Core Process, generate a sequence of n random numbers $(x_N)_i$ with $i = 1, \cdots, n$. If we consider each $(x_N)_i$ to be the result of random walk i, this will give us n N-step random walks to analyse.

Estimate the standard deviation $\ell_2(N)$ of this N-step process as

$$\ell_2(N) \approx \left[\frac{1}{n}\sum_{i=1}^{n}(x_N)_i^2\right]^{1/2}.$$

Complete the table for $N = 100$:

n	10	20	100	200	1000	100,000
$\ell_2(100)$						

Calculate $\ell_2(N)$ using the central limit theorem. What do you get for $N = 100$?

$\ell_2(N) =$ ________________, $\ell_2(100) =$ ________________.

[10 marks]

(b) Now choose $n = 100,000$. Estimate $\ell_2(N)$ for $N = 1, \cdots, 500$. Plot $\ell_2(N)$ as a function of N. Fit the result to

$$\ell_2(N) = D\sqrt{N}.$$

What is your estimate for the diffusion constant D? Calculate the exact diffusion constant D_{exact} and compare:

$D =$ ________________, $D_{\text{exact}} =$ ________________.

[10 marks]

MATLAB access
- Free installation using UoL site license
- MATLAB Online runs in Web browser using site license
- Alternative: python etc. through repl.it