Computational Science Assignment Overview

**Stats**

Weight: 100% of course

Task 1.1: 20 marks (5 marks for definitions of distributions and the reason behind the choice of distribution, Simulate and [plot the movements for 100 steps and plot movement)

Task 1.2: 30 marks (Repeat the above for 100 and 1,000 steps. Locate the common points in the traversal of the cell. Comment on the movements made)

Task 2.1 15 marks (10 marks for basic simulation, 5 marks for showing time to reach final time – you can also use analytical methods to the same. 5 marks each for choice of M on either side of the given value and commenting on simulation)

Task 2.2: 35 marks (5 marks for the part where you suggest what happens when the value of M changes, and why this is important)

Word Count: 1800

Deadline: 7th January 2025

Handin: PDF and GitHub Classroom

**Description**

**Part 1**

For this task assume that the cell is ready to move in one of the four directions. Use random processes to change this state

A blue grid with red arrows and a brown rectangle

Description automatically generated

If we ignore the state of the cells a movement algorithm could look like:

X = rand1; Y=rand2 /Binary numbers 0 or 1

If X=1 and Y=1; Move Up

If X=1 and Y=0; Move Down

If X=0 and Y=1; Move Left

If X=0 and Y=0; Move Right

These numbers can be generated using uniform distribution (numpy.random.unifrom)

For this exercise use uniform distribution

**Task 1.1**

Take a 100x100 grid. You will need to simulate the movement of a cell.

You will need to run the algorithm for a 100 steps and plot the movement of the cell

Include definitions of the 2 distributions mentioned. And state under which circumstance would you use these distributions.

Comment on the choice of distribution selected for random numbers

Comment on the computational complexity of each method (You have been asked to locate common-points which both methods reach)

**Task 1.2**

Instead of the four possible directions of movement you can have eight. Move diagonal is also possible.

Maybe use 000 – 111 binary for 8 moves

Do for 1,000 and 1,0000 steps

For both tasks screen shot the movements through the grid

Generate data to show that the directions are uniformly selected.

If you find they are not sufficiently uniform, suggest how you would do it and show that this happens. Provide reasoning

**Part 2**

Integrating a process for change of state of the cells

Consider the Gompertz model for the growth of cancer tumours

A white background with black and white clouds

Description automatically generated

N is the number of cells

K is the growth rate of cells and K>0

M is the capacity

Assume K=0.006; M=10^13; and N(0)=10^9

**Task 2.1**

Simulate the growth of tumour cells for t=1200.

Does the growth reach a steady state? If not, experiment with the final time and determine Time Required to reach a steady state.

What will happen if M is changed? Pick 2 values on either side of the value given

**Task 2.2**

Assume the host tissue is in the form of a grid

A blue grid with arrows and a hole in the middle

Description automatically generated

If the simulation starts in the canter, and when it reaches the steady-state value for the number of cells, the tumour moves to any one of the other eight cells of the grid. The choice of the cell to move is random.

When the growth moves to a second cell, your initial population of tumour is reset to the initial conditions

Carry on simulating the growth till a steady state is reached for 2 cells of the grid

Now the cell growth has to move to another cell in the grid, your choice of locations is now seven

Plot the movements of the tumour cell growth though the grid.

Start with a 100x100 grid.

Consider the issues associated with the numerical strategy you are using.

If the numerical methods are changed. What will be there change in the complexity of the simulation.

Note: this is a simulation of a non-linear function. So use small value of h (order 0.001)