MXB261 - Modelling and Simulation Science

Assignment 2 - A Simulation Project

Due Date: 11:59pm Wednesday 18 October 2023, (Week 12)
The group report and individual fortnightly reflections are elligible for the 48hr extension. The group presentation is not eligible for the 48hr extension

The theme of this project is the effect of parameter values on the behaviour of a parasite described by a mathematical model, in both a temporal and spatial setting.

This is a Group Project with 4 students per group and is worth 40% of your final grade. The groups have been set up on Canvas. There are four individual tasks available, and *each student must choose a different task* in discussion with your group. You are encouraged to help each other. If circumstances dictate that your group has only 3 students, then you may omit Task 3. Note: Tasks 1, 2 and 4 are still to be completed.

In this assignment, marks will be awarded for using github to store and collaborate on the project. The marks are for demonstrating a group effort on the code, for successfully committing (uploading) your code to github at least once and for successfully adding the markers (their github accounts can be found on Canvas). It is recommended that each group member set up a folder within the group repository and commit documents regarding their task into a folder called "Task X" for Task number X.

Marking calculation

The final mark for each student is made up of the score for their individual score (out of 20 marks), plus a group score (out of 8 marks), plus three reflection scores (out of 12 marks). Individual and group scores are awarded based on the Group Report and Group Presentation.

The **individual component** includes marks for the individual contribution to the Group Presentation (5 of the 20 marks). In the Group Presentation, each student should present a maximum of 1 slide on their task results. In the Group Presentation there should also be 1 introduction slide and 1 discussion/conclusion slide (aim for less than 8 slides) and the group can decide who presents the information on those slides. The Group Presentations will run in Week 12 and Week 13 Practicals. The remaining 15 marks of the inidividual component will be awarded based on the individual's code and analysis. These marks will be awarded based on the accuracy of the code, code commenting and also the use of github and committing.

For the **Group component**, marks will be awarded based on the report as a whole (8 marks total). You should write the group report like you would a self contained document, attempting to link together the findings from each of the Tasks and including an Introduction and Discussion section. We strongly recommend that if there are any issues with group members not contributing to the group project, then email Adrianne (adrianne.jenner@qut.edu.au) prior to the final submission.

Finally, the three **reflection scores** will be worth 4 marks each and will be submitted fortnightly through canvas. These scores will be made up of 1 mark for submitting a reflection with scores for your group members that match your reflection, and 3 marks for the average score awarded to you by your group members. For example, if there are four group members: Tim, Gab, Sarah and Harry and Tim is awarded 2/3 by Gab, 3/3 by Sarah and 3/3 by Harry for his contribution to the group project for that fornight, where Gab awarded him 2 because he wasn't contributing of helping with the code, he would receive 2.67 as his score from his group members.

More details on the marking breakdown are available on the last two pages.

Report submission

The group is to submit their Group Report in two ways. First, the markers must be added as collaborators to the github repository using their github accounts (see Canvas). In your github repository there should be all the Matlab m-files, movie files (.avi), and a pdf of the report. You do not need to submit the slides for their presentations.

Secondly, one member of the group must submit the report as a pdf to Canvas. It is imperative to follow the submission instructions as failure to do so will result in marks being deducted.

Oral Presentation Times

The oral presentation of your work will occur in Weeks 12 or 13 during the practical times. As a group you must discuss which week and which practical slot you would most prefer to present in. Once your group has decided when you would like to present, one member must email the Unit Coordinator (adrianne.jenner@qut.edu.au) to lock-in that time.

All groups must have set a presentation slot by Friday 6th October (end of Week 10) otherwise one will be assigned to your group. It is important that all group members agree on a presentation time because after Week 13 there will be no other times available for presentations. There will be no extensions to the Oral presentation timeslot.

The Parasite Model
Consider the following differential equation system

$$\frac{\mathrm{d}X_1}{\mathrm{d}t} = k_1 X_1 X_2 - k_2 X_1$$
$$\frac{\mathrm{d}X_2}{\mathrm{d}t} = k_3 - k_4 X_2 - k_5 X_1$$

where X_1 represents a population of parasites that feeds off a population X_2. Parameter k_1 represents the birth rate of X_1, k_2 represents the death rate of X_1, k_3 represents the rate of food growth, k_4 represents food decay, and k_5 represents food consumption by the parasites. All these constants are positive.

Task 1: Deriving the model and a Parameter Sweep

In this task, you will investigate the solution to the model above using Euler's method and `ode45` and discuss the long-term parasite and food behaviour.

(a) To begin, derive the explicit Euler's method of the 2D parasite/food system given above. In order to implement this scheme and solve the system, suppose the following parameters have values as indicated:

$$k_1 = 1,\ k_2 = 2,\ k_5 = 3$$

and that the initial values are $X_1(0) = 1,\ X_2(0) = 1$. The time span for the investigation is $[0, T]$ where $T = 20$ units, and the step size is $h = 0.01$.

(b) In addition to these values, consider first the case that $k_3 = 20,\ k_4 = 4$. Simulate this system using Euler's method and solve the system of ODEs with Matlab's built in `ode45`. Compare the two solutions with some form of accuracy measure.

(c) Now simulate your model (either using Matlab or Euler's method) for

$$k_3 = 0, 2, 4, \cdots, 48, 50$$

to find k_3-values that result in

$$(i)\quad 0 \le X_1(T) \le 0 + \mathrm{Tol}, \qquad \text{or} \qquad (ii)\quad 2 - \mathrm{Tol} \le X_2(T) \le 2 + \mathrm{Tol}$$

for tolerance $\mathrm{Tol} = 0.1$. It is also a requirement that both populations X_1 and X_2 do not drop below 0 at any time in the simulation; if this happens, you must discard those parameter choices. On a single plot, plot the k_3 values again which of the two outcomes above you obtain, i.e. (i) or (ii).You should determine the boundary of the regions that characterise k_3 with respect to the above two scenarios.

(d) As above, but now implement a parameter sweep on both k_3 and k_4 (over $[0, 50]$). Plot successful parameter pairs (k_3, k_4), showing the region(s) corresponding to the two different scenarios (i) and (ii).

(e) Write a concise paragraph to explain your results. Your report should include the following figures:

- a comparison of the two solvers for the given parameter regime,
- a parameter sweep of k_3,
- a parameter sweep of k_3 and k_4.

Task 2: Latin Hypercube Sampling in 2D

In this task, you will further examine how the behaviour of the parasites and food change over time by performing a Latin Hypercube sampling and comparing the results to the equilibrium solutions of the system.

(a) To begin, perform an analysis of the equilibrium solutions of the parasite model by finding the equilibrium of the model.

(b) Consider, that we can fix three of the parameters:$k_1 = 1$, $k_2 = 2$, $k_5 = 3$. What is the value of the two equilibrium's of the parasite and food model, i.e. X_1^* and X_2^*? Can you see any relationship between the equilibrium values and the analysis in Task 1, part (c)?

(b) You are then to implement Latin Hypercube Sampling on the 2D space of parameters k_3, k_4 (each in the range [0,50]). For an appropriate mesh size and number of trials, build a population of successful parameter pairs, that reflect the system of equations exhibiting the characteristics that either

$$(i) \quad 0 \leq X_1(T) \leq 0 + \text{Tol}, \qquad \text{or} \qquad (ii) \quad 2 - \text{Tol} \leq X_2(T) \leq 2 + \text{Tol}$$

with the constraint that neither X_1 nor X_2 drops below zero in $[0, T]$; if this happens, you must discard those parameter choices. Take $T = 20$ time units, and have $X_1(0) = 1,\ X_2(0) = 1$.

You are to write your own code to carry out the Latin Hypercube Sampling. You can check that your code is working by comparing results with the built-in MATLAB command `lhsdesign`, however this comparison should not be included as part of your report.

In your exploration of the 2D parameter space, you are to group your successful parameter pairs so that a region in the 2D space corresponds to particular characteristics of the system dynamics. In addition to this, you should find the boundary between these regions. You should then link your findings back to the equilibrium values you determined in part (a) and interpret the stability of these equilibrium. Demonstrate your results in a 2D visualisation that is appropriately labelled (axis labels and title). Write a concise paragraph to explain your results.

Task 3: Latin Hypercube Sampling and Orthogonal Sampling in 3D

This task requires a Latin Hypercube Sampling to be implemented as for Task 2, but over a 3D parameter space. Here $k_1 = 1$ and $k_2 = 2$. Again, the parameter space is explored to determine regions that correspond to certain system dynamics.

In this task you must also use a copy of your 3D Latin Hypercube Sampling to then develop an Orthogonal Sampler. Repeat your analysis over 3D parameter space and compare your results for Latin Hypercube Sampling and Orthogonal Sampling.

Visualisation of the successful parameter 3-tuples is required, with appropriate labelling. Discuss the approaches you take to represent the 3rd dimension in your plots in an effective and meaningful way. Write a concise paragraph to explain your results, and compare the two sampling methods. Make sure to then tie in the results of the sampler with those of Task 2 and Task 3 and discuss what this means for the equilibrium of the system.

The Latin Hypercube Sampling requirements of Task 3 are very similar to the coding required for Task 2. It is expected that the students involved in Tasks 2 and 3 may like to discuss their programming approach for the sampling, but then to develop their own visualisations.

Task 4: Spatial agent-based implementation

In this task, we'll be looking at a spatial stochastic implementation of the paraiste food model. A spatial implementation allows exploration of the system dynamics when interactions take place at an individual level rather than at population level.

Construct a grid of cells (200×200) and populate that grid with F agents for food and P agents for parasites, according to various densities (see below). The parasites will be positioned randomly, while the positions of the food will be placed according to two food-placement strategies: random, or localised around the two coordinates $(50, 50)$ and $(150, 150)$. There is to be one agent only per cell. Note that when choosing a cell for a localised food-placement strategy, if it is already occupied, place the new food agent in a nearby unoccupied cell. An example of the localised food-placement strategy is demonstrated in Figure 1.

The rules for the simulation are as follows:

(a) Each parasite, in turn, will attempt to move to a neighbouring cell that is N, S, E or W of its current position;
- if the parasite attempts to move through the boundary, it skips the attempted move and stays in its current location;
- if the new cell is empty, the parasite moves;
- if the new cell is already occupied by a parasite, the move does not take place;
- if the new cell is occupied by food, the food is consumed (the food is replaced by the parasite), and a birth event takes place with the new parasite being placed in the original cell.

(b) A parasite dies after f_1 iterations and is removed from the grid. Note that a parasite which has just been born does not count as having lived for the current step i.e. next step will be its first step.

(c) For all food agents, each agent dies if a uniform random sample ($u \sim U(0, 1)$) $u \leq f_2$, and it is removed from the grid. Note u has to be different for each food agent.

(d) After all the parasites and food agents have been processed for the current step, create f_3 new food agents and position them either randomly in empty cells, or localised (in empty cells).

For a selection of parameter values, and for various initial F and P population densities of 10%, and 40% of the grid (assume F and P have the same population density), simulate the evolution of the system and hence describe the relationship between initial population density, food-placement strategies, and the observed system dynamics. Consider two parameter regimes;

- $f_1 = 3,\ f_2 = 0.1,\ f_3 = 100$,
- $f_1 = 10,\ f_2 = 0.01,\ f_3 = 300$.

To demonstrate your simulation, track the abundance of parasites and food after every step for a simulation that lasts 400 steps (or shorter if it reaches equilibrium). Create two figures (one for each parameter regime) that are 2×2 subplots where the columns are the two densities (10% and 40%), and the rows are the two food-placement strategies (random or localised). These figures should be included in your report and referred to when discussing the effects of food-placement strategy, density, and parameter regime. Create a movie of the spatial stochastic model above, capturing the output at regular time points as the simulation evolves for each of the eight scenarios. Each movie should not be longer than forty seconds each (ten frames per second). Include a single frame from two of these simulations to demonstrate the food-placement strategies in the methods section of your report. The videos will be uploaded to github.

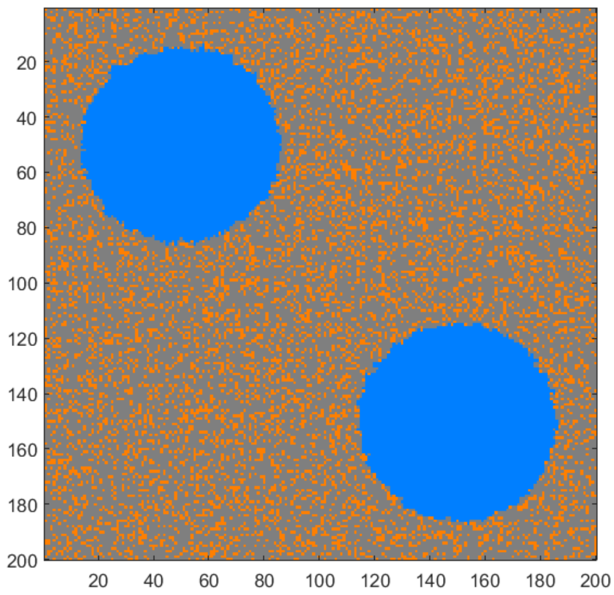

Figure 1: Parasite (orange squares) and food (blue squares) simulation initial frame with the localised food-placement strategy.

The Group Report

The purpose of the Group Report is to combine the results from the individual tasks, and to compare and contrast the results obtained from the different approaches and strategies.

The report (which should be approximately 10 pages) should have the following structure:

- an **Introduction**, setting the scene for the content (max. 1 page);
- a **Methods (by Task)** section, where you describe the approaches taken, for each Task; include here an analysis of the equilibrium solutions of the parasite model from Task 2, and the explicit Euler difference scheme from Task 1, and screenshots taken from the Task 4 movies to demonstrate your implementation of food-placement strategies (2-3 pages);
- a **Results and Discussion** section, where you combine, compare and contrast the results for parameter regions and the characteristics of the system dynamics from Tasks 1, 2 and 3; include here plots that justify your answers; also include results and figures from Task 4 (the spatial agent-based simulation) and the interpretation of the effect of initial population densities and food-placement strategies (5-6 pages);
- a **Conclusions** section, where you summarise the main results in no more than a few sentences (max. 1 page).

Note: Page limits are a guide. We only ask that you roughly aim to follow these limits.

The Oral Presentation

The purpose of the oral presentation will be to present your methods and key findings in an interesting and informative way to an audience of experts in your field (i.e. you can use technical jargon).

The presentation is intended to be a group effort and will go for a maximum of 6 minutes (aim for 5 mins, hard cut off at 6 mins) where each group member will present **one** slide each discussing their required task, and then a few extra slides for the group to present a brief introduction and their final conclusions.

The second part of the presentation will then consist of 4-5 minutes of questions from the audience.

Guide to the Marking Schedule

	Marks	Breakdown	
Individual component			
Structure	2	2	Code is well structured and well documented.
		0	Code is not structured and/or not documented.
Solution	6	6	Solution is correct, all aspects of the task have been considered.
		3	Parts of the solution may be incorrect, most aspects of the task have been considered.
		0	Little/no solution.
Methods (by task)	2	2	Methods for the task have been clearly and correctly outlined for reproducibility.
		1	Methods for the task have been outlined, but may not be correct, clear or reproducible.
		0	Little/no methods.
Results	2	2	Relevant and concise figures that clearly demonstrate the solution. Figures are clear, correctly and completely labelled.
		0	Irrelevant, excessive or no figures that do not clearly demonstrate the solution.
Github	3	3	Code has been committed to github at least once with commit comments that reflect the changes made to the code.
		0	No github commits or no reasonable commit comments reflecting changes made.
Oral component	**5**	5	Conveys a depth of understanding of the programming and issues for the Individual Task.
		2.5	Conveys some understanding of the programming and issues for the Individual Task.
		0	No oral discussion, or poor level of understanding conveyed.
Subtotal	**20**		

Group component			
Structure and presentation	1	1	Report has a clear and logical structure. Presentation is of a professional standard. No major spelling/grammatical errors.
		0	Report does not have a clear or logical structure. Presentation is not professional. Major spelling or grammatical errors.
Introduction	1	1	Introduction provides a short relevant background for the exercises performed in the report. Motivation for each task and an outline of the structure of the report is provided.
		0.5	Introduction missing key components, but outlines the main features of the report.
		0	Little/no introduction.
Discussion and comparison	4	4	Discussion shows concisely presented, but extensive, detailed and relevant insight. Results from individual tasks have effectively been compared. Plots, figures and tables are clear, concise and relevant.
		2	Discussion shows some relevant insight. Results from individual tasks have been compared. Plots, figures and tables may not be clear, concise and relevant.
		0	Little/no discussion or comparison.
Conclusions	2	2	Conclusions accurately and concisely summarise main findings of the project.
		1	Conclusions summarise some main findings of the project.
		0	Little/no conclusions.
Subtotal	**8**		
Total	**28**		

Reflection (individual) x4			
Structure and presentation	1	1	Reflection clearly articulates the progress made by the individual and group over the last week. The mark award to group members is clearly motivated.
		0	Reflection is not submitted or the mark submitted for group members is not clearly motivated.
Structure and presentation	3	3	Average of marks awarded by group members for an individuals contribution
Subtotal	**3 x 4**		
Total	**40**		