MATH1070 Assignment Questions

for Dr Christine Beveridge

Due: Wednesday 21st September in the Lecture

Please provide all answers in hard-copy only. Extensions will not be given without appropriate documentation Extensions will not be given on the full assignment

This assignment has three parts of equal value.

Part 1 will commence on 5th Sept. Part 2 will commence on 12th Part 3 in your own time.

Practical time on the 5th and 12th and 19th will be allotted primarily to Parts 1 and 2 of the Assignment.

Any questions, please email <u>c.beveridge@uq.edu.au</u>

MATH1070 Box Problem – Assessment Item 1 for Christine Beveridge

Due: 21st September in the lecture.

This exercise gives you some insight into the study of biology, or life on earth. You will learn how biologists deal with the fact that they are unable to measure everything they wish to and rarely have access to all the components in the system they study. Nevertheless those components may be very real and of crucial importance. For example, Mendel discovered the principals of genetic inheritance long before the first genetic code (DNA sequence) was determined.

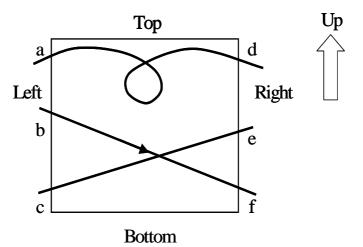
You will be split into groups. Each group will be given an enclosed box containing a network of interconnected tubes. The objective is to learn as much as possible about the contents of the box and to report your findings to the rest of the group.

- Take precise notes on your observations with the box.
 - Initial conditions (box orientation and location and number of objects)
 - o Movement 1 and new box orientation and location and number of objects;
 - Movement 2 and new box orientation and location and number of objects;
 - o etc
- Draw a diagram that describes the network inside the box.
- Describe the diagram with a list of hypotheses (statements).
- What sort of model could you make that describes those hypotheses?
- What features (level of abstraction) would you choose to represent in your model?
- How can you test that your model and hence whether your hypotheses are consistent with the box; what experiments could you design to test your hypotheses?
 - Make some notes on what happens if you start with the tubes facing down and the balls showing at the bottom and rotate 6 times to the left and 6 times to the right.

Next we will discuss how to create a computational model of this system.

MATH1070 Box Problem – Continued

Although we could not see or feel inside the box, several groups came up with the same hypothesis about the connections in the box. This is drawn below.



In summary, we decided that the box contained a direct connection between a to d, b to f and c to e, but that a to d had a loop. In some boxes, there was something blocking the flow of f to b, more so than b to f. That is, whereas 100% of the time, 100% of the balls could move b to f in the TOP-UP state, the reverse was not true for the BOTTOM-UP state.

If this system was very important to a biologist, they may wish to model it, even though they have no real data or detail on the connections within the box. What they want to model is their understanding of the connections between the letters shown above. The objectives would be to test whether the hypotheses of what is in the box are supported when implemented into a model and the model output compared to the "biological" data. A **mechanistic** model is therefore required.

What should such a model consist of and how do we do it?

We need to start asking some questions about the property of the network.

What are the objects we need to represent in the network? Are they simply *a*, *b*, *c*, *d*, *e*, and *f*? How would we deal with the "valve" between *b* and *f* and the loop between *a* and *d*?

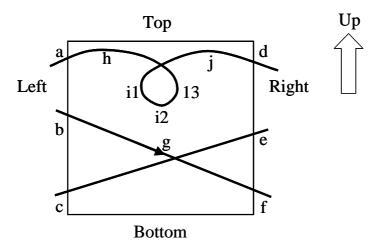
The answer is that we should consider the valve and the loop to be objects in the system even though we have no data for them. They are important features of the system and affect its properties.

How should we represent the loop? To answer this question, we need to consider **how we are going to describe the relationships between the objects** in the system.

Are the relationships between the objects always the same? They are always connected to each other in the same order. But the flow between objects is determined by the orientation of the box, or on the **state of the system** (which side of the box is facing up?). Furthermore, the flow of contents among different areas of the loop depends on the state of the system. The complexity arises from the properties of the objects changing for each state of the system (orientation of the box).

Although the loop is continuous, the model objectives are to achieve a largely qualitative rather than strictly quantitative output and therefore the different parts of the loop can be considered as discrete compartments rather than as a continuous connection. In order to represent the flow in the loop, the loop therefore needs to be divided into parts that represent arbitrary compartments in the loop. As shown in the figure below, 5 compartments (objects) h, i1, i2, i3 and j are sufficient to describe all parts of the loop within the box. Parts h and j are included because the balls often rested at that point rather than going directly from i1 to d or i3 to a.

MATH1070 Box Problem – Continued



How are we going to implement these concepts into a model? One possibility is to use a Boolean network to describe the state of the objects as containing or not containing balls. That is, on or off (1 or 0). Will that allow us to account for intermediate values, such as when only half the balls move as in from f to b, or if an odd number of balls are in h and the box is flipped from top bottom? Not easily.

As the hypothesis considers that the tubes are continuous, we could represent flows in and out of the compartments using differential equations. Is it necessary to represent continuous flow in the system? Not really. The system will quickly reach a steady state that can be represented with simple addition and subtraction and this also corresponds to the timeframe in which the data was collected (after contents had stopped moving).

We could consider the loop as a series of compartments that can only transfer balls to adjacent compartments. That is, when the box is turned from the topside up to the left side up, we could capture the mechanism that the contents move from a to h to i3 rather than simply stating that i3 becomes equal to a, by <u>explicitly representing the structure of the compartments</u> in the model. Time permitting; an L-system model will be presented to you in class that describes this approach.

An alternative approach to the approach above is to consider the mathematical relationships among the components in each state of the system rather than relying on representing the physical structure of the system.

For example, if Top is up then *c* will be it's value at the last step, plus the value of *e*; and *e* will become 0. As flow through *g* is uninhibited in this orientation, then *f* becomes it's value at the last step + g + b; and *b* and *g* become 0. In contrast, if Bottom is up, then we need to consider the valve. Lets say that only half the contents that reach the valve at a given rotation step can move through g. On this basis *b* becomes 0.5 x (*g* + *f*); *g* becomes 0.5 x *f* and *f* becomes 0.

Assessment Requirements

- 1) Hand-write or type a list of hypotheses that describe the system and can be used to achieve point 2 below.
- 2) Hand-write or type a list of algebraic equations that describe the hypotheses above and which could be used below (3) to create a rule-based mechanistic model that describes the simple relationships between the components for each state of the system.
- 3) Implement the model designed in (2) above in MATLAB. Prescribe an initial state of the box with the tubes facing down with all the balls showing at the bottom and print results for the contents of each compartment at each step of turning the box 6 times to the left and 6 times to the right. Compare the model output with your observed data. Do you have any further comments? Are there further tests you could perform with the model?

MATH1070 Membrane Transport 2 – Assessment Part 2 for Christine Beveridge

Due Wednesday 21st September in the lecture.

The transport of proteins across a membrane was given as an example in class. In class you were given a box containing pea seeds and a barrier with holes influencing the transport of the seeds from one side of the box (doner) to the other (receiver) through the holes.

- 1. Describe the system that you would like to model as a list of hypotheses.
 - a. Consider a constant energy state that is conducive to flow
- 2. Write a statement in the form of symbols and letters (as you have been shown in the lectures) that describes these hypotheses.
- 3. Write a differential equation that describes the change in the number of peas on the receiver side.
- 4. Use Eulers method to approximate the equation.
- 5. Write a Matlab model of this system.
- 6. Plot the number of peas in the receiver side over time given initial conditions of high and low numbers of transporters. Choose an initial number of peas that is in excess of the highest number of transporters.
- 7. Describe the emergent properties of this system what are the dynamics of the flow of proteins across the membrane under different conditions.
- 8. Name two other systems you can think of that may have these properties.

Eulers Method:

For $\underline{dy} = f(y)$; yn+1 = yn + hf(yn), where h is the step size. Take the function: $\underline{dy} = ky$ Its approximation is: $\underline{yi+1-yi} = kyi$ yi+1-yi = dt * kyiyi+1 = yi + dt * kyi

MATH1070 Exam-type Questions – Assessment Part 3 for Christine Beveridge

[Year 2004 MATH1070 Exam Question: Christine Beveridge] This question is part of your assignment due Wed 21st September during the lecture.

Read all questions in this section before commencing to answer the first part.

In a chemical context, A and B combine to produce C at a rate of k_1 . In this example, A and B are "consumed" in the production of C, just as carbon and oxygen and are used in the production of carbon monoxide. Write differential equations that describes the changes in A, B and C over time. 10 Marks

1/2 page

Write some Matlab code that describes this simple system.
 Marks
 page

2. What changes do you need to implement in the Matlab code if A requires two molecules of B to produce one molecule of C?
5 Marks
¹/₂ page

3. Write a new differential equation that describes the effect on an inhibitor, I, that competitively binds with B at a constant of k_2 .

5 marks.

3 lines

4. Is this system different to the transport of objects across a membrane or to chemical reactions that require enzymes – for example, if B was an enzyme? If so, how and why?
5 marks
10 lines