SCIE1000 Tutorial sheet 12

This tutorial contributes toward your final grade; see the Course Profile (https://www.uq.edu.au/study/course.html?course_code=SCIE1000). The tutorial will be marked out of 6, with 3 marks for completing the "Before class" work, and 3 marks for completing the "In class" assessment and working on the remaining "In class" questions until you finish them or the tutorial ends.

Goals: This tutorial sheet contains questions covering systems of differential equations, relating to modelling second-order chemical reactions and also from previous SCIE1000 exams. Take the exam seriously. Many people **think** that taking some notes into an exam makes it easier than standard exams, because there is no need to "cram" information. However, this type of exam is often harder, because there are no easy "memorisation marks". Have a look at previous papers, particularly from 2016, 2015 (which was a bit hard, perhaps), 2013 and 2012. Could you answer those questions, in 2 hours, if you didn't know what any of them were going to be? If not, then practise!

On this tutorial sheet and the final sheet next week, we will also work through the exam paper from 2014.

To be completed before class ¶

Complete the following questions before class, write (or type if you wish) your answers on a sheet of paper, put your name and student number on the top of the paper, and hand it to your tutor as you enter the room. **If you do not hand in the answers at the start of the class, as you enter the room, then you will lose the marks for this component.** Note that in some cases there are no "right" or "wrong" answers.

Polio

Read the following information, which appeared as the final page of the 2014 examination paper.

> **Background:** *Polio* is a highly contagious infectious viral disease, transmitted from an infected host to a susceptible individual via the faecal-oral route. Most people who suffer from polio will recover completely, but a small proportion will develop long lasting paralysis. Polio existed for thousands of years, but major epidemics did not occur until late in the 19th century. In the 20th century, major polio epidemics caused many thousands of children and adults to become paralysed, including in first world countries, and promoted widespread fear.
>
> **Epidemiology:** The typical infectious period for an individual with polio is 2 weeks, and on average 5 secondary infections will arise from a single infected individual in a fully susceptible population. In about 99 % of cases, an individual infected with polio will recover completely with no long term effects. However, in about 1 % of cases an infected individual will develop long term paralysis from the disease.
>
> **Polio eradication:** The possibility of developing paralysis makes polio a highly feared disease. In 1988, the World Health Organization, UNICEF and the Rotary Foundation commenced a global campaign to eradicate polio. The following table shows the global number of reported polio cases per year in a selection of years since 1988.

Year	Years since 1988	Number of recorded cases per year
1988	0	35251
1990	2	23484
1993	5	10487
1997	9	5185
2002	14	1922
2007	19	1387
2012	24	291

Vaccination: A cornerstone of the global polio eradication campaign is widespread vaccination, using the Oral Polio Vaccine (OPV) developed by Albert Sabin in 1957. There are three *serotypes* or variations of the polio virus, called *Sabin 1*, *Sabin 2* and *Sabin 3*.
A single OPV dose (usually two drops) contains 10^6 infectious units of the Sabin 1 strain, 10^5 infectious units of the Sabin 2 strain, and 6×10^5 infectious units of the Sabin 3 strain. Three doses of OPV produce protective antibodies to all three polio serotypes in about 95 % of recipients.

Polio test: In 1994-1996, the WHO conducted a trial to check the effectiveness of its world wide network of laboratories in which they test samples for polio. They prepared 500 uninfected biological samples, and then infected 61.2 % of these samples with at least one strain of polio virus. To make the test harder, many samples were infected with viruses similar to polio, but which were not actually polio. They sent these samples to 67 of their labs across the world, and each lab attempted to identify which of the samples they had been sent were infected with polio. Overall, the tests for polio undertaken in the network of laboratories had a sensitivity of 92 % and a specificity of 90 %.

Question (1)

Using the information about polio given above, answer the following questions which formed Question 1 on the 2014 exam paper. Marks that were allocated on the exam are shown, for your reference. Working time was about 1 minute per mark.

1. (**5 marks**) Oral Polio Vaccine (OPV) is distributed in vials with a volume of 1 fluid ounce that contain 10 doses. Find the concentration in mol/L of infectious units (of any kind of Sabin strain) in that vial. (Hint: there are about 33.8 fluid ounces in 1 litre. A *mole* of a substance, denoted mol, contains approximately 6.02×10^{23} constituent particles.)

2. (**7 marks**) Estimate the total volume of OPV (in litres) used world wide since 1957. Show working and state any assumptions. (Hint: note that 3 doses are typically administered to each individual.)

3. The OPV is only 95 % effective; that is, 5 % of vaccinated people will not develop immunity. The World Health Organisation (WHO) states that, in order to achieve *herd immunity* against polio, at least 80 % of people must be immune.

   A. (**2 marks**) Explain clearly why 80 % (rather than another value) is the minimum level of immunity to polio that is targeted by the WHO. (This question relies on something we may not have covered in class yet. If you cannot answer it, then leave it blank and your tutors will discuss the answer. The answer relates to the fact that, on average, 5 secondary infections arise from a single infected person in a fully susceptible population.)

   B. (**2 marks**) Given that the OPV is not 100 % effective at inducing immunity in vaccinated individuals, what minimum level of **vaccination** coverage should the WHO aim to achieve? Why?

   C. (**3 marks**) Should the WHO aim for a higher vaccination coverage than the minimum you identified in Part B? Give some arguments for and against.

Question (2)

This question uses the information on polio given above. Answer the following questions which formed Question 3 on the 2014 exam paper; marks that were allocated on the exam are shown, for your reference. Working time was about 1 minute per mark.

Run the program in the following Python cell, which plots the annual number of reported polio cases for various years from the table in Question (1), and also plots a graph of a model of these numbers,

$$P(t) = 35200e^{-0.2t},$$

where t is the number of years since 1988.

1. (**4 marks**) Demonstrate how the values 35200 and -0.2 in the function $P(t)$ were obtained. (It is **not** sufficient simply to substitute values of t into the equation.)

2. (**5 marks**) Use $P(t)$ to estimate the number of reported polio cases in 1975. Explain carefully the likely cause(s) of the difference between your estimate and the actual number which was 49293.

3. (**4 marks**) Use $P(t)$ to estimate the number of reported polio cases in 2013. Explain carefully the likely cause(s) of the difference between your estimate and the actual number which was 417.

4. (**2 marks**) Use $P(t)$ to predict the first year in which there will be only one reported case of polio.

5. Consider the following partial Python program.

```
def Pred(yr1):
    p = 35200*exp(-0.2 * (yr1-1988))
    return (p)

Yrs = array([ 1988, 1990, 1993])
NumC = array([ 35251, 23484, 10487])
i=2
tot = 0
while i>=0:
    diff = Pred(Yrs[i]) - NumC[i]
    if diff<0:
        diff = -diff
    print(diff)
    tot = tot + diff
    i = i-1
print("Total: ",tot)
```

```
  A. (**2 marks**) Explain clearly (in words) what the function $\texttt{Pred}$ doe
s.
```

```
B. (**6 marks**) Find all of the output produced by this program.
```

```
C. (**5 marks**) Explain clearly (in words) what the program does.
```

```
D. (**2 marks**) Write a brief comment that would be suitable to include in
```

the program, describing what the **while** loop does in the program.

In [ ]:

```
# Program to plot the numbers of reported annual polio cases from 1988 to 201
3, and
# also to plot an exponential model of these values.

from pylab import *

t=array([0,2,5,9,14,19,24])
N=array([35251,23484,10487,5185,1922,1387,291])

plot(t,N,"bx",mew=3,markersize=12,label="Cases per year")

t1=arange(0,24.05,0.1)
v1=35200*exp(-0.2*t1)
plot(t1,v1,"k",linewidth=3,label="P(t)")

legend(loc="upper right")
xlabel("Years since 1988")
ylabel("Polio cases per year")
title("Reported annual polio cases (1988-2013).")
grid(True)
show()
```

To be completed in class

Complete the following questions in class. They involve a mix of individual work, and discussions with others. Make sure that you read the questions before class and think about how you might approach answering them. Don't rely on someone else doing all of the work. You need to work by yourself on the final exam, so it is important that you work hard now.

Feedback: Be proactive!

Australian government research shows that students often feel they don't receive adequate feedback on their work. In a class of 800 students, it is not possible for the course coordinator to give direct feedback to each student. Instead, tutorial classes are designed to be the place in which you can get feedback on your work from classmates and the tutors. You can ask for help, show them your answers, and discuss your understanding of any of the course material. As an adult learner, the onus is on **you** to seek feedback; tutors and classmates are happy to give it, if you want it.

Question (3)

Your tutors will briefly discuss how to approach answering Questions (1) and (2). If you struggled with any of the questions then be sure to ask lots of questions.

Question (4)

Chemical reactions can be classified according to the properties of their reaction rates, as:

- **zero-order** if the reaction rate does not depend on the concentration of the reactant(s);
- **first-order** if the reaction rate depends on the concentration of only one reactant;
- **second-order** if the reaction rate depends on the square of the concentration of a single reactant, or the (multiplicative) product of the concentrations of two reactants; and
- **third-order** if the reaction rate depends on the (multiplicative) product of the concentrations of three reactants.

In lectures we have seen examples of zero-order reactions (for example, the metabolism of alcohol in the liver is effectively a zero-order reaction) and first-order reactions (such as metabolism of most other drugs). Consider the following second-order reaction - the formation of gaseous hydrogen iodide (molecular formula HI, molar mass 127.9 g/mol^{-1}) from gaseous hydrogen and iodine:

$$\mathrm{H}_2(g) + \mathrm{I}_2(g) \longrightarrow 2\ \mathrm{HI}(g)$$

Let $[H_2](t)$, $[I_2](t)$ and $[HI](t)$ be the concentrations of hydrogen, iodine and hydrogen iodide at any time t in seconds, with the initial concentrations of H_2 and I_2 equal. Then these concentrations satisfy the system of equations

$$[H_2]' = -k\,[H_2][I_2]$$

$$[I_2]' = -k\,[H_2][I_2]$$

$$[HI]' = 2k\,[H_2][I_2]$$

where k is the reaction rate. (Note that $[H_2][I_2]$ means the concentration of hydrogen **multiplied by** the concentration of iodine, whereas $[HI]$ means the concentration of hydrogen iodide.)

1. Interpret briefly what each equation in this system of DEs is saying. In particular, interpret the physical meaning of the terms containing $[H][I]$.

2. In this system of questions, at any time, $[H_2]' + [I_2]' = -[HI]'$. What does this mean, and why is it expected?

3. If the concentration of reactants and products is measured in mol L^{-1} and the most appropriate unit of time for the above reaction is seconds, what are the units of k? (Show working.)

Question (5)

This question extends the content of Question (4).

Chemical reactions rarely, if ever, proceed to completion; that is, the concentration of any of the reactants rarely reaches zero. Instead, the reaction typically reaches a state called *chemical equilibrium*, where the concentrations of reactants and products remains constant with respect to time. In other words, reactions are occurring in **both** a **forward** and **reverse** direction, with reactant(s) R transforming into product(s) P, and the product(s) P themselves becoming reactant(s) which react to produce new product(s) R. Consider again the formation of gaseous hydrogen iodide, but in terms of both the forward and reverse reactions.

$$\mathrm{H_2}(g) + \mathrm{I_2}(g) \rightleftharpoons 2\ \mathrm{HI}(g)$$

Let $[H_2](t)$, $[I_2](t)$ and $[HI](t)$ be the concentrations of hydrogen, iodine and hydrogen iodide at any time t in minutes (with the initial concentrations of H_2 and I_2 equal). Then these concentrations satisfy the following system of DEs, where k_f is the forward reaction rate and k_r is the reverse reaction rate.

$$[H_2]' = -k_f\,[H_2][I_2] + k_r\,[HI]^2$$

$$[I_2]' = -k_f\,[H_2][I_2] + k_r\,[HI]^2$$

$$[HI]' = 2k_f\,[H_2][I_2] - 2k_r\,[HI]^2$$

1. Find the values of $[H_2]'$, $[I_2]'$ and $[HI]'$ at equilibrium.

2. Show why the following is true at equilibrium and explain in words what this means:

$$k_f[H_2][I_2] = k_r[HI]^2.$$

Question (6)

This question extends the content of Question (5).

For a given reaction at equilibrium, scientists can define an equilibrium constant, K. One reason that the equilibrium constant is of significance is that at a given temperature, regardless of the initial concentrations of reactants and products in the system, the equilibrium constant will remain the same. In other words there is one equilibrium constant for a given system at a particular temperature. Consider the following reaction type:

$$x\text{A} + y\text{B} \rightleftharpoons z\text{C}$$

where A, B and C represent the reactants and products and x, y and z are coefficients. The equilibrium constant, K, for such a reaction is given by:

$$K = \frac{([C]_e)^z}{([A]_e)^x([B]_e)^y}.$$

Note that the concentrations of reactants and products in this equation are those at equilibrium.

1. Calculate the equilibrium constant for the formation of gaseous hydrogen iodide, given that at 700 K, $k_f = 6.3 \times 10^{-2}$ and $k_r = 1.8 \times 10^{-3}$. (Hint: use the final part of Question (5).)

2. Predict the equilibrium concentrations of H_2, I_2 and HI at 700 K, given the following initial concentrations:

$$[H_2]_0 = 1\,\text{mol}\,\text{L}^{-1} \quad [I_2]_0 = 1\,\text{mol}\,\text{L}^{-1} \quad [HI]_0 = 0\,\text{mol}\,\text{L}^{-1}$$

   (Hint: the number of molecules in the system is constant. Also, $[H_2] = [I_2]$ at all times. Finally, the solutions to the quadratic equation $31x^2 + 8x - 4 = 0$ are $x = 0.2527$ or $x = -0.5107$.)

Question (7)

This question is a required, in-class assessment piece. To receive the marks for this component, you and your partner must show your answers to a tutor during your tutorial.

(This question was on the final examination in 2009, and worth 16 marks. Expected working time for this question was about 16 minutes.)

Here are the general forms of six equations used for modelling in SCIE1000. In each case, let y be the phenomenon being modelled, t be the variable time, and a, b and c be positive constants.

- (1) $y(t) = a\sin(bt)$
- (2) $y(t) = at + b$
- (3) $y(t) = at^b e^{-ct}$
- (4) $y(t) = ae^{bt}$
- (5) $y(t) = at^b$
- (6) An equation $y(t)$ that satisfies $y' = ay\left(\frac{b-y}{b}\right)$

1. *Moore's law* says that the processing power of computers roughly doubles every 2 years. Let $y(t)$ be processing power, where t is in years from now on.

   A. If Moore's Law is true, which of the Equations (1) to (6) best models y? Briefly justify your answer.

   B. Some experts predict that processing power will continue to increase, but at a continually decreasing rate. If so, which equation could best model y? Briefly justify your answer.

   C. Sketch rough graphs of your equations from Parts A and B on a single set of axes with appropriate labels, clearly identifying each graph.

2. In *autocatalytic* chemical reactions, one or more reaction products catalyse the reaction, so the rate of reaction at any time is proportional to both the amount of reaction product and the amount of original substance remaining. *Tin pest* (https://en.wikipedia.org/wiki/Tin_pest) is an autocatalytic chemical reaction in which the element tin transforms to a brittle form.

   In a certain experiment the **proportion** of a tin sample that is in brittle form is initially 1 %. Over time this proportion initially rises slowly, then rises at an increasing rate until half of the sample is in brittle form, and then this proportion rises more slowly and gradually approaches 100 %.

   Let $y(t)$ be the proportion of the tin sample that is in the brittle form at any time t.

   A. Which of the Equations (1) to (6) best models y? Briefly justify your answer.

   B. Chemists trial a treatment for tin that may reduce the effect of tin pest. In a treated tin sample, the reaction still follows the same general mechanism but occurs with a slower reaction rate, and a state with 60 % of the tin in brittle form is ultimately approached, rather than 100 %.

   This reaction will be modelled by the same equation as in Part A. Explain whether the values of any constants (a, b, c) would be larger than, unchanged, or smaller than those in Part A, and why.

C. Sketch rough graphs of your equations from Parts A and B on a single set of axes with appropriate labels, clearly identifying each graph. Mark any values that you know.

Extra questions

Here are some extra practise questions, for you to do in class (if you have time), or outside class. You do not need to do them all, but may like to choose some to help with your preparation for the final exam.

Question (8)

(This question was on the final examination in 2012, and worth 31 marks. Expected working time for this question was about 31 minutes.)

Let $F(t)$ represent a population of foxes (predators) and $R(t)$ represent a population of rabbits (prey). The population of rabbits is limited by a maximum carrying capacity, K. Researchers propose the following **new** predator/prey model of the populations, as a **variation** of the Lotka-Volterra model. Note that a, b, c and d are positive constants.

$$R' = aR\left(\frac{K-R}{K}\right) - bRF$$

$$F' = -cF + dFR$$

1. Explain briefly how the equation for R' in the above model includes competition between rabbits.

2. Rather than being dimensionless quantities, let the units of R and K be "rabbits", the units of F be "foxes", and let time be measured in "years". Find the units of each of: R', F', a, b, c and d.

3. What does the model predict would happen to the fox population if all rabbits died suddenly? Explain your answer, and draw a rough sketch of the predicted fox population.

4. What does the model predict would happen to the rabbit population if all foxes died suddenly? Explain your answer, and draw a rough sketch of the predicted rabbit population.

5. Consider a population in which $R = 100$, $F = 9$, $K = 1000$, $a = 1$, $b = 0.1$, $c = 0.1$ and $d = 0.001$, all with appropriate units. Apply **one step** of Euler's Method with a step size of 2 to predict both population sizes at time $t = 2$.

6. Interpret your answer to Part 5. Explain carefully what this means biologically, for both populations and for their predator/prey interactions.

7. For both parts of this question, let $K = 1000$, $a = 1$, $b = 0.1$, $c = 0.1$ and $d = 0.001$, all with appropriate units, and assume that the size of the fox population is 20.

   A. Find the size(s) of the rabbit population in order for each of:

   - the fox population to decrease;
   - fox population to remain unchanged; and
   - the fox population to increase.

   B. Show that the rabbit population will decrease, irrespective of the number of rabbits.

Question (9)

Consider the following life table for fleas.

Time period	Developmental stage	Number alive
1	Eggs	10,000
2	Larvae	500
3	Pupae	50
4	Adults	30

The male:female ratio of adult fleas is 1:1, and adult female fleas lay a total of 2,000 eggs each.

1. Draw a life-cycle diagram showing the transitions the fleas make between stages. Label each stage, with E denoting eggs, L denoting larvae, P denoting pupae and A denoting adults. (Hint: fleas that do not transition to another stage all die.)

2. Write a system of DEs to model this flea population.

3. You bought a new bed for your dog from friends but it contained 100 eggs, 50 larvae, 10 pupae and 2 adult fleas (1 male, 1 female) at time $t = 0$. Apply one step of Euler's method, with a step size of 1 time period, to estimate the population of fleas in each stage at time $t = 1$. (Show all work.)

Question (10)

In a population at high risk of developing cancer, each individual is classified as: Undiagnosed (U), Positive (P), Treatment (T) or Deceased (D). There is a test for the cancer, but there are false positive and false negative test results. Each month:

- Each Undiagnosed person will either test positive and move to the Positive category (10 % likelihood), return a false negative test result and Die (3 %) or return a true negative test result (87 %) and remain Undiagnosed.
- Each Positive person will move to the Treatment category (70 % likelihood), or move to the Undiagnosed category (30 %) because their earlier test result was a false positive.
- Each person in the Treatment category will either recover and move to the Undiagnosed category (40 % likelihood), require treatment for another month (40 %), or Die (20 %).

Researchers wish to develop a model based on a system of differential equations.

1. Draw a life-cycle diagram showing all possible transitions between the four categories "Undiagnosed" U, "Positive" P, "Treatment" T, and "Dead" D, including the probability of each transition.

2. Let $U(t)$, $P(t)$, $T(t)$ and $D(t)$ be the number of people in each category at any time t. Equations for U' and D' are as follows. Write similar equations for P' and T'.

$$U' = -0.13U + 0.3P + 0.4T \qquad\qquad D' = 0.2T + 0.03U$$

3. In a particular population, at time $t = 0$, the functions and derivatives have the following values. Apply **two** steps of Euler's method with a step size of one month to estimate the number of people in each category at time $t = 2$ months.

   - Function values: $U(0) = 800$, $P(0) = 100$, $T(0) = 50$, $D(0) = 0$
   - Derivative values: $U'(0) = -54$, $P'(0) = -20$, $T'(0) = 40$, $D'(0) = 34$

4. Run the Python program in the following cell, which applies Euler's method to these equations for a period of 12 months. (Note that the initial populations in this question are different from those in Part 3.) The four curves on the graph correspond to $D(t)$, $P(t)$, $T(t)$ and $U(t)$ in some order. **From the graph**, identify which graphs correspond to $D(t)$, $P(t)$, $T(t)$ and $U(t)$ respectively, and explain your answers.

In [ ]:

```
# Euler's method to solve system of DEs modelling cancer.
from pylab import *

# Initialise variables.
maxstep = 41
D1=zeros(maxstep)
D2=zeros(maxstep)
D3=zeros(maxstep)
D4=zeros(maxstep)

D1[0] = 1000
D2[0] = 900
D3[0] = 500
D4[0] = 200
h = 0.3
times=zeros(maxstep)

# Step through Euler's method with stepsize h
i = 0
times[0]=0
while i<maxstep-1:
    dD1 = -0.13 * D1[i] + 0.3 * D2[i] + 0.4*D3[i]
    dD2 = -D2[i] + 0.1* D1[i]
    dD3 = -0.6*D3[i] + 0.7 * D2[i]
    dD4 = 0.2 * D3[i] + 0.03 * D1[i]

    D1[i+1] = D1[i] + h * dD1
    D2[i+1] = D2[i] + h * dD2
    D3[i+1] = D3[i] + h * dD3
    D4[i+1] = D4[i] + h * dD4

    times[i+1] = (i+1) * h

    i=i+1
# Output graphs.
grid(True)
plot(times, D1, 'k-', linewidth=3)
plot(times, D2, 'k-', linewidth=3)
plot(times, D3, 'k-', linewidth=3)
plot(times, D4, 'k-', linewidth=3)

xlabel('Time (months)')
ylabel('Number of people')
title('Population and disease status')
text(6.2,870,"Graph 1")
text(4.3,1300,"Graph 2")
text(4.5,250,"Graph 3")
text(2.5,50,"Graph 4")
show()
```