**Homework 3, Math 450, Spring 2018**

*Instruction:* Answer each of the following questions, showing and explaining your work as you go. Partial credit will be awarded based on how well I can follow your work and how far you get, so please use sentences, description, diagrams, and clear definitions to communicate your results as best you can. All diagrams and plots should be labelled, for example.

1. Translate the following compartmental model into a set of reactions, labelling each reaction arrow with its corresponding rate constant. Then use the reaction network to construct the corresponding system of differential equations.

![Compartmental Model Diagram]

2. Compartmental differential equation models have also been applied to the theory of war.

   (a) Lanchester famously proposed the following equations for the destruction of rival air-forces during World War I. Let $A(t)$ and $B(t)$ be the sizes of rival air-forces over time.

   $$
   \frac{dA}{dt} = -gB, \quad \frac{dB}{dt} = -rA.
   $$

   The constants $g$ and $r$ are called “force multipliers”, and represent things like technological advantages. The “loser” is the first air-force to be destroyed. Find an equality involving only the initial sizes of each air force $A(0)$ and $B(0)$, along with the constants $g$ and $r$ that predicts how big air force $A$ has to be to win the war.

   (b) Guerilla warfare is often contrasted from traditional warfare because the enemy can be hard to locate when in small numbers. This can be applied in the context of the American revolution or the Vietnam war. One way to represent this is with the law of mass action.

   $$
   \frac{dA}{dt} = -gBA, \quad \frac{dB}{dt} = -rA.
   $$

   Find an equality involving only the initial sizes of each air force $A(0)$ and $B(0)$, along with the constants $g$ and $r$ that predicts how big air force $A$ has to be to win the war.

3. Data from Kermack and McKendrick’s 1927 paper on epidemic modelling includes data on the number of new cases each week during a plague epidemic in Bombay: [http://www.math.psu.edu/treluga/plague_data.txt](http://www.math.psu.edu/treluga/plague_data.txt)

   (a) Plot the data points $(t_i, y_i)$ where $y_i$ is the number of new cases of plague and $t_i$ is the time, measured in weeks.

   (b) The simplest modern compartmental model of epidemic dynamics is the SIR model

   $$
   S(0) = S_0, \quad \dot{S} = -\beta SI,
   $$

   $$
   I(0) = I_0, \quad \dot{I} = \beta SI - \gamma I,
   $$

   where $\beta$, $\gamma$, $S_0$, and $I_0$ are unknown parameters. In this model, the rate of new infections is $\beta SI$. Plot $\beta S(t)I(t)$ for the same values of $t$ that are observed in the data when $\beta = 3 \times 10^{-5}$, $\gamma = 0.01$, $S_0 = 9000$, and $I_0 = 30$. 
(c) Calculate the absolute error

\[ E_1 = \sum_i |y_i - \beta S(t_i)I(t_i)| \]

and the square error

\[ E_2 = \sum_i (y_i - \beta S(t_i)I(t_i))^2 \]

between the data and the model’s predicted rate of new cases.

(d) Use ‘scipy.optimize.fmin()’ to minimize the square error \( E_2 \) over the 4 parameters \( \beta, \gamma, S_0, \) and \( I_0 \). Plot the best fit and the data on the same plot for comparison, and state the best estimates for each of the 4 parameters.

(e) One imperfect but commonly used measure of goodness of fit is the “coefficient of determination”, which for this problem can be written

\[ R^2 = 1 - \frac{\sum_i (y_i - \beta S(t_i)I(t_i))^2}{\sum_i y_i^2} \]

You can think of \( R^2 \) as the fraction of the data’s information successfully explained by our model; the closer \( R^2 \) is to 1, the better the model fits the data. Calculate the coefficient of determination for your best parameter estimates. (It should be better than 0.95 if you’ve gotten a good fit.)

4. Imagine an autocatalytic reaction between two chemicals is described by the system of ordinary differential equations

\[ x(0) = x_0, \quad \dot{x} = a - x + x^2y \]
\[ y(0) = y_0, \quad \dot{y} = b - x^2y \]

where \( a \) and \( b \) are the rates at which the chemicals \( x \) and \( y \) flow into the system. The concentration \( x(t) \) is observed over time, giving the data in http://www.math.psu.edu/treluga/450/autocatalytic_data.csv

Repeat parts (a), (d), and (e) of the previous problem for this data.

5. Using montecarlo simulation, estimate the distribution for the maximum number of sequential heads in 100 flips of a fair coin. Perform atleast 100,000 simulation runs. Present your results as a plot the number of runs with fewer than \( n \) heads in a row as a function of \( n \).

6. Montecarlo simulations can also be used to calculate things like the area of a unit circle \( \pi \).

(a) If you draw a square circumscribing a unit circle, and then pick a point \((x, y)\) uniformly randomly from that square, then according to the principle of indifference, the chance that point is in the unit circle itself is \( \pi/4 \). Write a python program that samples 10 million points from this square, counts how many are in the unit circle, and uses this to estimate \( \pi \). The pythagorian theorem can be used to check if a point is inside the unit circle. How many digits of accuracy does you estimate achieve?

(b) For comparison, use the formula

\[ \arctan \left( \frac{\sqrt{3}}{3} \right) = \frac{\pi}{6} \]

and the Taylor series of \( \arctan \) around \( x = 0 \) to estimate \( \pi \). How many terms do you need to use to obtain the same accuracy as your Montecarlo simulation?

(c) Which approach is a better way to calculate \( \pi \)?