Math 2208: Ordinary Differential Equations

Project 5: An Application from Chemistry - The Brusselator and Hopf Bifurcation

Spring 2020 **Subhadip Chowdhury** **Due: May 6**

The **Brusselator model** is a famous model of chemical reactions with oscillations. The dynamics and chemistry of oscillating reactions has been the subject of study for the last almost 60 years, starting with the work of Boris Belousov. While studying the Kreb's cycle, he witnessed a mixture of citric acid, bromate and cerium catalyst in a sulphuric acid solution undergoing periodic colour changes. These changes indicated the cycle formation and depletion of differently oxidized Ce(III) and Ce(IV) ions. This was the first reaction, where biochemical oscillations was observed in 1950. In 1961, Zhabotinsky reproduced Belousov's work and showed further oscillating reactions. The reaction mechanism is an example of an autocatalytic, oscillating chemical reaction. Autocatalytic reactions are chemical reactions in which at least one of the reactants is also a product and vice versa. The rate equations for autocatalytic reactions are fundamentally nonlinear.

Consider a Brusselator whose equations are given as follows[1]:

$$\begin{gathered}
\mathbf{A} \xrightarrow{k_1} \mathbf{X} \\
\mathbf{B} + \mathbf{X} \xrightarrow{k_2} \mathbf{Y} + \mathbf{D} \\
2\mathbf{X} + \mathbf{Y} \xrightarrow{k_3} 3\mathbf{X} \\
\mathbf{X} \xrightarrow{k_4} \mathbf{E}
\end{gathered}$$

where **A** and **B** are reactants (substrates), **D** and **E** are products and **X** and **Y** are the autocatalytic reactants of the set of reactions. Also k_1, k_2, k_3 and k_4 are the rate of reactions for each component reaction.

The governing equations of the Brusselator are obtained using law of mass action (the rate of a chemical reaction is directly proportional to the product of the concentration of reactant) and the set of equations for the change in concentrations of **X** and **Y** are found to be (after some scaling):

$$\begin{aligned}
\frac{dx}{dt} &= a - (1+b)x + yx^2 \\
\frac{dy}{dt} &= bx - yx^2
\end{aligned}$$

where x and y represent the concentrations of the autocatalytic reactants and $a, b > 0$. Because of obvious reasons, we are only going to be interested in the case where x and y are positive.

We will be using `Desmos` and `PPlane` for this project.

§A. Equilibrium Point Analysis

Read the above text and watch the linked video

https://www.youtube.com/watch?v=wHKnZl3FslU

before you begin! The video uses different compounds than the original experiment by Belousov but the theory is still the same.

[1] https://en.wikipedia.org/wiki/Brusselator

Question 1. (1+1+2 points)

Find the equation of the nullclines and the equilibrium point in terms of a and b.

Question 2. (2+1+1 points)

Find the Jacobian of the system at the equilibrium point. Show that its trace is

$$\mathbf{T} = b - 1 - a^2$$

and determinant is

$$\mathbf{D} = a^2$$

§B. Bifurcation

Question 3. (2+2+2 points)

Suppose we keep a fixed and vary b. Write down the type of phase portrait that occurs at the point of equilibrium in the following three cases. Also mention their stability type.

a) $a = 1$ and $b = 1$.

b) $a = 1$ and $b = 3$.

c) $a = 1$ and $b = 5$.

Question 4. (1+3+2 points)

We conclude that there are at least two bifurcation values of b when a is fixed at 1.

(a) Check that $\mathbf{D}$ is always positive, so the equilibrium is source or sink based on values of $\mathbf{T}$.

(b) Draw the curves $\mathbf{T} = 0$ and $\mathbf{T}^2 = 4\mathbf{D}$ in the (a, b)-parameter plane.

(c) Find the bifurcation values of b when $a = 1$.

Question 5. (4 points)

Find all possible behaviour of the system as a function of parameters a and b. In particular, draw the regions in (a, b)-plane (remember that $a, b > 0$) that correspond to stable/unstable node or spirals.

§C. Nullclines and Direction Field

Question 6. (2+2 points)

Use `Desmos` to draw the nullclines. Set sliders for a and b.

(a) Move the slider to check that the nullclines intersect only once for all values of a and b. How does changing a and b change the x and y coordinates of the point of intersection? Is this consistent with the formula of equilibrium point you obtained above?

(b) Set $a = 1, b = 2.5$ and copy the resulting graphs of the nullclines on to paper. Draw the direction field along the nullclines.

Question 7. (4 points)

Find whether x' and y' are positive or negative in other regions (4 of them) and use this information to draw the direction field arrows in those regions (on your paper).

§D. **Phase Portrait**

Question 8. (2+2+2 points)

Something very interesting happens in the phase portrait as the equilibrium becomes unstable. Let's use `pplane` to draw the phase portrait in each of the three cases from question (3). You may need to change the window width in each case for a comfortable viewing size.

Include a printout of the phase portrait with some sample solution curves in each case. You can collect all three on one page using e.g. MS Word to save paper.

§E. **Existence of a Limit Cycle**

In the second picture above, solution curves that start near the equilibrium point go to a limit cycle. Could we have predicted that we would be getting a limit cycle when the equilibrium becomes unstable? Recall the four possibilities for a trajectory of a solution curve for a nonlinear system as a consequence of **Poincaré–Bendixson** theorem (look in the last worksheet). Assuming the requirements hold, the only possibilities for solution curves that start near $(a, b/a)$ are that either they become unbounded or they spiral towards a limit cycle. How do we know they are not going to infinity? In the following steps we will work this out.

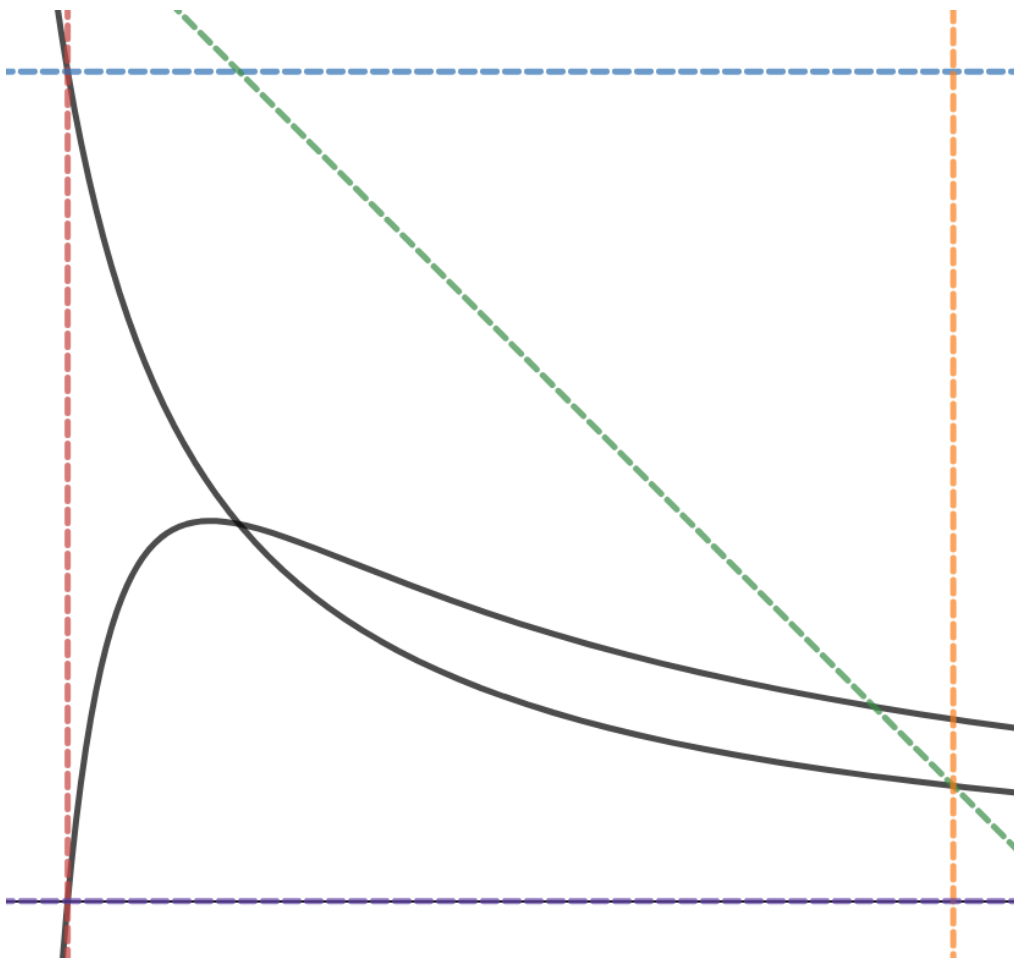

Figure 1: Trapping Region

Consider the five dotted lines that we have drawn along with the nullclines in figure 1. We will describe and find equations for them in the next problem.

■ Question 9. (1+1+1+1+1 points)

(a) The red dotted line is vertical and it passes through the point of intersection of the x-nullcline and the x-axis. Find it's equation in terms of a and b.

(b) The blue dotted line is horizontal and it passes through the point of intersection of the red line and the y-nullcline. Find it's equation in terms of a and b.

(c) The green dotted line has slope -1 and passes through the point $\left(a, \frac{b(b+1)}{a}\right)$. Find it's equation in terms of a and b.

(d) The orange dotted line is vertical and passes through the intersection of the green line and the y-nullcline. Find it's equation in terms of a and b.

(e) The purple dotted line is just the $\mathbf{X}-$axis. Mark the region bounded by the five dotted straight lines.

■ Question 10. (2+2 points)

We are going to find the direction field along the boundary of this region. Arrows along the horizontal and vertical segments are easy to find. So we only need to check the diagonal segment.

(a) Show that $-y' > x'$ if $x > a$. [Hint: Calculate $x' + y'$.]

(b) Explain how this inequality implies that the vector field points inward on the diagonal green line.

[Hint: What is dy/dx for $x > a$?]

■ Question 11. (2 points)

Draw the arrows along the five boundary (dotted) line segments. What can you say about the long-term behavior of a solution curve that crosses into the region? Can it ever leave the region?

The region we have constructed above is called a **Trapping Region**. It 'traps' the trajectories inside as all the arrows are pointing inward! On the other hand, when the equilibrium point is a spiral source, all trajectories that start near the point are going outwards. Since they can't escape the trapping region, they are doomed to converge towards a limit cycle! Note that the requirement of being a repelling equilibrium point is crucial, since otherwise all trajectories could have converged to a point.

§F. Hopf Bifurcation

The kind of bifurcation you observed above is called a **Hopf Bifurcation**. The uniqueness of such bifurcations lies in two aspects: unlike other common types of bifurcations (e.g. pitchfork, saddle-node or transcritical) Hopf bifurcation cannot occur in one dimension. The minimum dimensionality has to be two. The other aspect is that Hopf bifurcation deals with birth or death of a periodic solution or limit cycle as and when it emanates from or shrinks onto a fixed point, the equilibrium. Recently, Hopf bifurcations of some famous chaotic systems have been investigated and it is becoming one of the most active topics in the field of chaotic systems.