Complex Systems - TP20 - Brusselator

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1 Introduction

The practical work that we were given regards the Brusselator theoretical model for a type of autocatalytic chemical reaction. The main objective of this work is to study the model mentioned above in the matter of long-term behaviour for different values of the parameters, a and b, of the x and y concentrations over time. Also, we will determine if this dynamical system presents oscillatory behaviour.

$$\dot{x} = a - (b+1)x + x^2 y$$
$$\dot{y} = bx - x^2 y$$

2 Experimental Setup

2.1 Frameworks and Tools

To run our simulations we decided to use the *simcx* python framework as the simulation and visualization core. Then, we implemented the simulators and visuals that we needed to visualize the behaviour over time, the sensitivity to the initial conditions of the simulation, the phase space of the system, a bifurcation diagram in 3D and other needed visuals. The programming language used was python.

2.2 Integration methods

As previously stated, we had to implement a numerical integration method in order to obtain the x, y values of the system. This was the factor that made us implement most of our simulators, because there is not a simulator with numerical integration already implemented in the *simcx* framework. We created a class with the numerical integration methods (*NumericalIntegration*), where each method receives a state, a function (the brusselator function) and the step to be used in the integration. This method then returns the new state based on the given state. The forward euler method and the Runge-Kutta fourth-order method were implemented. On our simulations, we used a step of 0.01.

3 Visual Analysis

3.1 System behavior

To understand the behavior of the system over time empirically, we ran several simulations, from which two can be seen in the figure 1.

In figure 1 (left) we can see that the simulation, for 16 different initial states, converged into the fixed point $(0.2, 0.5)$. For this simulation, the initial points were sampled from $x \in [-4, 4[, y \in [-4, 4[$ with step equal to 2.

For figure 1 (right) the case is different, also for 16 initial states, the system did not converge into a fixed point, but instead presents a oscillatory behavior. Differently from the previous simulation, the initial points were sampled from $x \in [-4, 4[, y \in [0, 8[$ with step equal to 2.

By analysing these two figures, one can assume that the convergence of the system does not depend on the initial states, but on the parameters specified on the brusselator model.

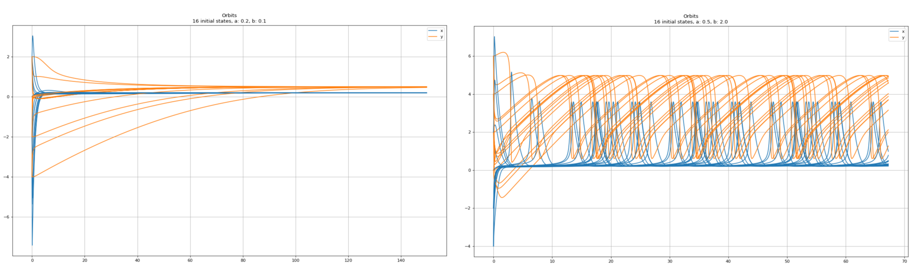

Fig. 1. On the left, we have the behavior of the system over time for $a = 0.2$ and $b = 0.1$. On the right the behavior of the system over time for $a = 0.5$ and $b = 2$

3.2 Sensitivity to the initial conditions

With the goal of understanding how the initial conditions influence the behavior of the system in mind, we performed simulations where the difference of two seeds was plotted, along with the respective orbits.

Figure 2 shows us that, for those parameters, the differences between different seeds go to 0, meaning that the system converges for the same point. We can conclude that, in this case, the system is not sensitive to the initial conditions.

In figure 3 we get a completely different result. The orbits do not converge to the fixed point, instead they enter into a oscillatory behavior and they never overlap each other. We can see that they do not overlap, because the differences between the orbits do not converge to 0, but also present a oscillatory behavior. The orbits are the same, but shifted (the size of the shift stays the same over time). Since the shift size does not change (can be seen by the periodicity of the differences over time), we can say that the system is not sensitive to the initial conditions, because, over time, its behaviour is unchanged.

Figure 4 shows us another type of behaviour of our system. For these parameters the system converges to the fixed point but in spiral. This is easier to see in a phase space plot. The differences between orbits are getting lower and eventually will become 0 when the fixed point is reached, so we can say that the system does not depend on the initial conditions.

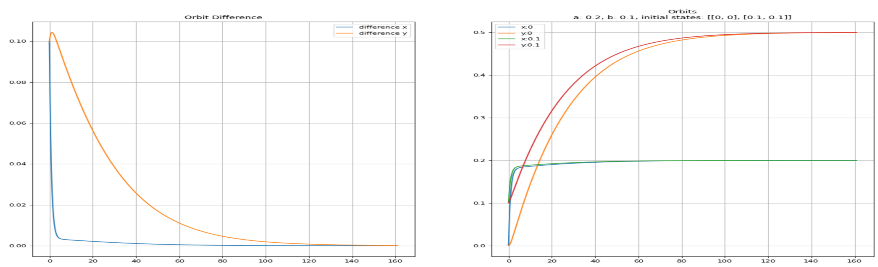

Fig. 2. Difference of the orbits (on the left) and the respective orbits (on the right) for seeds $(0, 0)$ and $(0.1, 0.1)$, with $a = 0.2$ and $b = 0.1$.

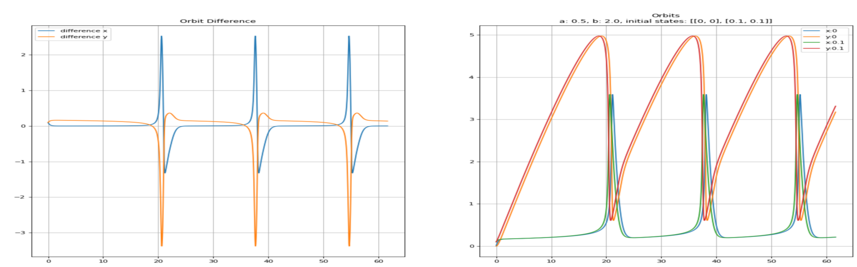

Fig. 3. Difference of the orbits (on the left) and the respective orbits (on the right) for seeds $(0, 0)$ and $(0.1, 0.1)$, with $a = 0.5$ and $b = 2$.

3.3 Phase Space

The phase space in figure 5(1,1) is another way to show that, for those parameters, the system does converge to the fixed point, independently of the seed.

Previously we stated that the orbits, when the behaviour is oscillatory, are equal between different seeds, but are shifted in time. Figure 5(1,2) corroborates this, because after a while all the orbits have the same trajectory. We are in the presence of a limit cycle. No matter the seed, the system goes to it.

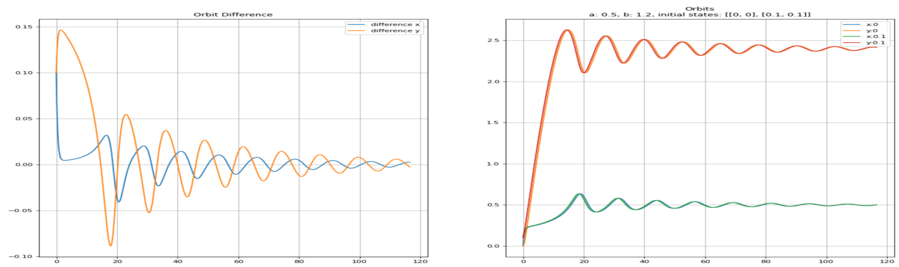

Fig. 4. Difference of the orbits (on the left) and the respective orbits (on the right) for seeds $(0, 0)$ and $(0.1, 0.1)$, with $a = 0.5$ and $b = 1.2$.

Figure 5(2,1), as we stated previously, is a superior way to show how, for certain $a's$ and $b's$, the system converges in a spiral to the fixed point.

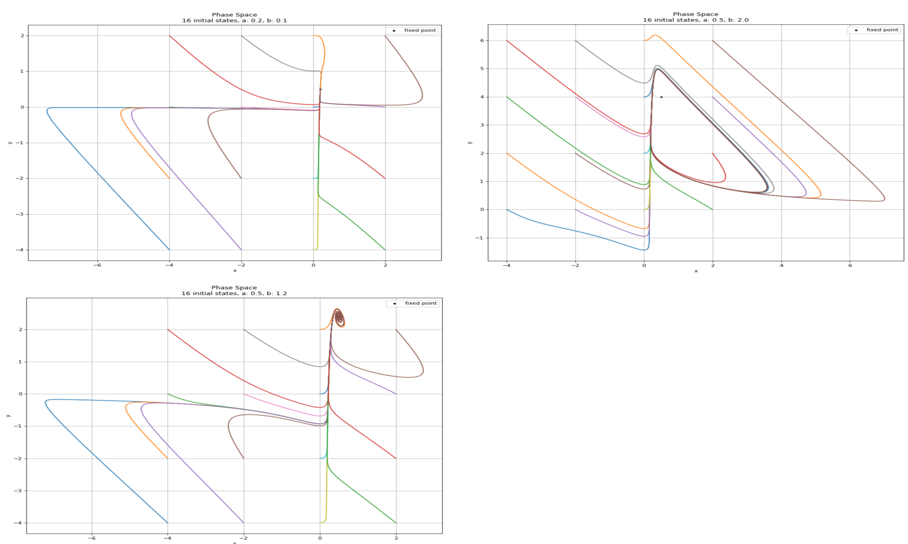

Fig. 5. (1,1) Phase space for $a = 0.2$ and $b = 0.1$. (1,2) Phase space for $a = 0.5$ and $b = 2$. (2,1) Phase space for $a = 0.5$ and $b = 1.2$.

3.4 Bifurcation Diagram

In order to see how the system behaves for several values of a and b we decided to a 3D plot present in figure 6. We can see that the oscillatory behavior appears in a certain region of the space (a, b). Later a analytical analysis will be presented, showing the boundary where the system goes from one behavior to another.

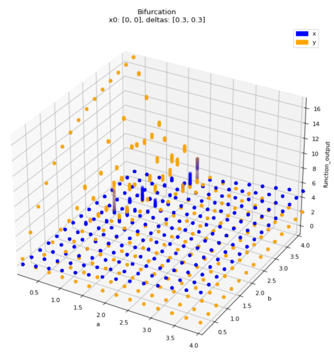

Fig. 6. Bifucartion diagram in 3d.

4 Analytical analysis

After the visual analysis, we will inspect the model through the use of mathematical tools, looking for a better understanding and explanation of the observed results as we dive deeper in complex systems theory.

4.1 Description

The model above presents itself as a non-linear, first order, autonomous, continuous-time 2D dynamical system that has x and y as variables of state and a and b as *parameters*. Since the dimensions of this continuous-time dynamical system are 2D, only fixed and periodic long-term behaviours are possible, rejecting the possibility of chaos.

4.2 Fixed Points

In order to calculate the fixed points, the model needs to be solved as a system of equations, where there are no changes in the values of the state variables from one step to another, i.e. the derivatives of x and y over time are equal to zero:

$$\begin{cases} \dot{x} = a - (b+1)x + x^2 y \\ \dot{y} = bx - x^2 y \end{cases} \implies \begin{cases} 0 = a - (b+1)x + x^2 y \\ 0 = bx - x^2 y \end{cases} \iff$$

$$\iff \begin{cases} 0 = a - bx - x + x^2 y \\ 0 = x(b - xy) \end{cases} \iff \begin{cases} \dots \\ x = 0 \vee y = \frac{b}{x} \end{cases}$$

For x = 0:

$$0 = a - b \cdot 0 - 0 + 0^2 y \iff a = 0$$

which is impossible, since a > 0.

For $y = \frac{b}{x}$:

$$0 = a - bx - x + x^2 \frac{b}{x} \iff$$
$$\iff 0 = a - bx - x + bx \iff$$
$$\iff 0 = a - x \iff$$
$$\iff x = a$$

After some algebraic manipulation, it is possible to reach the solution of the equation system above (x,y) = (a, $\frac{b}{a}$), which is the only fixed point of the brusselator model.

As seen in the visual analysis, on one hand, the system presents convergence towards this stability point for some combination of the parameters. On the other hand, other parameter combinations may cause the model to periodically repeat the same trajectory around the fixed point, never experiencing convergence. This fact calls for a stability analysis around the fixed point, for an enhanced insight into the system.

4.3 Stability

After having the fixed point of the model, it is of most importance to understand its stability. The stability around a fixed point, which is unique in this system, gives useful insights on what the system's long-term behaviour is going to be. In order to determine the stability of the system around the fixed point $(x, y) = (a, \frac{b}{a})$, we need to first calculate the values of the eigenvalues of the Jacobian matrix of the system at the fixed point.

$$J|_{(a,\frac{b}{a})} = \begin{bmatrix} \frac{\delta \dot{x}}{\delta x} & \frac{\delta \dot{x}}{\delta y} \\ \frac{\delta \dot{y}}{\delta x} & \frac{\delta \dot{y}}{\delta y} \end{bmatrix} |_{(a,\frac{b}{a})} = \begin{bmatrix} 2xy - b - 1 & x^2 \\ b - 2xy & -x^2 \end{bmatrix} |_{(a,\frac{b}{a})} = \begin{bmatrix} b-1 & a^2 \\ -b & -a^2 \end{bmatrix}$$

$$det(J - \lambda I) = 0 \iff \begin{vmatrix} b - 1 - \lambda & a^2 \\ -b & -a^2 - \lambda \end{vmatrix} = 0 \iff \lambda^2 - Tr(J)\lambda + Det(J) = 0 \iff$$

$$\iff \lambda = \frac{Tr(J) \pm \sqrt{Tr(J)^2 - 4 \cdot Det(J)}}{2}$$

Where $Tr(J)$ and $Det(J)$ are the trace and determinant of the Jacobian matrix:

$$Tr(J) = (b - 1) + (-a^2) = -a^2 + b - 1 \tag{1}$$

$$Det(J) = (b - 1)(-a^2) - (-b)(a^2) = -ba^2 + a^2 + ba^2 = a^2 \tag{2}$$

The stability condition of the system is given by:

$$Re(\lambda_d) < 0$$

where λ_d is the dominant eigenvalue. Hence, if $Tr(J)^2 < 4 \cdot Det(J)$, the stability condition becomes:

$$Tr(J) < 0$$

else, the condition is [2]:

$$Det(J) > 0 \qquad \wedge \qquad Tr(J) < 0$$

In summary, the system becomes stable under two conditions:

$$Tr(J)^2 < 4 \cdot Det(J) \qquad \wedge \qquad Tr(J) < 0$$

or

$$Tr(J)^2 \geq 4 \cdot Det(J) \qquad \wedge \qquad Det(J) > 0 \qquad \wedge \qquad Tr(J) < 0$$

Solving the first condition, by substituting $Tr(J)$ and $Det(J)$ by equations 1 and 2:

$$\begin{cases} Tr(J)^2 < 4 \cdot Det(J) \\ Tr(J) < 0 \end{cases} \iff \begin{cases} (-a^2 + b - 1)^2 < 4a^2 \\ -a^2 + b - 1 < 0 \end{cases} \iff \begin{cases} b < (a+1)^2 \\ b > (a-1)^2 \\ b < 1 + a^2 \end{cases} \tag{3}$$

Applying a similar procedure to the second condition:

$$\begin{cases} Tr(J)^2 \geq 4 \cdot Det(J) \\ Det(J) > 0 \\ Tr(J) < 0 \end{cases} \iff \begin{cases} b \geq (a+1)^2 \vee b \leq (a-1)^2 \\ a^2 > 0 \\ b < 1 + a^2 \end{cases} \tag{4}$$

As we may observe from the unfolded conditions, the equation $b < 1+a^2$ appears in both. In the second condition, note that $a^2 > 0$ is always true. Since $b < 1+a^2$ defines the plane of a and b parameters that cause the system to be stable in both conditions and taking into consideration that in the first condition $(a-1)^2 < b < (a+1)^2$ and that in the second, b is defined by the set of points that complement the previous, like so

$$\neg((a-1)^2 < b \qquad \wedge \qquad b < (a+1)^2) \qquad = \qquad b \leq (a-1)^2 \qquad \vee \qquad b \geq (a+1)^2$$

the equation $b < 1 + a^2$ properly defines stability for every $a, b > 0$. If this equation is satisfied and b belongs to $[(a-1)^2, (a+1)^2]$ then the dominant eigenvalue contains complex conjugate values, hence the system will converge in a spiral into the fixed point. If it is satisfied and b does not belong to that interval, the system will converge into its fixed point. If the equation is not

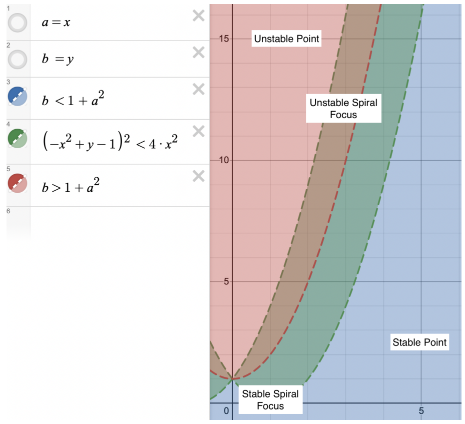

Fig. 7. Stability regions for b = f(a), from desmos.com

satisfied and b belongs to that same interval, then the system will diverge from the fixed point in a spiral manner. Else, the system will be unstable, and diverge from the fixed point. The 7 explains it better graphically.

This stability analysis has explained the convergence that we witnessed in the visual analysis, as well as the oscillatory long-term behaviour. Nonetheless it did not explained the appearance of a limit cycle in the phase space, which was brought a several change in the phase space. The bifurcation plot showed us that there are values of a and b that cause bifurcations to happen. Therefore, a bifurcation analysis makes sense.

4.4 Nullclines

In order to get a general explanation and understanding of the phase space behaviour, as the system is continuous, we may define regions where every seed inside it behaves asymptotically similarly, through the computation of the nullclines for each state variable, which are lines in the phase space where some of the state variables derivative value is 0, i.e., there is no variation for that state variables. The intersection of the nullclines for both state variables also gives us the location of the fixed point. For that, we may solve each of the equations used in the subsection above solely:

$$
\begin{aligned}
\dot{x} &= a - (b+1)x + x^2 y & \dot{y} &= bx - x^2 y \\
0 &= a - (b+1)x + x^2 y & 0 &= bx - x^2 y \\
(b+1)x - a &= x^2 y & 0 &= x(b - xy) \\
y &= \frac{(b+1)x - a}{x^2} & x = 0 \vee y &= \frac{b}{x}
\end{aligned}
$$

The equations above result in 3 nullclines:

For $\dot{x} = 0$:

$$y = \frac{(b+1)x - a}{x^2}$$

For $\dot{y} = 0$:

$$x = 0 \qquad \vee \qquad y = \frac{b}{x}$$

This way, we can better visualize the general phase phase and have a general idea of it. These results may be visualized in the picture below. The arrows directions are estimated through the signal of the derivatives of both state variables.

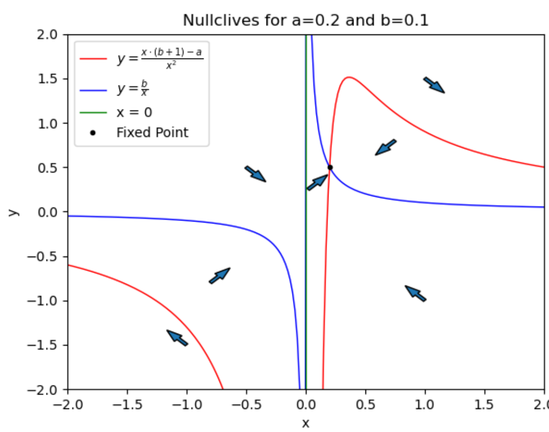

Fig. 8. Nullclines and Phase Space Asymptotic Directions

4.5 Bifurcations

Since the system shows oscillatory behaviour around the fixed point for $b < 1 + a^2$, and close enough changes its stability, into what seems to be an unstable spiral focus enclosed by a limit cycle in the phase space it is fair to guess that the resulting bifurcation is a Hopf bifurcation, and that the critical condition is $b = 1 + a^2$. In order to find out if it is this type of bifurcation, the dominant eigenvalues must have a pure imaginary non-zero value, i.e.

$$Re(\lambda_d) = 0 \qquad \wedge \qquad Im(\lambda_d) \neq 0$$

Applying a similar process to 3, since that is the only condition branch of $Re(\lambda_d) = 0$ that will have non-zero imaginary values,

$$\begin{cases} Tr(J)^2 < 4 \cdot Det(J) \\ Tr(J) = 0 \end{cases} \iff \begin{cases} (-a^2 + b - 1)^2 < 4a^2 \\ -a^2 + b - 1 = 0 \end{cases} \iff \begin{cases} b < (a+1)^2 \\ b > (a-1)^2 \\ b = 1 + a^2 \end{cases} \iff$$

$$\iff b = 1 + a^2$$

As we can see, our suspicions where correct, having a Hopf Bifurcation at

$$b = 1 + a^2$$

5 Conclusions

In terms of studying the behaviour of the system for different values of the parameters, we conclude that the model presents different behaviours for a and b, from fixed point convergence to fixed point spiral divergence into a limit cycle. We have also concluded that the system, in the long-term, does not depend on initial states.

Now we can answer the question ”Is it possible for the system to have an oscillatory behavior?” with ”yes”, as seen in previous sections, since the system has presented us with a oscillatory behaviour, for a certain set of parameters, which we have analytically showed that it does in fact happen.

References

1. Ault, S., Holmgreen, E.: Dynamics of the brusselator (2003)
2. Sayama, H.: Introduction to the Modeling and Analysis of Complex Systems. Open SUNY Textbooks, Milne Library (2015)