Analysis of Chaos in Willamowski-Rossler Chemical Reactions

Dynamical Systems Final Project

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1 Introduction

Rossler and Willamowski [1] found a chaotic behaviour in the rate equations of a series of chemical reactions:

$$A_1 + X \underset{k_{-1}}{\overset{k_1}{\longleftrightarrow}} 2X \tag{1}$$

$$X + Y \underset{k_{-2}}{\overset{k_2}{\longleftrightarrow}} 2Y \tag{2}$$

$$A_4 + Y \underset{k_{-3}}{\overset{k_3}{\longleftrightarrow}} A_2 \tag{3}$$

$$X + Z \underset{k_{-4}}{\overset{k_4}{\longleftrightarrow}} A_3 \tag{4}$$

$$A_5 + Z \underset{k_{-5}}{\overset{k_5}{\longleftrightarrow}} 2Z \tag{5}$$

Where X, Y, Z are some compounds with varying concentrations and the concentrations of $A_1, ..., A_5$ are remaind constant.
Reactions of the form of (1), (2), (5) are called autocatalytic reactions because there is the same compound in both the reactant side and the product side.
From chemical kinetics, we know that the rate of an elementary reaction $aA \xrightarrow{k} B$ is $\frac{d}{dt}[B] = k[A]^a$ (further discussion on chemical kinetics can be found on [2]).
Generalizing this, we can derive the rate equations for the varying compound concentrations x, y, z:

$$\begin{aligned} \dot{x} &= k_1 a_1 x - k_{-1} x^2 - k_2 xy + k_{-2} y^2 - k_4 xz \\ \dot{y} &= k_2 xy - k_{-2} y^2 - k_3 a_5 y + k_{-3} a_2 \\ \dot{z} &= k_5 a_4 z - k_{-5} z^2 - k_4 xz + k_{-4} a_3 \end{aligned} \tag{6}$$

In [1]'s discussion, Rossler and Willamowski noted that the system's chaotic behaviour is conserved when taking small k_{-2}, a_2, a_3. In [3] (which would soon be discussed extensively) Bodalea and Oacea followed their footsteps and set $k_{-2}, a_2, a_3 = 0$ during their whole analysis. While it might seem obvious that a_2, a_3 does not affect the system's dynamics, the affect of k_{-2} is not so clear, and would be the subject of the first analysis in this work.

Following with Bodalea and Oacea, they set those parameters to zero and combined the remaining constants in order to get:

$$\begin{aligned} \dot{x} &= k_1 x - k_{-1} x^2 - k_2 xy + k_{-2} y^2 - k_4 xz \\ \dot{y} &= k_2 xy - k_3 y - k_{-2} y^2 \\ \dot{z} &= -k_4 xz + k_5 z - k_{-5} z^2 \end{aligned} \tag{7}$$

These equations describe chaotic behaviour that eventually comprise a strange attractor. Numerically integrating these equations with the parameters in Table 1 yields the strange attractor in Figure 1.

k_1	30
k_2	1
k_3	10
k_4	1
k_6	16.5
k_{-2}	10^{-4}
k_{-5}	0.5

Table 1. *Parameter values*

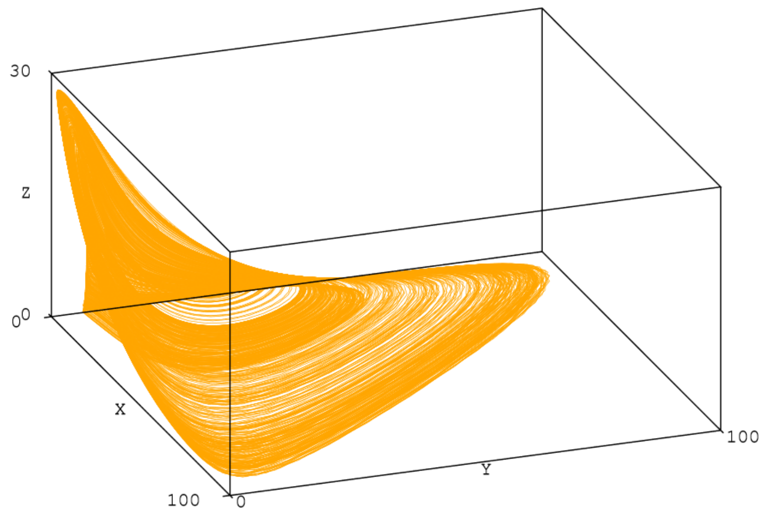

Figure 1. *The strange attractor for the parameters in table (1).*

The Minimal Willamowski Rossler (MWR) system that Bodalea and Oacea considered in [3] is equations (7) with $k_{-2} = 0$. Bodalea and Oacea showed that synchronized chaos can be achieved between two MWR systems. Not only that, they could accomplish it using only one control parameter. Following the method beautifully presented by Hu and Xu [4], we consider two MWR systems denoted by $\{x_1, x_2, x_3\}, \{y_1, y_2, y_3\}$. The x system would be called 'master' system and the y system is the 'slave' system that is imitating the master system. The synchronization would be through the addition of control parameters z_1, z_2, z_3 that would track the differences between x_i and y_i. The full mathematical model considered is:

$$\dot{\vec{x}} = \vec{f}(\vec{x}) := \begin{pmatrix} k_1 x_1 - k_{-1} x_1^2 - k_2 x_1 x_2 - k_4 x_1 x_3 \\ k_2 x_1 x_2 - k_3 x_2 \\ -k_4 x_1 x_3 + k_5 x_3 - k_{-5} x_3^2 \end{pmatrix} \tag{8}$$

$$\dot{y}_i = f_i(\vec{y}) - z_i \cdot (y_i - x_i), \quad i = 1, 2, 3 \tag{9}$$

$$\dot{z}_i = -c_i (y_i - x_i)^2 \tag{10}$$

With k_i, c_i constants. This model ensures that the slave MWR system $\vec{y}(t)$ would synchronize with the master system $\vec{x}(t)$. It would be analyzed in parts 2 and 3 of this work.

2 Analysis of k_{-2} affects

As mentioned above, k_{-2} has been 'ignored' in the [1] and [3], although it is quite important. It describes the rate of the reverse reaction (2), and it is the coefficient of the nonlinear term y^2 in the chaotic equations (7). Without it, we are diminishing the reverse reaction and therefore change the whole system. For brevity of notation, in this section I would write $k = k_{-2}$ and analyze equations (7) with the parameters described in table (1) (treating $k_{-2} = k$ as a variable).

Using numerical methods, I have found that for values of k greater in order than 10^{-2}, the system is not chaotic at all. In fact, there is a critical value above which the system is at a stable fixed point $k > k_1^c = 0.056$.
We can be convinced of k_1^c existence by looking at k's bifurcation diagram in Figure 2:

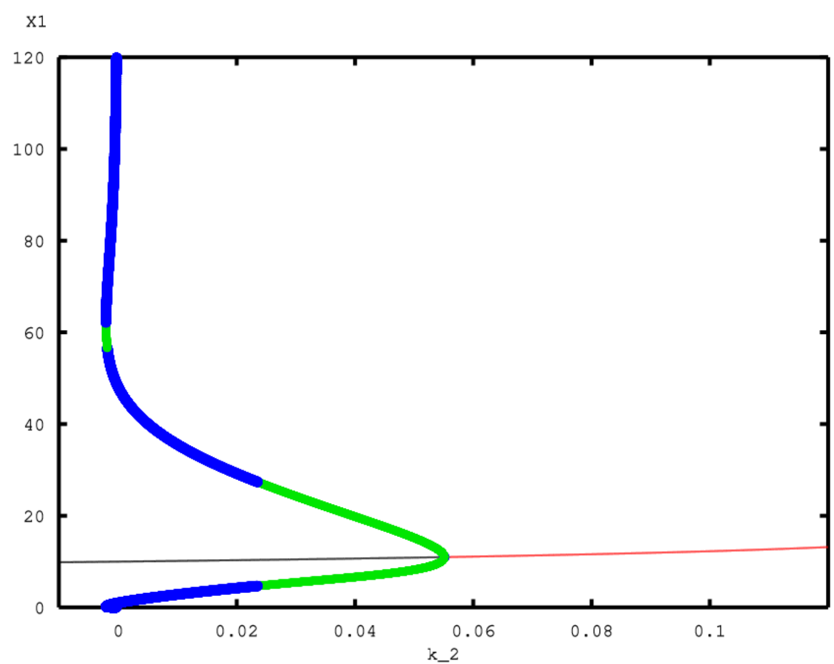

Figure 2. *Bifurcation diagram for k_{-2}. Red - stable point, Black - unstable point, Green - stable limit cycle, Blue - unstable limit cycle*

In the diagram we can clearly see a Hopf Bifurcation at a point $k = k_{-2} = k_1^c$. For $k > k_1^c$ the system is in a stable fixed point (red line). For $k < k_1^c$ the system is 'running away' from an unstable fixed point (black line) towards a limit cycle or strange attractor (green lines or blue lines). Note that the numerical program used to derive this has its limitations, so the transition between the blue and green lines is to be taken with a grain of salt and checked manually. In order to see the limit cycles, you are referred to supplementary video A in [5] (in which $k = 0.05$), or Figure 3.

As we decrease k below the first critical value, we find that the limit cycle slowly turns to the strange attractor that we see in Figure 1. We can see this effect demonstrated in Figure 3, where one stable limit cycle evolves and takes another shape. The limit cycle branched and changed its shape.

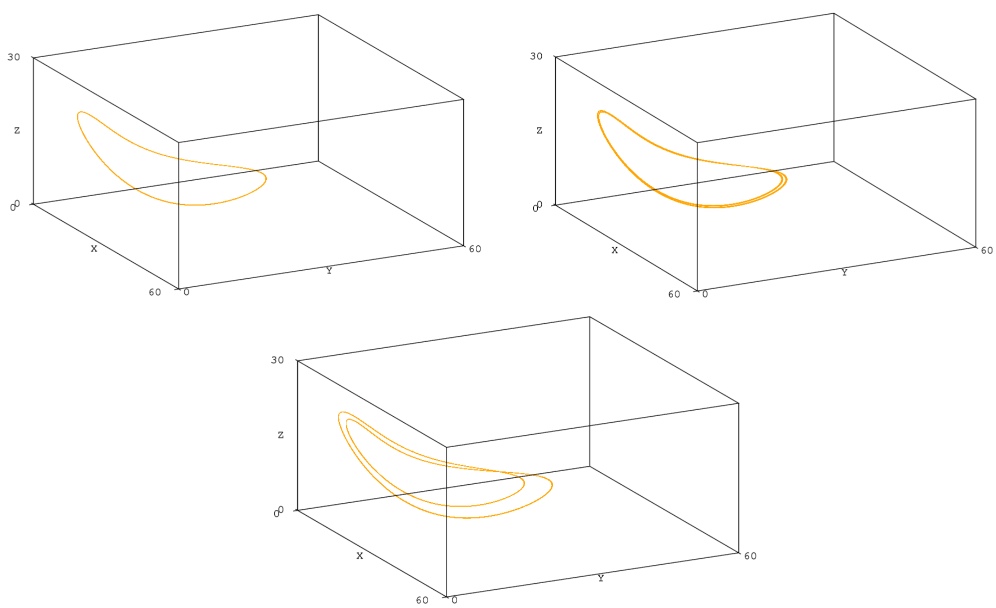

Figure 3. *Development of limit cycle to strange attractor as we decrease k. Upper left $k = 0.024$, upper right $k = 0.0235$, down $k = 0.023$. Notice the separation of the limit cycle in upper right.*

As we continue to decrease k, the limit cycle branch out and expand gradually until it becomes a strange attractor. The first form of the strange attractor is slightly different from the expected one (Figure 4 left), but around the point $k_2^c = 1.95 \times 10^{-3}$, the strange attractor finally changed into the known strange attractor of the Willamowski-Rossler system (Figure 4 right).

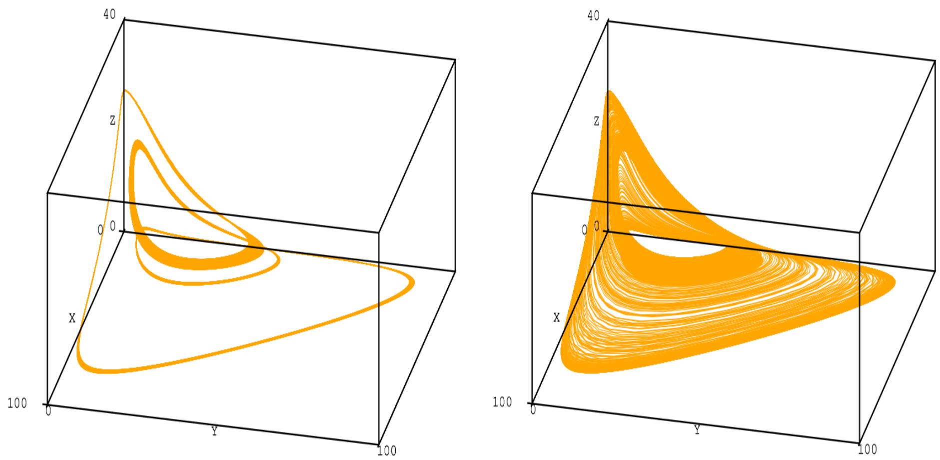

Figure 4. *Development of strange attractor as we decrease k. Right $k = 2 \times 10^{-3}$, Left $k = 1.95 \times 10^{-3}$*

Note that the change from limit cycle to strange attractor happened before $k = k_2^c$. I did not find the exact point of change due to the fact that the cut between evolved limit cycle into strange attractor is unclear. You can also see the strange attractor in Figure 4 left in supplementary video B in [5]. Also in [5] is the .ODE file that was used with XPPAUT to produce these simulations.

3 Synchronisation Transient Time

Coming back to Bodalea and Oacea in [3], we consider two MWR systems interacting according to the mathematical model described in the introduction with equations (8-10). Using this model, we can set the two chaotic systems with different initial conditions and after some integration steps (transient time) they reach into good synchronisation, meaning $y_i = x_i \pm O(\alpha)$ where α is some tolerance. Bodalea and Oacea showed that they could synchronize the two systems using only one control constant (one of the c_i's). I replicated those results and was interested in their remark in section 5, which directed the affect of c_i's on the time till synchronization. That would be the topic of this section - analysis of the transient time (integration steps required until sync) dependence on control strengths c_i's.

First let's look at the replicated results. Using equations (8-10), the parameters in table (1), the constants $c_i = 1$ and the initial conditions $\{x_i^0, y_i^0, z_i^0\} = \{1, 50, 0\} \quad i = 1, 2, 3$, we find:

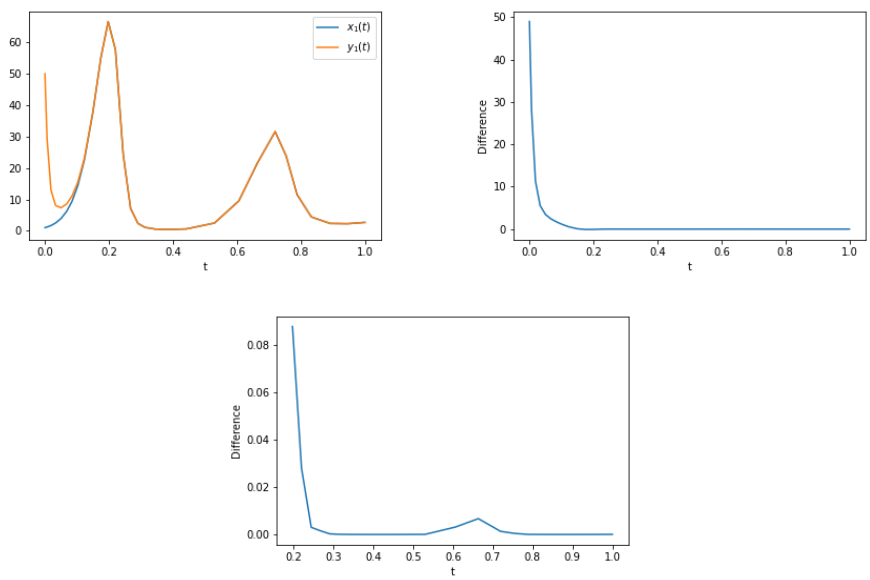

Figure 5. *x_1 compared to y_1 according to the description parameters in section 3. Left - x_1 and y_1, Right - difference $|y_1 - x_1|$, Bottom - zoom of rght.*

Notice in Figure 5 how little time it takes for the systems to catch up and sync - it happens after very few time steps. In the bottom part of the picture, we can see that the error (difference after synchronization) peaks at around $\alpha \approx 0.01$. Considering the fact that x_1 and y_1 range between 1 and 30, it is quite a small error.
If we'd set c_2, c_3 to zero we will also find synchronization, but it would take much longer to reach it. In Figure 6 we see just that:

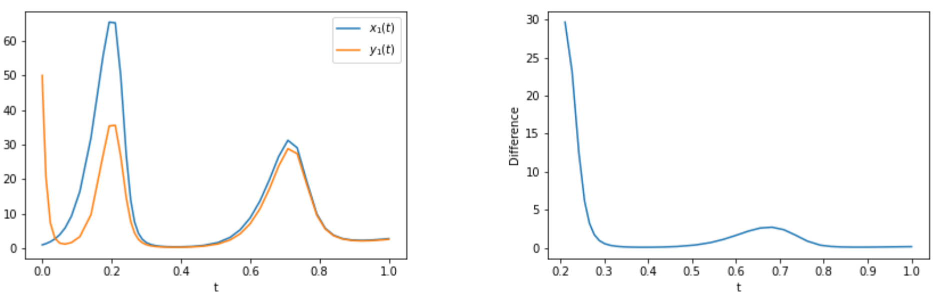

Figure 6. *x_1 compared to y_1 according to the description parameters in section 3 but with $c_1 = 1, c_2, c_3 = 0$. Left - x_1 and y_1, Right - difference $|y_1 - x_1|$ zoomed in.*

The transient here is about $T = 0.3s$, which is about three times the value of the one with $c_2, c_3 = 1$. Bodalea and Oacea noted in [3] that they could achieve the same effect with c_2 turned on instead of c_1 (considering their modified system), but I was not able to replicate that. Instead, I found that each pair of control constants could synchronize the system. So no matter which one of the c_i's is set to zero, the systems would sync. It is worth noting that the transient times of the pairs is about the same as the transient time of working only with c_1.

I wanted to find the smallest transient, so taking $c_2, c_3 = 0$, I computed the transient of the system for different values of c_1 (using a python script that can be found in the supplementary material [5]). In Figure 7 we can see that the minimum is in the range of $c_1 = 3$. It means that if we want the systems to synchronize as fast as possible, while controlling the least amount of variables, we should choose $c_1 = 3$.

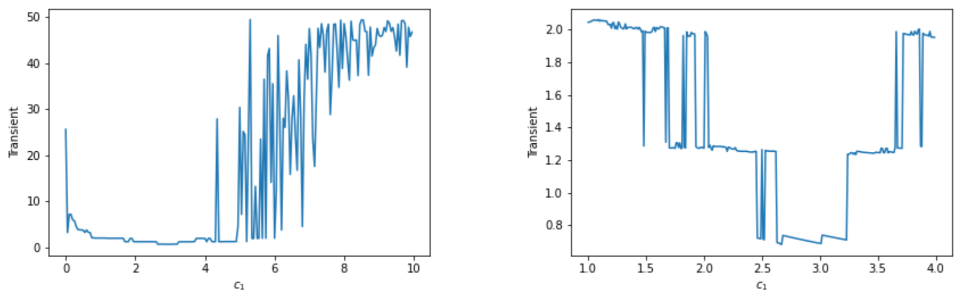

Figure 7. *Transient of system (time until sync) for different values of c_1. Left - low resolution, Right - zoomed in with finer resolution.*

Note in Figure 7 that the saturation at 50 or 2.0 is a product of the numericall simulation I ran and has no physical meaning.
Finally, I went ahead and tested the same effect - transient as a function of control constants, only now for the case of $c_1 = c_2 = c_3$. Surprisingly, it seems that the transient is monotonically decreasing and reaching zero, as we can see in Figure 8. Although setting the control constants this high does not seem practically plausible, it is interesting to see that the mathematical model does converge towards zero. At least in theory, it seems that we can get the system to synchronize after every small length of time ϵ to our choosing.

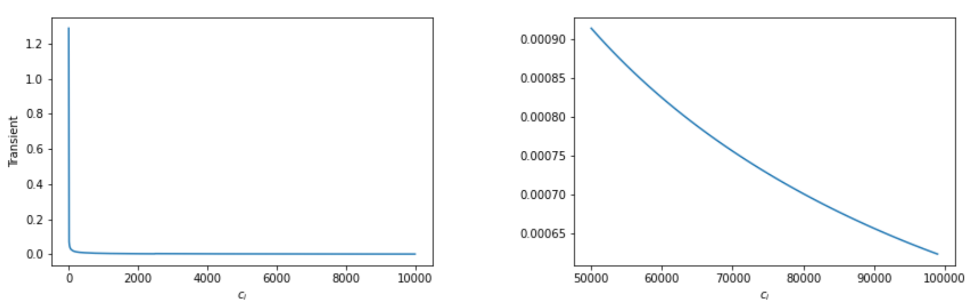

Figure 8. *Transient of system (time until sync) for different values of $c_1 = c_2 = c_3$. Left - low resolution, Right - zoomed in with finer resolution.*

4 Initial Conditions Affect on Control Values

The general method of synchronization using the control parameters z_i's that is partially presented in [4] and followed by Bodalea and Oacea in [3], generates seemingly arbitrary final values for z_i. Because $\dot{z}_i \propto (y_i - x_i)^2$, then as the two systems sync, $\dot{z}_i \to 0$ and we'd always get that z_i converged towards some constant. So in this section I will consider the dependence of the initial conditions on the final values of z and hopefully would find a reasonable connection.

The system is equations (8-10), the parameters in table (1), the constants $c_1 = 1, c_2, c_3 = 0$ and the initial values $\{x_i^0, y_i^0, z_i^0\} = \{1, 1, 0\}$, except x_1^0, y_1^0 which would be a variables. Since $c_2, c_3 = 0$ than $z_2(t), z_3(t) = 0$ for every t, it would make the analysis easier.
The first thing I found is that when we keep the difference $y_1^0 - x_1^0$ constant, the final values of z_1 would depend on the size of x_1^0, y_1^0. If the difference is small compared to the sizes, meaning $|y_1^0 - x_1^0| \ll x_1^0, y_1^0$, than the final values of z_1 would be close to zero. This makes sense because z_1 seems to play the role of the 'correction' between the different systems. Also, its derivative $\dot{z}_1$ is determined by the difference, so if the difference is small compared to the actual values, the amount of 'correction' needed is small, therefore z_1 is small. This could be seen in Figure 9:

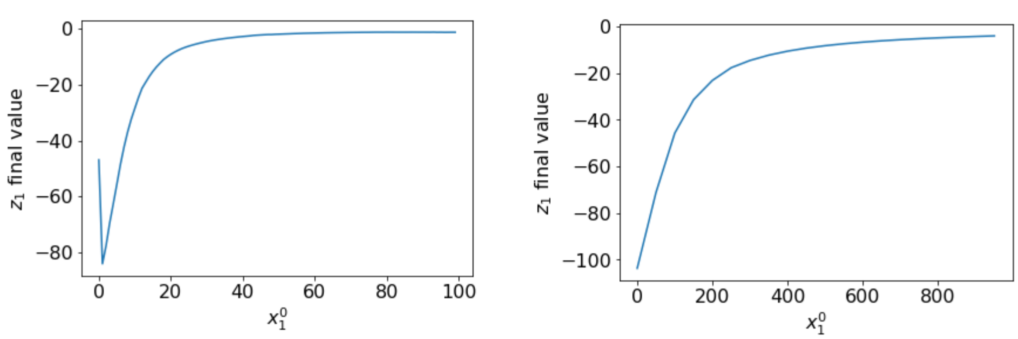

Figure 9. *Initial condition values x_1^0 vs z_1 final values with a constant difference in initial conditions $e = |y_1^0 - x_1^0| = const.$ Left - $e = 5$, Right - $e = 50$.*

Now we let go of the constraint $|y_1^0 - x_1^0| = const$ and change x_1^0 while keeping $y_1^0 = 1$ so the difference would grow up. We find that z_1 final values decrease proportionally with x_1^0, as we can see in Figure 10:

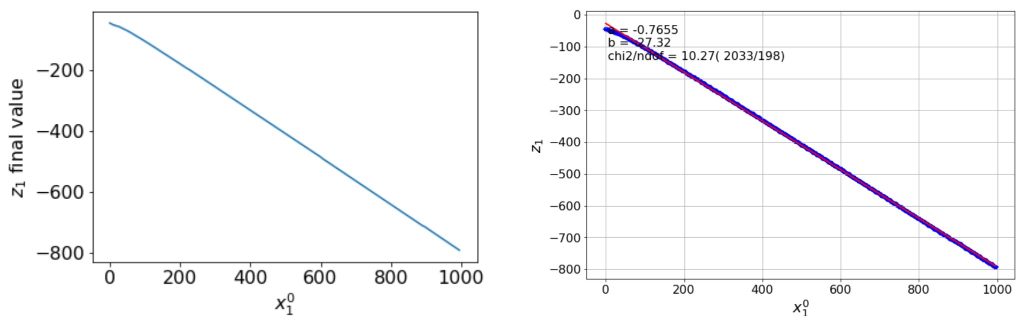

Figure 10. *Initial condition values x_1^0 vs z_1 final values. Left - plain, Right - numerical fit (blue is data, red is fit).*

Surprisingly, the values of z_1 are linear with respect to x_1^0. We found $z_1 \approx -0.77x_1^0 - 27$. Interestingly I found that we get the same linear dependence even for large c_1's (more on that in the discussion). Moreover, I had run the same analysis for negative values of x_1^0 and found that their dependence is a bit different, we can see that in Figure 11:

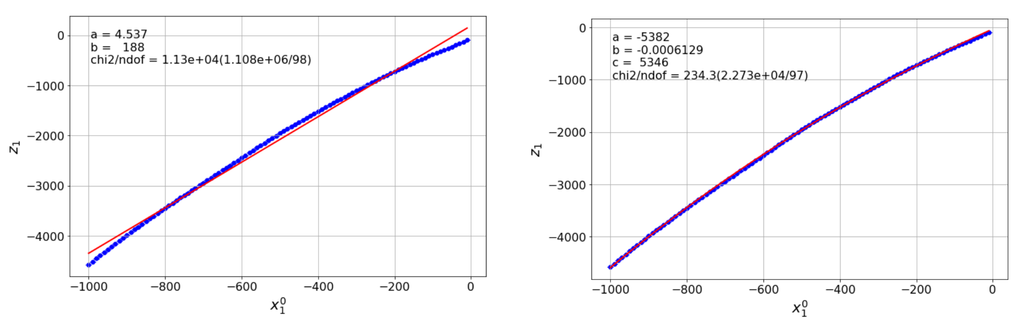

Figure 11. *Initial condition values x_1^0 vs z_1 final for negative IC. Left - linear fit, Right - exponent fit. Data in Blue and fit in Red.*

I fitted the data for both a linear function and an exponential function and found - based on χ^2_{red} - that the exponential fit is much better (although it is still not great). The exponential fit is: $z_1 = a \cdot e^{b \cdot x_1^0} + c$. Also we can see that the values of z_1 at $x_1^0 = \pm 1000$ are vastly different. We can conclude - at the very least - that the system is not symmetrical in x_1^0.

5 Summary and Discussion

During this work I had delved into the Willamowski-Rossler system and numerically investigated its chaos and strange attractor. I followed Bodalea and Oancea [3] and had seen for myself the fast synchronization that happens between the systems.

In section 2, I had used the program XPPAUT to analyze the affects of k_{-2} on the regular WR system. I was surprised to find out that this parameter that was completely neglected in [3] had a big impact on the system. Using XPPAUT's graphical interface I could see the limit cycle evolve into a strange attractor. The graphical interface helped me study the system and provided better understanding of it.

In section 3, I started working with XPPAUT but quickly discovered that I need more computational freedom in order to investigate what caught my eye. Using a small python script that could be found in [5] I managed to create two systems and synchronize them in accordance with [3]. I was surprised to see how fast the systems synchronized, so I wanted to analyze it. I was pleased to find out that the results confirmed my intuition - that there is a c_1 'sweet spot' for which the synchronization was the fastest.

In section 4, I was interested in the behaviour of the final values of z_i's. My explanation for the linearity that was found between z_1 and x_1^0 was that because $\dot{z_1}$ was directly related to the difference $|y-x|$, within few a iterations it will take a value related to the difference, so it is only dependent on the difference. So the linearity was caused by fast synchronization. But I found that we get the same linear dependence even for large c_1's, and from section 3 we know that for large c_1 there is a large transient - so the hypothesis fails and I remained without a satisfying explanation.

In order to learn the mathematical method of chaos synchronization, I followed Bodalea and Oancea citation and studied the first sections of [4] by Hu and Xu, which was beautifully written. This method provided me with great intuition on the topic, and it was a good extension to the material studied in the course. The only thing I had wished were more apparent in this work and in [3] is the physical (or chemical) conclusions of the analysis.

6 Bibliography

[1] Willamowski KD, Rossler OE. *Irregular oscillations in a realistic abstract quadratic mass action system.* Z Naturforsch 1980

[2] Steinfeld J.I., Francisco J.S. and Hase W.L. *Chemical Kinetics and Dynamics* 2nd ed., 1999.

[3] I.Bodalea, V.A.Oancea, *Chaos control for Willamowski–Rössler model of chemical reactions*, Chaos, Solitons and Fractals, 2015.

[4] Hu M, Xu Z. *Adaptive feedback controller for projective synchronization*, Nonlinear Anal: Real World Appl 2008.

[5] Supplementary material - click here. By Nadav Porat.