Deterministic Modeling - Project 2 (Biology)

Marta Gacek

January 2024

1 Introduction

The aim of this project is making use of mathematics in biology. Precisely - modeling the process of originating the pattern on animal's skin. We will use the Gierer - Meinhardt system of equations, so called "reaction-diffusion model".

In order to carry out the experiment, we will start with drawing the scheme of the animal which is going to be the object of study. I have chosen a bear. In the picture below there are some parameters describing the exact location of each body part.

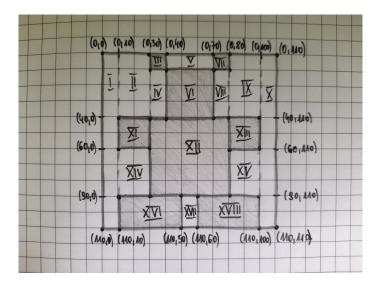


Figure 1: The diagram of the bear

2 Creating an animal

The next step is writing a class in Python, which will "create" an animal. We can use it to see the scheme of the bear - it will be useful later, during the calculations. The class is stored in the file called *class_bear.py*.

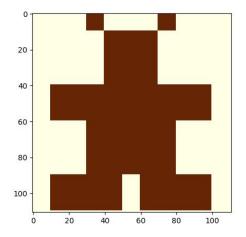


Figure 2: The bear

3 The mathematical part

First of all we will analyse the equations of Gierer - Meinhardt model. There are many modifications of this system of equations. The model which we are going to use is one of them. It is shown below:

$$u_{t} = D_{u}\Delta u - C_{1}u + \frac{C_{2}u^{2}}{v} + C_{3}$$
$$v_{t} = D_{v}\Delta v + C_{4}u^{2} - C_{5}v$$

The model is related to the process of diffusion. The pattern on the skin is the result of two substances diffusing with different rates.

The variable u describes the activator (short-range autocatalytic substance) and the variable v means a long-range inhibitor, which is an antagonist to the activator. The activator regulates the production of the inhibitor. The derivative u_t characters a change of activator concentration in some unit of time and similarly v_t shows a change of inhibitor.

The number of molecules that decay in some time unit is proportional to the decay rate C_1 and to the number of present molecules (u). The $\frac{C_2u^2}{v}$ part describes the production rate, depending in a non-linear way on the activator concentration and is slowed down by the inhibitor. The D_uu_{xx} term enables the exchange of molecules. The C_3 parameter is a small activator-independent production rate of the activator. Its task is initiating the activator autocatalysis at very low activator concentration, for example when the organism needs to regenerate. The parameters of the second equation can be analogously determined in case of the inhibitor change.

We assume that there are no special changes of the pigment on the "edges" - that is on the fragments connecting body parts together. It means that every part of the body is individual; for example the pigment on the head doesn't "mix" with the pigment on the belly. We can treat the edges as blockades separating the body parts and their amounts of the pigment.

As an unit we will be using $\frac{kg}{m^2}$. Therefore u_t and v_t are measured by $\frac{kg/m^2}{s}$. We need to write a numerical scheme which will be used to solve the system of equations. First of all we notice that:

$$\begin{split} \Delta u(x,y,t) &\approx \frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2} \approx \\ &\approx \frac{u(x+h_x,y,t) - 2u(x,y,t) + u(x-h_x,y,t)}{h_x^2} + \\ &\quad + \frac{u(x,y+h_y,t) - 2u(x,y,t) + u(x,y-h_y,t)}{h_y^2} \end{split}$$

We assume that $h_x = h_y$, so:

$$\Delta u(x,y,t) \approx \frac{1}{h_x^2} \Big(u(x+h_x,y,t) + u(x-h_x,y,t) + u(x,y-h_x,t) + u(x,y+h_x,t) - 4u(x,y,t) \Big)$$

Similarly:

$$\Delta v(x,y,t) \approx \frac{1}{h_x^2} \Big(v(x+h_x,y,t) + v(x-h_x,y,t) + v(x,y-h_x,t) + v(x,y+h_x,t) - 4v(x,y,t) \Big)$$

Now we can rewrite the first equation using the definition of the derivative.

$$u_t = \lim_{h_t \to 0} \frac{u(x, y, t + h_t) - u(x, y, t)}{h_t}$$

$$\frac{u(x,y,t+h_t) - u(x,y,t)}{h_t} = \frac{D_u}{h_x^2} \left(u(x+h_x,y,t) + u(x-h_x,y,t) + u(x,y-h_x,t) + u(x,y+h_x,t) - 4u(x,y,t) \right) - C_1 u(x,y,t) + \frac{C_2 u(x,y,t)^2}{v(x,y,t)} + C_3$$

Differently:

$$\frac{u_{i,j,k+1} - u_{i,j,k}}{h_t} = \frac{D_u}{h_x^2} \left(u_{i+1,j,k} + u_{i-1,j,k} + u_{i,j-1,k} + u_{i,j+1,k} - 4u_{i,j,k} \right) - C_1 u_{i,j,k} + \frac{C_2 u_{i,j,k}^2}{v_{i,j,k}} + C_3 u_{i,j,k}^2 + C$$

After some modifications:

$$u_{i,j,k+1} = h_t \left(\frac{D_u}{h_x^2} \left(u_{i+1,j,k} + u_{i-1,j,k} + u_{i,j-1,k} + u_{i,j+1,k} - 4u_{i,j,k} \right) - C_1 u_{i,j,k} + \frac{C_2 u_{i,j,k}^2}{v_{i,j,k}} + C_3 \right) + u_{i,j,k} + C_3 u_{i,$$

Similarly we can get the second equation:

$$\frac{v(x,y,t+h_t) - v(x,y,t)}{h_t} = \frac{D_v}{h_x^2} \Big(v(x+h_x,y,t) + v(x-h_x,y,t) + v(x,y-h_x,t) + v(x,y+h_x,t) - 4v(x,y,t) \Big) + C_4 u(x,y,t)^2 - C_5 v(x,y,t)$$

$$\frac{v_{i,j,k+1} - v_{i,j,k}}{h_t} = \frac{D_v}{h_x^2} \left(v_{i+1,j,k} + v_{i-1,j,k} + v_{i,j-1,k} + v_{i,j+1,k} - 4v_{i,j,k} \right) + C_4 u_{i,j,k}^2 - C_5 v_{i,j,k} + C_4 u_{i,j,k}^2 - C_5 v_{i,j,k} + C_5 v_{i,j,k}$$

$$v_{i,j,k+1} = h_t \Big(\frac{D_v}{h_x^2} \Big(v_{i+1,j,k} + v_{i-1,j,k} + v_{i,j-1,k} + v_{i,j+1,k} - 4v_{i,j,k} \Big) + C_4 u_{i,j,k}^2 - C_5 v_{i,j,k} \Big) + v_{i,j,k} + v_{i,j,k} + v_{i,j+1,k} - 4v_{i,j,k} + v_{i,j+1,k} - 4v_{i,j,k} \Big) + C_4 u_{i,j,k}^2 - C_5 v_{i,j,k} \Big) + v_{i,j,k} + v_{i,j+1,k} - 4v_{i,j+1,k} - 4v_{i,j,k} \Big) + v_{i,j,k} + v_{i,j+1,k} - 4v_{i,j+1,k} - 4$$

The above equations for u and v work almost for every case, but there are some exceptions (the edges of matrices), therefore we have to add some conditions.

$$u_{i,j,0} = u_0(x,y)$$

$$v_{i,j,0} = v_0(x,y)$$

$$u_{0,j,k+1} = u_{1,j,k+1} + h_x g(t_{k+1})$$

$$u_{-1,j,k+1} = u_{-2,j,k+1} + h_x g(t_{k+1})$$

$$u_{i,0,k+1} = u_{i,1,k+1} + h_x g(t_{k+1})$$

$$u_{i,-1,k+1} = u_{i,-2,k+1} + h_x g(t_{k+1})$$

$$v_{0,j,k+1} = v_{1,j,k+1} + h_x g(t_{k+1})$$

$$v_{-1,j,k+1} = v_{-2,j,k+1} + h_x g(t_{k+1})$$

$$v_{i,0,k+1} = v_{i,1,k+1} + h_x g(t_{k+1})$$

$$v_{i,-1,k+1} = v_{i,-2,k+1} + h_x g(t_{k+1})$$

4 Measuring of the diversity

We will measure the diversity of patterns using variance, which informs about the size of differences in a set of observations. Therefore it is a good tool to compare the results and how they change in time. In order to do this we will try different values of parameters and examine their impact on final results.

At first I chose values $h_t = 0.1$, $D_u = 0.4$, $D_v = 0.6$, $h_x = 1$, $C_1 = 0.5$, $C_2 = 0.7$, $C_3 = 0.4$, $C_4 = 0.6$, $C_5 = 0.3$, to check the behaviour of the solutions. At first the diagram looks like below:

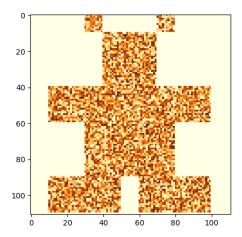


Figure 3: The bear at the beginning

It is a gathering of arbitrary points in various shades of brown, orange and yellow. We will see that after using the numerical method the pattern will become more consistent and organized.

The two pictures on the next page show the solutions after some time. The bear is brown, but it has some light patterns. They often align in a shape of circles. Each time we run the code, the bear is slightly different. Sometimes it even turns out to be orange or yellow - the intensity of the color is different each time, despite having the same parameters. Therefore we have an explanation why animals of the same species can look differently.

We can see that as the time passes, the solutions start to be more and more intentional. They form the light pattern on the fur. The pattern is similar in both cases - for u and v solutions. We can also see a small prove of the adversarial work of the inhibitor and activator - on the leg there is one bigger contrasting part. In places where the pigment for v is greater, the color for u is weaker and vice versa. It happens every time we draw the solution - always in different places on the body of course. For bigger lags of time the fur is darker and leads up to be plain.

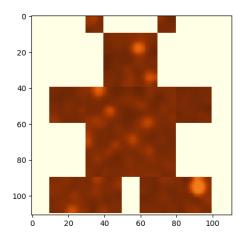


Figure 4: The bear after some time - solution for \boldsymbol{u}

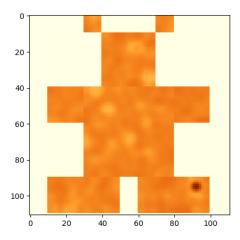


Figure 5: The bear after some time - solution for \boldsymbol{v}

In the *Variance* file we compute the variance of the solutions, to measure their diversity. We do it for "C" parameters and both D_u and D_v values. The algorythm computes the variance for different sizes of each parameter and draws the plot of it. The rest of the parameters remain the same - 0.5 - in order to avoid inaccurate results.

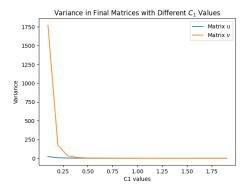


Figure 6: Variance for different C_1

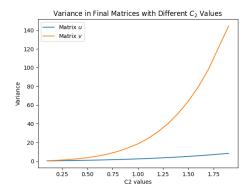


Figure 7: Variance for different C_2

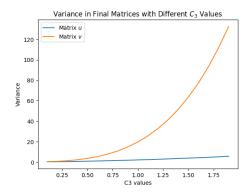


Figure 8: Variance for different C_3

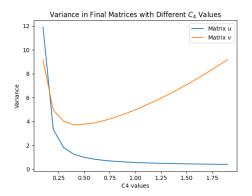


Figure 9: Variance for different C_4

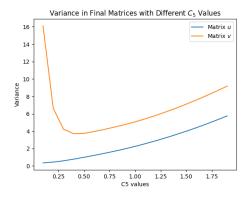


Figure 10: Variance for different C_5

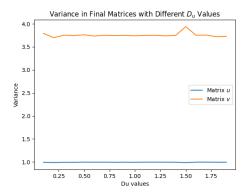


Figure 11: Variance for different D_u

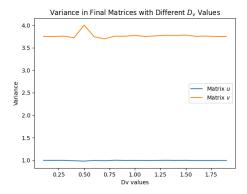


Figure 12: Variance for different D_v

We see that in case of parameters C_2 and C_3 the variance of inhibitor strongly increases, while for the activator it remains at the same (or slightly higher) level. It is logical, because those parameters are related to the production rate of the substances. When the values are higher, the rate is bigger and the diversity increases.

An opposite situation is shown on the first plot, presenting the variance for different values of C_1 . This parameter represents the decay rate, what explains the decreasing level of variance for the inhibitor solutions. The variance of the activator remains on the same level.

The fourth and fifth pictures look similarly. The line connected to v results is decreasing at first, but then it begins to rise. The difference is in the behaviour of the variance for the activator - in case of C_4 it goes down and in case of C_5 it increases. The explanation can be the fact, that the C_5 parameter describes the rate of first-order degradation of the inhibitor. Because it doesn't increase as strongly as in previous pictures, it is a chance of growth for the activator, which works as an antagonist. Therefore the diversity increases.

The situation of variance in case of different values of D_u and D_v is very similar. The variance remains on the same level with small deviations, but the level for the inhibitor is a few times higher. It seems that the size of both diffusion coefficients' values don't have a big impact on the diversity.

All in all, the values of parameters are important - some have bigger, some have smaller impact on the solutions of the model. However they all decide about the appearance of the animal.