Chapter 237

Discrete mathematical modeling of biological phenomena: Case of drug concentration in the organism

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ABSTRACT
At first, mathematical modeling is a tool used to understand the occurrence of phenomena, and through the existence of a pattern in the recurrences, it is possible to formulate a recurrence expression where the phenomenon is modeled in such a way, understanding its behavior and predicting certain situations. In the study of biological phenomena, there is a need to understand a certain action in such a way, thus, to understand the process is given by Mathematical Modeling applying the equations of differences, in this way resulting in linear or non-linear functions, because of this modeling with N applications in the biological field, the study of the research project at UFDPar will be discussed as an example.

Keywords: Modeling, Phenomenon, Mathematics, Recurrence.

1 INTRODUCTION

The research project on Biomathematics at UFDPar studied the application of the equations of differences for the study of biological phenomena. Modeling is the closest form to the true essence of mathematics because it is based on creating a model to exemplify real-world situations, and along with computer modeling it is possible to represent, through equations, graphs, and other ways of demonstrating factors that occur, in the recurrence relationship model, always revolves around a certain regular pattern that is present in n repetitions, where it is observed that in fact, the resulting data have a pattern in

familiarity, so they are means of better understanding the phenomena that are happening in reality, such as the variation of the concentration of a drug "x" in the organism of a person over time, possessing an initial value and a final value, resulting in a system of linear and nonlinear equations, which are ways to understand the path that information is taking. The theme for the realization of the modeling, was based on the application of the equations of differences for the study of a problem found in the material "APPLICATIONS IN BIOLOGICAL PROCESSES USING MATHEMATICAL AND COMPUTATIONAL MODELING" (NASCIMENTO; SANTOS; NASCIMENTO, 2020), on the variation of the concentration of a drug in the body of a person, in such a way that there is a sum of the amount of medication inserted in each application, with a loss in each cycle due to natural factors of the body, having a search for the best method of analysis.

Through studies and algebraic artifices to formulate a recurrence expression for the phenomenon, in such a way that one could make a progression in the Python programming environment.

2 DEVELOPMENT

Given the research means, it is clear that the methodology applied to the study of the project was made through didactic material "Differential Equations with Applications" (BASSANEZI, FERREIRA JR, 1988), and for the formulations of the models "Mathematical models in Biology" (EDELSTEIN-KESHET, 2005), these articles of equations of differences were of great importance for research, the classes on the formulation of graphs in the Python programming language, to better understand the issue of nonlinear functions, to make the progression of the points of the image before the points of the domain informed, because there is a question of understanding the mathematical functions within the computer language, such as sum, method of least squares, are specific methods of each syntax, before the teacher left the student researcher with a programming language that had knowledge, thus being able to explore new ideas, with more applications, occurring periodic meetings, to talk and address how the subject of the research was, being the theme of the study of modeling, on the variation of the concentration of a drug in the body of a person, in such a way that occurs a sum of the amount of medication inserted in each application, having a loss at home cycle due to natural factors of the body, in collecting the data, choosing a better method of analysis. A phenomenon that was addressed by the article, equations of Differences was the use of a drug, where the patient will receive n applications of the same, which has an initial amount $Q0$ and will be the same amount applied in each cycle, but at a rate of elimination of the body denoted of r, the question is the amount of this drug that will be present in the individual's body at the end of these applications denoted Qn, by the placement of the variables, if you have an initial model of this recurrence:

$$Q_{n+1} = (1 - r)Q_n + Q_0$$

After a calculation made by induction and putting the factor in evidence through remarkable products, one finds the equation of recurrence of the system:$\frac{Q0}{r}$

$$Q_n = \left(1 - \frac{1}{r}\right)(1 - r)^n Q_0 + \frac{Q_0}{r}$$

Assuming that Q *0* is the amount of drug that will be applied in each cycle, and *Q* n is the amount of drug present in the body at the time of that application, the *r* will be the rate of natural elimination made by the body, and n the cycle which is present the application.

The representation of the number of drugs in the individual's body after n applications, making one more observation the rate of elimination r, can not be 0 and 1, because then the substance would be eliminated in 0 % or *100%,* so we will calculate the limit of this equation for *n* tending to infinity, and *0 < r < 1*.

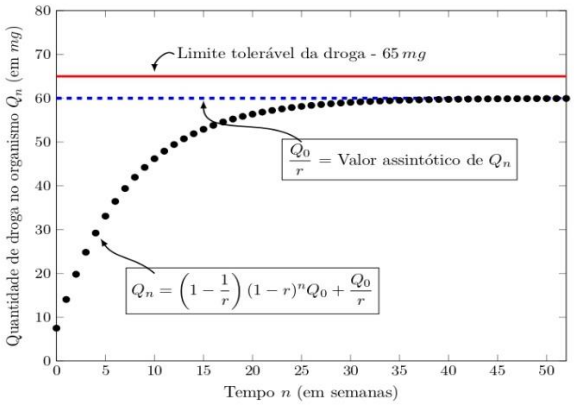
$$\lim_{n \to +\infty} Q_n = \lim_{n \to +\infty} \left[(1 - \tfrac{1}{r})(1 - r)^n Q_0 + \tfrac{Q_0}{r}\right] = \tfrac{Q_0}{r}$$

Therefore, Q n converges on, the asymptotic value of $Q\frac{Q_0}{r}n$. It is soon deduced that the amount of drug tends to stabilize in the body over time, thus opening new questions, how does the variation of the amount of drug behave over time? We have to converge, the amount of drug is directly linked to the number of applications, so in one case which was given by the article on applications in biological processes.

To exemplify our modeling, let's consider that a patient of the State General Hospital (HGE) is placed on medication that in turn is taken once a week and will have *52* applications. The dose applied to the patient is *7.5 mg*. Also, consider that each week your metabolism burns *12.5%* of the drug in your body. If the level of medicine in the body reaches *65 mg* the consequences are very serious. Is it safe for the patient to take this medication indefinitely?

Given the following data: *r = 0.125, n = 52* and *Q0 = 7.5*. The graph formed in the jupyter, is based on the graph found in the article Equations of differences and systems with biological applications (NASCIMENTO; SAINTS; BIRTH, 2020). As can be seen that in fact, it converges in 60 mg, with 52 weeks of application, and the value was $\frac{Q0}{r}$ very close to 60, but did not exceed, the value was approximately *59.94935 mg* (Graph 1).

Graph 1 \u2012 Trajectory of the concentration of medication "x" with the variation of applications.



Source: Own authorship.

3 FINAL CONSIDERATIONS

The data obtained were satisfactory and the objectives set out in the project menu were achieved, thus obtaining success. Some problems found as the question of the equation of recurrence as well as the study of the function of the trajectory of the concentration of the drug in the body, in view of all the predicted modeling, and having in vista a point of convergence**, the** study was made by the property in having a regular factor, which is in the relationship between the constant amount that is being injected and the amount after the cycle, **in the case** Q **n** as a function **of Q** 0 **, in** this case of the expression of recurrence of the issue of drug accumulation in the body, where a progression of how the accumulation would occur over time was created, with losses **s** and gainss in value in the variable $Q\ n$, in the study of biological phenomena if it has that often the result can arrive in a linear or nonlinear function, through computer modeling it is possible to design a graph **of the** functions**, and** make a search for the values of an expression through the method of least squares, the Python language coupled with many libraries were of extreme importance in understanding the behavior of the function and seek the means of development lver the expression of recurrence, which makes it possible to understand the path that the next data will take, being possible to make a progression.

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