EXPLORATIONS OF MATHEMATICAL MODELS IN BIOLOGY WITH MAPLE™

Mazen Shahin

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MAZEN SHAHIN
Department of Mathematical Sciences
Delaware State University
Dover, DE, USA

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EXPLORATIONS OF MATHEMATICAL MODELS IN BIOLOGY WITH MAPLE™

PREFACE

MAIN GOALS

The main goal of *Explorations of Mathematical Models in Biology with Maple*™ is to offer students a textbook to help them explore and discover mathematical concepts and utilize these concepts in building and analyzing mathematical models of life science disciplines such as biology, ecology, and environmental sciences. The main mathematical tools utilized in this text are difference equations and matrices. The use of the mathematics software Maple is an integral part of exploring and analyzing the models. It is important to stress that this text is neither a text on difference equations nor a text on how to use Maple.

THE NEED FOR A TEXTBOOK IN ELEMENTARY MATHEMATICAL MODELING AND MATRIX ALGEBRA

The Mathematical Association of America (MAA) published *Math & Bio 2010: Linking Undergraduate Disciplines* in 2005. *Math & Bio 2010* envisions a new educational paradigm in which the disciplines of mathematics and biology, currently quite separate, will be productively linked in the undergraduate science programs of the twenty-first century. As a science, biology depends increasingly on data, algorithms, and models; in virtually every respect, it is becoming more quantitative, more computational, and more mathematical.

One of the recommendations of the Curriculum Renewal Across the First Two Years (CRAFTY) of the MAA published in 2004 was the inclusion of mathematical modeling, discrete mathematics, and matrix algebra in the mathematics curriculum for biology majors.

Following recommendations of these professional organizations, we believe that there is a need for a course in elementary mathematical modeling and matrix algebra for biology and life science majors. Traditionally, mathematical models utilize differential equations. A differential equations course is usually offered after calculus I and calculus II. Consequently, there is a great need to offer a course in mathematical modeling that utilizes difference equations rather than differential equations. Difference equations and matrix algebra are simple, yet powerful, tools in modeling discrete time dynamical systems. These tools are accessible to students with high school algebra II or college algebra and do not require calculus and differential equations.

Since one of the main objectives in writing this book is providing students with a self-contained textbook, we included the background materials necessary to understand the main topics in the text. For example, we presented necessary materials from linear algebra.

APPROACH

In this text, we introduce the modeling of real-life situations with difference equations and matrices using Maple. We emphasize the use of graphical and numerical techniques, rather than theoretical techniques, to investigate and analyze the behavior of solutions of the mathematical models. We also investigate interesting linear and nonlinear models from diverse life science disciplines such as biology, ecology, and environmental sciences.

We utilize a discovery pedagogical approach. To introduce a concept, first we investigate a model numerically and/or graphically and recognize a pattern or certain properties that characterize that concept. Then we give a definition of the concept with examples and applications. For example, to introduce the eigenvalues and corresponding eigenvectors of a square matrix, we investigate an age-structure population model with different initial population vectors that lead to a visualization of an eigenvalue and corresponding eigenvectors. Then the definition of the eigenvalues and eigenvectors is introduced and some properties are discussed.

WHY MODELING WITH DIFFERENCE EQUATIONS AND MATRICES?

Difference equations represent a very sophisticated and powerful mathematical tool to model a wide range of real-life discrete time situations in diverse areas, including the life sciences. And matrices provide an excellent tool in modeling linear problems. Moreover, these powerful tools do not require a sophisticated mathematics background, being accessible to anyone who has successfully completed high school algebra or college algebra.

WHY DO WE USE MAPLE?

All the models presented in the text require the use of computers. For example, in order to investigate and analyze a model, it is often required to iterate the difference equation(s) or the matrix difference equation(s) that represent the model and graph it. Sometimes, it is required to find the eigenvalues and the corresponding eigenvectors in order to investigate the long-term behavior of a dynamical system. In other instances, in order to investigate the sensitivity of a dynamical system to certain parameters, it is required to change the parameters of the dynamical system and find the corresponding numerical solutions. All these computational activities require a software that is easy to learn and to use. In this text, we utilize Maple, which is a very user-friendly and powerful mathematics software with excellent graphing capabilities. The use of Maple frees students from tedious calculations, thus allowing them to focus on translating a problem into mathematical notation, finding a solution, interpreting the numerical and the graphical information provided, and then making conjectures and writing about their findings and observations. With the use of Maple, the students focus on building and analyzing the models.

ORGANIZATION

The materials in the text follow a logical order.

Chapter 1 introduces the mathematical modeling process, basic difference equations terminology, and getting started with Maple.

Chapter 2 introduces modeling with linear and nonlinear first-order difference equations. Sections 2.1 and 2.2 focus on models with linear difference equations such as population dynamics of a single species, the concentration of a drug in blood stream, radioactive decay and carbon dating, and forensic applications of Newton's law of cooling. Section 2.3 introduces modeling with nonlinear difference equations where logistic growth models with and without harvesting are investigated. Section 2.4 is an intuitive introduction to chaos.

Chapter 3 introduces the basic concepts of matrix algebra. Section 3.1 introduces the systems of linear equations having unique solutions with models on nutrition. In Section 3.2, we discuss the Gauss–Jordan elimination methods with models such as allocation of resources, balancing chemical equations, and determining the death time of a murdered person. In Section 3.3, we introduce the standard matrix notation and the basic matrix operations, such as addition, subtraction, scalar multiplication, multiplication, and the inverse of a square matrix. Section 3.4 is a simple introduction to the main concepts of determinants and their role in finding the inverse of a matrix and in determining whether a system of linear equation has a unique solution, many solutions, or no solution. In Section 3.5, we intuitively introduce the concept of eigenvalues and eigenvectors, and then investigate the methods to determine the eigenvalues of a square matrix and the associated eigenvectors. In Section 3.6, we investigate the use of eigenvalues to determine the long-term behavior of a system of linear equations.

Chapter 4 concentrates on modeling with systems of linear difference equations. In Section 4.1, we discuss a special class of finite stochastic processes and modeling with Markov chains. Section 4.2 provides investigations of Leslie's age-structured population models. In Section 4.3, we investigate modeling real-life situations with second-order linear difference equations, such as seal population dynamics and a plant population model. The eigenvalues and eigenvectors are efficiently utilized as a tool to study the long-term behavior of the models discussed in Chapter 4.

Chapter 5 introduces modeling with nonlinear systems of difference equations. Section 5.1 is devoted to investigating the dynamics of interacting species, such as predator–prey and competing species. In Section 5.2, we investigate some models of the spread of contagious diseases such as the SIR and SIS models. Section 5.3 considers some models represented by second-order nonlinear difference equations, such as delayed logistic models.

THE INTENDED AUDIENCES

The intended audiences are life sciences, mathematics, and mathematics education majors. The life sciences include biology, ecology, environmental science, and forensic science. The text can serve as a mathematics course in the liberal arts core or a general education requirement mathematics course. It can also serve as an honors mathematics course for all majors.

SUPPORT WEBSITE

Supplementary material for this book can be found by entering ISBN 9781118032114 at booksupport.wiley.com. This website contains solutions to selected problems, worksheets, and Maple code for many programs used in the text.

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1

OVERVIEW OF DISCRETE DYNAMICAL MODELING AND MAPLE™

1.1. INTRODUCTION TO MODELING AND DIFFERENCE EQUATIONS

In this section, we introduce dynamical systems, discuss discrete dynamical systems versus continuous dynamical systems, and informally define a mathematical model.

1.1.1. Model 1: Population Dynamics—A Discrete Dynamical System

Consider the population of a city with a constant growth rate per year. The populations are counted at the end of each year. For simplicity, we assume that there is no immigration to or emigration from the city.

i. Model the population dynamic and predict the long-term behavior of the system.
ii. The population of a city is 100,000 in year 2010. The natural annual growth rate of the population is 1% per year. Predict the city population in 2020. Find the population over the next 30 years and graph it. What is the long-term behavior of the population?

Explorations of Mathematical Models in Biology with Maple™, First Edition. Mazen Shahin.

Discussion

i. We will measure the population at discrete time intervals in one year units. Let

p_n = population size at the end of time period (year) n
p_0 = the initial population size
r = the constant growth rate per period (year)

The relationship between the current population, p_n, and the next population, p_{n+1}, is

$$p_{n+1} = p_n + rp_n$$
$$p_{n+1} = (1+r)p_n \tag{1.1}$$

Therefore, the population dynamics can be modeled by equation (1.1).

Equation (1.1) is a ***difference equation*** (or recurrence equation). The system (1.1) and the initial value p_0 represent the population dynamic. Since the population changes over time, this system is a ***dynamical system***. Since this dynamical system changes over discrete time intervals, the system is called a ***discrete dynamical system***. We say that the population dynamics is ***modeled*** by the discrete dynamical system (or the difference equation 1.1).

To find p_k, use p_0 in equation (1.1) to find p_1, then use p_1 to find p_2 and so on until p_k. This process is called ***iteration*** of the difference equation (1.1); and the sequence (1.2),

$$p_0, p_1, p_2, \ldots, p_k \tag{1.2}$$

for any value of k (positive integer) is called a ***solution*** or ***numerical solution*** of the given difference equation (1.1).

From equation (1.1), if the current value of p_n is known, the next value p_{n+1} can be calculated. For example, if we have p_5, we can calculate p_6. However, if we have p_0, equation (1.1) does not allow us to calculate, for example, p_6 in one step. Therefore, we are in need of a closed form to calculate p_n in one step if we know the values of p_0 and n. It can be easily proven that

$$p_n = (1+r)^n p_0 \tag{1.3}$$

Equation (1.3) is called the ***analytical solution*** of the difference equation (1.1).

Equation (1.3) is an exponential function and will grow or decay exponentially depending on the value of r. If $r > 0$, then $(1+r) > 1$, and therefore population size p_n grows unbounded when n is very large. If $r < 0$, then $(1+r) < 1$, and consequently, the population size approaches zero when n is very large.

ii. Let us apply the aforementioned model to the given information where $r = 0.01$ and $p_0 = 100,000$. The city population is modeled by the system

$$p_{n+1} = 1.01p_n, \quad p_0 = 100{,}000 \tag{1.4}$$

To find the population in 2020 (10 years from 2010), we use equation (1.3) with $n = 10$ and $p_0 = 100,000$. We are looking for p_{10}. We have

$$p_{10} = (1.01)^{10} 100,000 = 110,462.$$

One way to find the values of $p_1, p_2, \ldots, p_{30}$ is to iterate equation (1.4). Then graph the ordered pairs (n, p_n). To illustrate how the iteration works, let us see how to calculate, for example, p_3. Set $n = 0$ in (1.4) to get p_1,

$$p_1 = 1.01 p_0 = 1.01(100,000) = 101,000.$$

Then set $n = 1$ in (1.4) to get p_2,

$$p_2 = 1.01 p_1 = 1.01(101,000) = 102,010.$$

Finally, setting $n = 2$ in (1.4) gives p_3,

$$p_3 = 1.01 p_2 = 1.01(102,010) = 103,030.$$

In particular, to find P_{10}, the answer to the original question, we can use the difference equation (1.4) and the initial condition to find the sequence p_0, $p_1, p_2, \ldots, p_{10}$ which is 100,000; 101,000; 102,010; 103,030; 104,060; 105,101; 106,152; 107,213; 108,285; 109,368; 110,462. Thus $p_{10} = 110,462$.

Usually we use Maple to iterate a difference equation. We will introduce Maple in Section 1.3. The graph of p_n, $n = 0, 1, 2, \ldots, 30$ versus n is shown in Figure 1.1.

The analytical solution and numerical solution of (1.4) show that the city population slowly grows unbounded as n becomes very large.

1.1.2. Model 2: Population Dynamics—A Continuous Dynamical System

Consider the following situation. There are some bacteria in a tube with nutritive solution. As time progresses, the bacteria reproduce by splitting and dying. Assuming that there is enough food and space for the bacteria, model the dynamics of the bacteria. Investigate the long-term behavior of the model.

Discussion

Let $p(t)$ be the bacteria's population size (number of bacteria) at time t and $p(0) = p_0$. Assume that the growth rate $r = b - d$, where b is the birth rate and d is death rate. The assumption that there is enough food and space means that there is no restriction on the increasing number of bacteria. Therefore, the rate of change of bacteria's population size (dp/dt) is proportional to the bacteria's population p. Consequently, the dynamic of the bacteria is modeled by the dynamical systems (1.5) and (1.6)

$$\frac{dp}{dt} = (b-d)p = rp \tag{1.5}$$

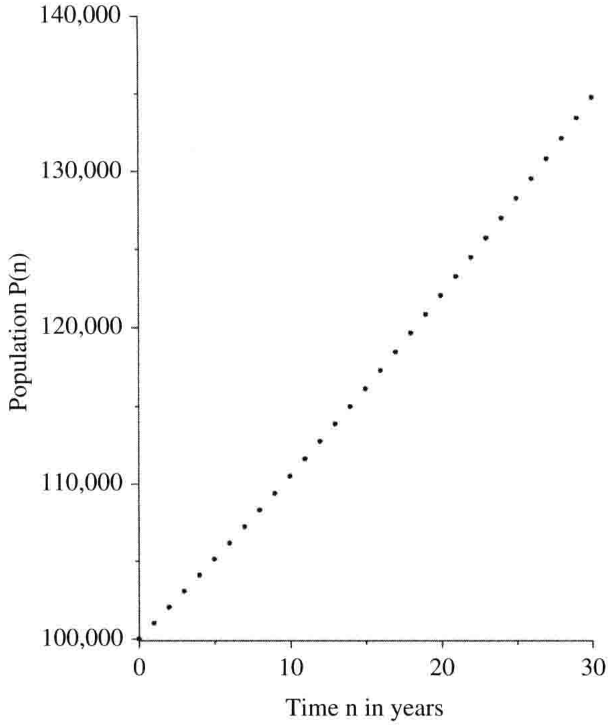

FIGURE 1.1. Graph of a city's population after n years, p_n, versus time n in years. The population is modeled by the difference equation $p_{n+1} = 1.01p_n$, with the initial population $p_0 = 100,000$, and $n = 0, 1, \ldots, 30$.

$$p(0) = p_0 \tag{1.6}$$

Equation (1.5) is a ***first-order ordinary differential equation***, and equation (1.6) is called the initial value (condition). From the basics of differential calculus or differential equations, the solution of the systems (1.5) and (1.6) is

$$p(t) = e^{rt} p_0 \tag{1.7}$$

Knowing the values of r and p_0, the population $p(t)$ can be evaluated at any time t. For $r > 0$, equation (1.7) implies that the population size $p(t)$ increases and grows unbounded as $t \to \infty$, while $r < 0$ implies that the population size decreases and approaches zero as $t \to \infty$.

Since the change in the system (1.5) is continuous, this system is called a ***continuous dynamical system***. Usually continuous dynamical systems are represented by one or more ordinary or partial differential equations. Note that the models discussed in this text are restricted to discrete dynamical systems. In other words, we will discuss in this text only models represented by difference equations.