BASIC METHODS OF THE DEVELOPMENT AND ANALYSIS OF MATHEMATICAL MODELS

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Summary

We study the main classical mathematical methods for the study of discrete recurrence equations or continuous differential equations, arising in mathematical modeling.

1. Discrete Time Models

We will see in this section the basic tools for the development and analysis of such mathematical models. We will restrict ourselves to a rather general framework, because more specialized models are described in the following chapters, and after. As often in mathematics, the study of linear systems will give the grounds on which the study of more complex nonlinear models is based. The exposition will be at an elementary level.

1.1. Making a Model

The first steps of the modeling of a dynamical real system has been discussed already (see *Mathematical Models, Basic Principles of Mathematical Modeling*); without entering into details, it consists of isolating the system to be modeled from the rest of the world, and selecting inside this system some variables, called state variables, that will give a good description of the state of the system at time k. The time will be considered as discrete, i.e. we consider only the sequence of instants 0,1,...,k,..., and describe the system for these instants only.

It remains to write the equations giving the state at the instant (k+1) in function of the state x(k). In general, the state x(k) at time k will be a vector of n variables $(x_1(k), x_2(k), \dots, x_n(k))$, and the general system will be (if there is no input):

$$\begin{aligned} x_1(k+1) &= f_1(x_1(k), x_2(k), \dots, x_n(k)) \\ \vdots &\vdots &\vdots \\ x_n(k+1) &= f_n(x_1(k), x_2(k), \dots, x_n(k)). \end{aligned}$$
 (1)

Each domain has its own methodology for building models; in general, there is some laws giving part of the dynamics; moreover, a complex model is done often of more elementary parts, describing the interactions inside some subsystems of the system, and involving a limited number of variables. These parts or subsystems are often added with some weights describing the importance of the dynamic of the subsystem in the whole dynamic. The model can be linear (cf. the example below) or not.

The discrete model can be also the result of the discretization of some continuous model, with the goal of making it simpler or more easily implementable on a computer.

For example, a dynamical model written as an ordinary differential equation with continuous time needs to be discretized in some way to be simulated on a computer; a numerical integration method (Euler, Runge-Kutta, ...) is needed to do that in the most accurate way.

Partial differential equations, having continuous variables in time and space, for example, need also to be discretized in time and space to be implemented on a computer.

The model obtained after discretization is often of large dimension, and the solutions should be compared to the solutions of the original continuous model: the aim being that, for, in general, a small step size for the discretization, the two kinds of solutions are very similar. We here enter the large domain of numerical analysis.

1.2. The State Space: Basic Vocabulary

Consider the general system (1); it can be written in the more concise form

$$x(k+1) = f(x(k)),$$

where *f* is some function associating an *n*-vector to another. Given an initial vector condition $x(0) = x_0$, the solution will be some vector $(x_1(k), x_2(k), ..., x_n(k))$ evolving with time *k*.

(2)

The usual graphical representation of this vector is the representation with respect to time : the time is on the X-axis, and the n variables on the Y-axis. The state space is another way of seeing the system, very efficient, particularly for the low dimensions.

The state space for the dimension 2 (two variables $x_1(k), x_2(k)$) is the representation in the plane of the point of coordinates $x_1(k), x_2(k)$: the time does not appear explicitly. The dynamics is clear from this Figure 1: starting from a point (initial condition x_0), the dynamical system "jumps" to another point, and so on.

This representation enables to see (with the help of a computer) a more geometrical vision of the behavior; moreover, as will be seen in the next section, a classification is possible in this space. This space is also named the phase space.

A point that does not move is called an equilibrium; it satisfies $x^* = f(x^*)$; a sequence of points jumping from one to the next (given by the equation of the system) is a solution. The initial point x_0 at time t = 0 is called the initial condition.



Figure 1. Time (left) and phase (right) representation in dimension two

A point that does not move is called an equilibrium; it satisfies $x^* = f(x^*)$; a sequence of points jumping from one to the next (given by the equation of the system) is a solution. The initial point x_0 at time t = 0 is called the initial condition.

In some cases, the system can be submitted to the action of external variables, that do not belong to the state variables: it could be, for example, the external temperature that will change the survival and reproduction rates in the Leslie models; these external variables are called inputs in the language of control theory (see *Basic Principles of Mathematical Modeling*). If there is some input u(k) depending on the time k, the new system is x(k+1) = f(x(k), u(k)).

1.3. Linear Discrete Equations

Let us consider the simple example of the geometric growth (see *Classification of models*). The model is

x(k+1) = ax(k) .

In particular, we wish to know if the population will decline or increase, and how it behaves for large times. This formalism and study is in fact at the basis of all the models we will write in the following. The model describes how the variables determining the state of the system at time k will evolve at next time (k+1). The initial condition gives the value of the state variables at time 0. We wish to study the behavior of a solution starting from the initial condition, and describe it for any time.

For the above example, the answer is simple, because the solution is $x(k) = a^k x(0)$ and therefore:

- if a > 1, then the solution grows without limits (if x(0) is not zero)
- if a = 1, then the state stays always at the initial value x(0)

• if a < 1, then the solution goes to zero: the population goes to extinction.

Even in this very simple discussion, we have used our knowledge of the physical meaning of the parameter a: we know that a is positive because it represents a number of cells.

Now we can consider the more general case (several variables) of a linear discrete system, also called difference equations. It plays a prominent role in the study of mathematical dynamic discrete models (similarly to its continuous analog: the linear differential equation).

The system is supposed to be described by *n* state variables $x_1(k), x_2(k), ..., x_n(k)$ at instant *k*. We first list the variations around linear models. The simplest case is the case of a linear square constant matrix *A* with *n* rows and *n* columns.

1.3.1. The Homogeneous Constant Linear System

A homogeneous constant linear system is described by x(k+1) = Ax(k). The matrix A is given by

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{pmatrix} .$$

To define a solution, we must give us an initial condition $x(0) = x_0$. As an example, consider the Leslie model (see *Classification of Models*):

$$x(k+1) = Ax(k)$$

with

$$A = \begin{pmatrix} 0 & F_2 & F_3 \\ P_1 & 0 & 0 \\ 0 & P_2 & 0 \end{pmatrix}.$$

1.3.2. The Homogeneous Time-varying Linear System

A homogeneous time-varying linear system is described by

$$x(k+1) = A(k)x(k).$$

The matrix A(k) depends on the time k. Of course, it is a generalization of the above constant case.

As an example, let us imagine that the parameter of survival and reproduction and the Leslie model vary with the time (let us say the year) because of the variation of climate.

1.3.3. The Non-homogeneous Linear System

A non-homogeneous linear system is described by

x(k+1) = A(k)x(k) + b(k),

where b(k) is some forcing vector of dimension *n* depending (possibly) on time. As an example, in the Leslie model, the vector

$$b = \begin{pmatrix} 0 \\ b_2 \\ 0 \end{pmatrix}$$

could represent the immigration of individuals coming from outside in the second age class.

1.3.4. The Controlled Linear System

In the above, the vector b(k) can be seen as an input, and can be written to make explicit the connection between the actual inputs of the system u(k) of dimension m, and the evolution equation. Thus we define a matrix B(k) of n lines and m columns, and write:

$$x(k+1) = A(k)x(k) + B(k)u(k)$$
.

This system is now relevant for Control Theory (see *Basic Principles of Mathematical Modeling, Controllability, Observability, Sensitivity and Stability of mathematical models*); we may also add outputs, describing the available measurements:

$$y(k) = C(k)x(k).$$

1.3.5. Conversion to Matrix Linear Form

The model can sometimes be described by an equation involving the state variable at different times k. Let us take the example of the linear difference equation:

$$y(k+n) + a_{n-1}y(k+n-1) + \dots + a_0y(k) = u(k)$$
.

The model depend on the variable y taken at times between k and k+n, n is a given integer.

Define the new state variable x(k) of dimension n by:

$$x_1(k) = y(k)$$

$$x_2(k) = y(k+1)$$

$$\vdots$$

$$x_n(k) = y(k+n-1).$$

Then the system is a linear homogeneous system

$$x(k+1) = Ax(k) + Bu(k)$$

with

$$A = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ -a_0 & -a_1 & -a_2 & \dots & -a_{n-1} \end{pmatrix} B = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}.$$

1.4. Basic Study of the Homogeneous Constant Linear System

This case is the simplest one, but also the most important as a basis for the study of dynamical systems, either linear or nonlinear (the linear system being obtained by linearization of the nonlinear one, see below).

The considered system is

$$x(k+1) = Ax(k)$$

with an initial condition $x(0) = x_0$. The explicit solution is easily written as:

$$x(k) = A^k x_0.$$

We suppose that the matrix A-I is bijective for simplicity, then the origin is the only equilibrium, because the equation x = Ax only has one solution.

The following theorems give the basic behaviors of such systems: they are based on the notions of eigenvalue and eigenvectors.

Theorem 1 Case 1 (asymptotic stability): if all the eigenvalues of the matrix A are strictly less than 1 in modulus, then the solution goes to zero.

Case 2 (*instability*): *if one eigenvalue of the matrix is greater that one (in modulus), then the solution is not bounded for almost any initial condition.*

It is possible also to classify the behavior in the phase space (the space of the state

variables) into some cases giving a good and intuitive view of the situation. In the case of two variables, we obtain (we have concentrated on generic cases for simplicity):

Proposition 1 *Classification of behavior in the plane:*

- stable node: if the two eigenvalues are real of modulus lower than one, the solution converge toward the origin with two principal directions (the two eigenvectors).
- stable focus: if the two eigenvalues are complex and conjugated with a real part lower than one, the solution converges along a kind of spiral towards the origin.
- *unstable node: if the two eigenvalues are real and of modulus greater than one, the solution becomes unbounded with two principal directions (the two eigenvectors).*
- stable focus: if the two eigenvalues are complex and conjugated with a real part greater than one, the solution converges along a kind of spiral towards the origin.
- saddle : if one eigenvalue is real and greater than one in modulus, and the other real and lower than one in modulus, then the phase space has one attractive direction, and one repulsive, along two lines (the two eigenvectors).

There exist algebraic tests to study the location of the eigenvalues, and conclude concerning the stability. In dimension two, they are simple:

Proposition 2 The second order matrix A is asymptotically stable if |trace(A)| < 1 + determinant(A), determinant(A) < 1

1.5. Basic Study of the Non-homogeneous Constant Linear System

The basic equation is:

$$x(k+1) = Ax(k) + b$$

where the vector b is constant also. In fact, the study of this system amounts to the study of a translated linear homogeneous system.

Proposition 3 Consider the unique equilibrium x^* such that

 $x^* = Ax^* + b$

then the new variable $y = x - x^*$ is solution of the system:

$$y(k+1) = Ay(k).$$

This system is studied as above.

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Biographical Sketches

Jean-Luc Gouzé is a Senior Research Scientist at INRIA (National French Institute for Computer Science and Control), and the head of the research team COMORE (Control and Modeling of Renewable Resources, see http://www.inria.fr/comore).

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