BASIC PRINCIPLES OF MATHEMATICAL MODELING

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Summary

In this chapter we try to introduce the reader to the main features of Mathematical Modeling. Modeling is now a very fashionable word and is widely used to name a complex scientific activity where the computer plays a central role. But actually mathematical modeling is not a new activity and was practiced for a long time by scientist.

Among them, engineers developed a theory called *Mathematical Systems theory*. It was developed, mostly during the twentieth century for the purposes of understanding the dynamics of complex man-made devices. It was a theory for engineers and was mainly developed in electrical engineering departments. It is now a mathematically sophisticated science.

By the middle of the twentieth century two major events had taken place: The development of computer facilities and the rise in interest in the dynamics of life systems. For these reasons Mathematical Systems theory became more and more used for the modeling of natural systems as opposed to artificial ones and we decided to focus on this aspect of mathematical modeling. Of course this is not the only possible approach.

The chapter is divided in four sections. The first and the last are devoted to methodological issues and the two intermediate ones to more technical aspects of Mathematical Systems Theory. In the first section we insist on the need for mathematics in modeling activity. The first ingredient of Mathematical Systems Theory is the classical mathematical concept of dynamical system, either continuous or discrete with respect to time, finite or infinite-dimensional with respect to the state space, deterministic or stochastic.

This is described in Section 2. The second ingredient, described in Section 3, comprises the concepts of input and output, which are absolutely necessary to define what a feedback is. We will see how these concepts are useful for the modeling of few natural systems. After this introduction to the major concepts of systems theory we shall give a very brief account on controllability, observability and stabilizability. We shall explain the major results for the case of linear systems and give few indications on the possible generalization to nonlinear systems. In the last section we come back to modeling and consider the various possible uses or misuses of a model.

1. Introduction

1.1 A Fashionable Word

The use of the word “modeling” in sciences is relatively recent. Scarcely used during the last century it is now a fashionable word, but “mathematical modeling” is not a new activity, even if had not appeared under this name before. As we know, the classical theories of physics express their law through a mathematical apparatus, the “equations” as we used to say formerly, that could be called a “mathematical model” in our present language. But we are not mainly concerned with this kind of model in the present chapter, despite the fact we often shall refer to them for comparison purposes.

We shall consider the word “model” in the engineering tradition of the last century, who, before the computer achievement, used to build “reduced models”. Nowadays, the models used by engineers are symbolic representations, expressed in a language that is possibly recognized by a computer, of some complex and changing real system. The computer simulations of the dynamic generated by the model are used to solve a great variety of practical questions.

In his classical mathematical text-book, “Ordinary Differential Equations”, the famous mathematician Pontryagin relates an important practical problem which was solved thanks to a mathematical model: The question of the stability of Watt’s governor for steam engines. The Watt governor was invented by the end of the eighteenth century and was perfectly suitable for its purposes for some time. It turned out that, by the middle of the nineteenth century, the functioning became worse and worse. A mathematical model of the motion of the steam engine with its governor was elaborated, and a mathematical theory of the stability of motion was simultaneously elaborated by the Russian Wischnegradsky and the famous physicist J. C. Maxwell around 1870.

In that case the mathematical model was a set of three differential equations established on the basis of Newton’s laws of mechanics for an artificial apparatus designed by man. Since that time, “Automatic Control Theory” has become the science whose aim is to provide engineers with the tools for achieving the regulation of more and more complex systems as in modern aircraft, industrial processes, electrical networks, etc.

During a little more than one century, automatic control theory has developed for its own use a theory of mathematical modeling with efficient concepts and highly mathematically sophisticated developments. This theory was well developed when the computer appeared at the middle of the twentieth century and was able to incorporate this revolution harmoniously. We call this theory *Mathematical Systems Theory*.

More recently, say for half a century, there has arisen a need for a more quantitative theory of the dynamics of complex natural systems. (The existence of the EOLSS is a good example of this new important challenge facing humanity and we do not pursue on this point here). The representation of ecological systems dynamics through mathematical equations was present a long time ago, at the beginning of the century, but the nonlinear equations were too complex for a mathematical treatment. Thanks to the fantastic computing power of modern computers one can simulate more and more

complex systems of equations. Thanks to the low cost of modern personal computers and to the facilities of new computer languages, more and more people conduct simulations for various purposes. What is the scientific value of such simulations? This is a big issue and mathematical modeling is a way, if not the only way, to address it.
In this introduction we shall describe what mathematical modeling is in the spirit of the traditional training of automatic control engineers and try to see to what extent this methodology is suitable for areas of research other than industrial production.

1.2 Modeling: A Complex Activity

A picture like the one in Fig. 1 is by itself all a philosophical program! We begin by some comments about it. In this picture we observe a first ensemble called “piece of reality” which feeds (arrow 1) another ensemble called “discourse about reality”. This possibility of a crude separation between an objective “reality” which exists independently and previously to any discourse, and the “discourse about this reality” is quite questionable.

The question of the existence of an objective world, and the possibility of a non-subjective analysis of it, is a formidable philosophical question that we shall not consider here. We shall adopt the following pragmatic point of view. We accept that there are circumstances where the existence of an object to be studied, the piece of reality, is quite clear.

For instance if the problem is to realize a flight simulator for an aircraft, say an Airbus A320, the piece of reality is well defined. Small ambiguities, like what kind of engine or instrumentation is used, will be easily clarified. Another example: Make a model of the growth of the temperate-climate oak.

In this case also, even if it seems a little more difficult to agree on what an oak is and what means its growth, clearly a general consensus is possible.

But, “set up a model of the functioning of the tropical forest” is clearly a different question. If the rain forest is a relatively well understood object, what does it mean, “its functioning”? Are we speaking of productivity or are we interested by the biodiversity it can sustain?

The question about the “good” use of such a tropical forest might be different if you are a poor peasant of Brazil or a rich citizen of an industrialized country. Different points of view, even contradictory points of view are to be expected.

Even more difficult is the problem of the separation between a subject and an object when considerations about human psychology are concerned. Is it possible to make a model of the behavior the Stock Exchange, since people who know the model will change their behavior?

Mathematical modeling assumes that there is an “object” and a “subject” making a discourse on this object. We know that it is not always the case but we do as if it were the case.

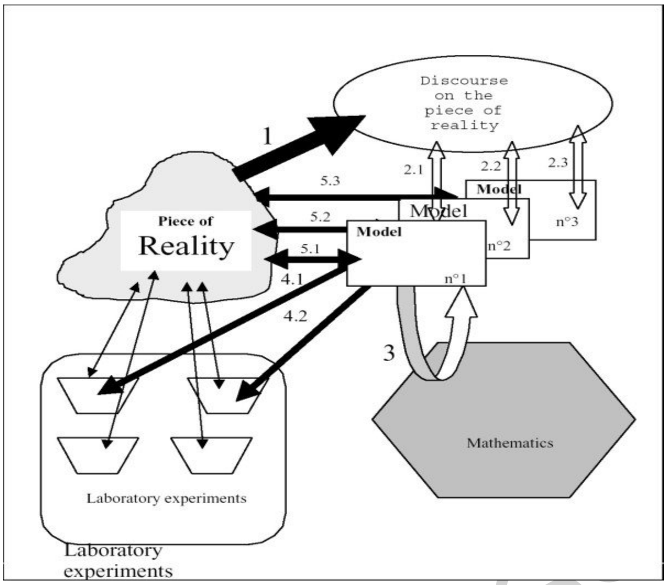

Fig. 1: The model and the real world

In Fig. 1 we have drawn some rectangles to indicate "models". There are several models, $n^\circ 1, n^\circ 2\ldots$ recalling the fact that, for the same object, there are many different viewpoints and by the way many different models. By this we mean that, in mechanics for instance, we do not use the full equations of relativity to represent the motion of an airplane, but Newton's equations, which comprise a simplified model. But we do not mean only this. We mean that some objects may have several models which are both necessary to describe it and not reducible one to each other. The best instance for this fact is probably quantum mechanics, where wave and particle models are both necessary to describe the same reality.

The arrows 2.1, 2.2, … define a connection between the model and the discourse about the reality. This is the work of interpretation. By the interpretation we mean the following point. Suppose that we are interested in two interacting populations, say a prey and a predator. The number of prey is of the order of magnitude of 10^9 and the predators of 10^6 (this is plausible in the case of a relation between fishes and small plankton) and choose the 10^9 as unity for the prey and 10^6 for the predators. Denote by $x(t)$ and $y(t)$ the quantity of prey and predators in these units. Because of this choice $x(t)$ and $y(t)$ appear to be real numbers, (i.e. numbers with decimals). Assume that we build a model in terms of differential equations and that the model has the property that, when t tends to infinity, $x(t)$ tends to zero. The "first degree" interpretation of this application of the model is that the prey population extinguishes. But one must be careful since the justification for working with real numbers was the fact that the numbers of prey was large, of the order of 10^9 which will no longer be the case if $x(t)$ tends to 0. So, when $x(t)$ decreases, it follows that at some moment the model is no longer appropriate to represent reality and we must think about it. Thus $x(t)$ tending to 0 in this model means that the population of prey decreases below some threshold, no more. In some sense, what we call interpretation is the art of modeling itself, but we prefer to keep the word modeling for the more complete process that we are presently describing than just for the activity of interpretation of mathematical results. Another reason why we do not want to call modeling the activity of giving sense to mathematical facts is because in this respect astrology could also be called modeling, since it is an activity in which one gives interpretations of fact about celestial objects that can be predicted mathematically!

In the scientific modeling activity the predictions of the model are to be compared to reality by means of empirical data. This is shown through arrows 4.1, 4.2… that concern empirical data that are produced in laboratories where the "piece of reality" is extrapolated, or data produced directly by the "piece of reality itself" (arrows 5.1, 5.2…). We make a distinction between data that are produced directly by reality and those that are produced in a laboratory. The second are very secure while the first are subjected to errors of various origins. Most of "life support systems" are complex systems in the sense that we cannot reduce them to the laboratory and by the way they often lack of good data. This is a reason why we try to understand large complex systems but we must remember that no model can replace good data.

1.3 The Need for Mathematics

By definition a *mathematical model* must have a strong connection with mathematics! This is represented by the arrow 3. A mathematical model is by itself an object, which is inserted in a more or less well-developed theory. It is this mathematical theory that gives to the model its utility. Let us consider an example. In a lake (which water is supposed to be at rest), one represents by $U(t,x,y)$ the concentration of some pollutant at the point of coordinates (x,y) at time *t*. The pollutant diffuses in the water, and the evolution of this concentration during time can be represented by the system of equations:

$$\frac{\partial U(t,x,y)}{\partial t} = k^2 \{ \frac{\partial^2 U(t,x,y)}{\partial x^2} + \frac{\partial^2 U(t,x,y)}{\partial y^2} \} + \phi(t)\delta_{x_0,y_0}$$

$$(x,y) \in \partial\Omega \Rightarrow \ \frac{\partial U}{\partial \vec{n}} = 0$$

which express that the flux at the boundary of the lake is null and that the pollutant source is located at the point (x_0, y_0). From the knowledge of the function $\phi(t)$, one can compute (analytically in some cases, with computer simulations in other cases) the value of *U* at any point at time *t*. From the knowledge of the position of the emission of pollutant one can deduce the future pollution at each point. This is not very surprising; we are accustomed to longstanding successes in celestial mechanics, that mathematical models predict the future motion. Maybe more surprising is the following: Assume that we know the intensity of the pollution at one, or some points, in the lake; is it possible to recover, from this information, the position and the intensity of the emission of pollutant? The answer is 'yes'. These kinds of problem, known as inverse problems in mathematics, have a long history, and have been solved recently for wide classes of useful equations. It must be noticed that if the question of prediction of future pollution from the knowledge of the pollutant source requires relatively few mathematical technicalities and can be implemented on a computer quite easily, the solution of the inverse problem requires high mathematical sophistication.

There is another reason why a mathematical theory is necessary when we develop models. As we said we need to make simulations and we need to interpret them. Since the simulation is done on a computer that is not able to compute with ideal real numbers there are numerous artifacts related to the computation itself, which must not be interpreted as properties of the model. The way to measure the distance between mathematical ideal solutions and the actual simulations comprise a wide body of knowledge that was developed for the use of computers and is called *numerical analysis*.

Becoming more and more common are models of simulation, *computer models*, which are built directly from the discourse about reality, using high-level languages that fit perfectly with the purpose of modeling. The temptation, for non-mathematicians, is to try to avoid mathematics. Our position here is that a model, by itself, needs a theory. The physical theory that explains how the electron microscope works has nothing to do with the biology of cells that are observed but it is necessary to understand the image that one sees. Computer simulation is to the knowledge of the dynamics of complex systems what the microscope is to the vision of the infinitely small: It is a tool that also needs its own theory. The theory of the model, which must not be confused with the theory of the piece of reality which the model describes, must be done in the language of mathematics.

1.4 Orientation of the Chapter

We first (Section 2) give an account of the concept of mathematical dynamical systems, including infinite dimensional systems and stochastic processes. The importance that we give to each aspect of dynamical systems does not reflect the importance they occupy in the mathematical world because our objective is not to give a fair description of the subject but to introduce the mathematical tools that are useful for modeling. We tried to explain concepts through examples that we choose more in the life sciences than in physics since we think that people trained in the exact sciences have already a general understanding of the subject.

In the Section 3 we give an extensive account of mathematical systems theory for the reasons we explained earlier. The basic concept developed in this section is the concept of an input-output system.

In the forth and last section we ask the question: A model for what purposes? We suggest the following classification.

- Models for understanding, where the model has no pretension of being in accordance with empirical data but simply sheds light on the discourse.
- Models for description and prediction which have qualitative and quantitative connections with the real world.
- Models for purposes of control.

2. The Mathematical Concept of Dynamical System

Every scientist has his own idea of what an actual *dynamical system* is. For a physicist it could be a set of point masses interconnected by strings, occupying various places through time. For an oceanographer it could be the displacement of masses of oceanic water. For the agricultural engineer, who fights against insects, it could be the evolution during the season of their number in response to his action. For an economist it could be the evolution of prices of goods related to their production. It is not useful to multiply these kinds of examples. But now consider the following sentence: “The spirit of this man has changed: he was careless and casual but now we can be confident in him”. This sentence says that something changed during the time: the spirit of a man. But, opposed to the preceding examples, where there was something to quantify, the position, the production, etc… there is hardly something comparable in the case of the spirit. This is the reason why the mathematical concept of a dynamical system is not very useful in such questions. In the game of love mathematicians have no more nor less success than anyone!

The mathematical concept of a dynamical system was certainly elaborated in view of the development of classical mechanics since the discovery of its laws by Newton. We shall not attempt in this chapter to recall the history of this mathematical concept, which we assume to be more or less familiar to the reader. We just want to recall what the various types of dynamical systems are and fix some notation. A most important concept in the theory of dynamical system is that of state and state space. We try to make this concept clear in this section.

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Biographical Sketch

Claude Lobry, was born in 1943 and got a “thèse d’état” at the university of Grenoble, in optimal control, in 1972. He was then appointed as professor at the University of Bordeaux and joined the University of Nice in 1981. His main interest is mathematics applied to automatic control and natural systems where he became a specialist of controllability. During the eighties he used the tools of Nonstandard Analysis in some problems of singular perturbations of differential systems.From 1990 to now he has been very active in creating interdisciplinary teams or networks with the Centre National de la Recherche Scientifique, the Institut National de Recherche Agronomique, the Institut National de Recherche en Informatique et Automatique. Besides his scientific activities he has a strong involvement in the promotion of mathematical research in developing countries, especially Africa.