MATHEMATICAL MODELING OF LIFE SUPPORT SYSTEMS: CLASSIFICATION OF MODELS

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Contents

Summary

Deep investigation of a process, phenomenon, or object requires its mathematical description that leads to a clear understanding of its key features, which in turn, allow us to predict the further behavior of the object, to give recommendations on its control, and so on. Such a description is just a *mathematical model* of the object (process, phenomenon). We deal first of all with mathematical problems that are generated by applied researches. During a practical investigation a mathematical model of the object (phenomenon, process) under investigation is constructed. At the theoretical level of researches the mathematical model reflects the most important features of the object under investigation. In the form of mathematical correlations (equations, inequalities, functionals, etc) the fundamental laws of the applied field, the connections between separate components of the investigated object, the conditions (real or forecast) of the object existence, etc. are expressed in appropriate mathematical form.

We often seek the simplest possible mathematical models whose investigation allows us to draw only some qualitative conclusions without quantitative information. This is because, in particular, the fundamental laws of the applied field, as they are, do not possess an exact quantitative character. We speak in this case about qualitative mathematical models. The adequacy of the mathematical model is one of the basic

requirements. Mathematical problems of large dimension are, as a rule, more adequate but they are more difficult for investigation. This circumstance is called as curse of dimensionality. The principle of simplicity is to construct a mathematical model satisfying two, generally speaking, contradictory conditions. On the one hand, the mathematical model must be sufficiently complete, i.e., must give an adequate description of the investigated object. On the other hand, the mathematical model should have maximum of simplicity for the investigation (analytical or numerical). An applied mathematical model may include elements that account for the uncertainties of nature - random scalar and vector values, random functions, etc. In this case we speak about probabilistic (stochastic) mathematical models. The deterministic mathematical models do not contain the element of probabilistic nature. For linear mathematical models the superposition principle holds, that is, any linear combination of solutions (e.g., their sum) is also a solution of the problem. Using the superposition principle it is not difficult, starting form a solution in a particular case, to construct the solution in a more general situation.

It is necessary to specify the models with lumped parameters (point models) and the models with distributed parameters. Point models do not take spatial effects into account; they are usually connected with systems of algebraic equations and with systems of ordinary differential equations. A real applied model is often connected with the construction of a geometric model, by taking into account the dependence of the investigated phenomenon and process behavior on a spatial point. In this case the key feature of the mathematical model is its use of partial differential equations (distributed models). The stationary and non-stationary mathematical models are distinguished according to the influence of time. Realistic mathematical models of real world systems and processesare, as a rule, nonlinear. Linear models are often considered as particular cases and usually they serve as the first approximation to the reality. Nonlinear mathematical models are invariably more complicated for investigation by both numerical and, analytical methods, even more complex in the latter case. A mathematical model may be well-posed (correct) if its solution exists, this solution is unique, and it continuously depends on input data (i.e., small perturbations of input data cause small perturbations of the solution). Otherwise the mathematical model is called ill-posed.

An elaboration of effective computational algorithms is always a key problem of mathematical modeling. Formulation of such models is based on conversion from a continuous argument (continuous domain) to grid functions (discrete domain). A discrete mathematical model may also be also considered on its own for the investigation, but in most cases we deal with continuous models.

The investigated object may be too complicated for theoretical investigation, and there is no opportunity to use an analytical description on the basis of earlier known fundamental laws. Such a situation is typical for the stage of collecting the experimental data, natural experiments. In order to describe the collection of experimental data, to perform their analysis, and to make a reasonable forecast for the behavior of the investigated object in the new conditions, special mathematical models are constructed. Such models mainly are only of mathematical character without any connection with the nature of the investigated object. Such a modeling is called *imitation modeling.* The term as it is reflects the peculiarities of imitation modeling. In some sense this is a defective mathematical modeling. It is possible to say that we deal not with a real mathematical model but only with its imitation. So, we arrive at the approximation of mathematical models, which reflect as far as possible certain specific features of the actual system; they usually regard the object as a "black box". Empirical formulas, which are typical in the treatment of experimental data, serve as an example of approximating models.

1. Introduction

Scientific foundations of life support systems are based on using the vast complex of knowledge of natural sciences, engineering and technology, humanities and economical sciences, medicine, etc. Nowadays theoretical and experimental investigations involve extensive use of modern information technologies. Collection, storage, analysis and processing are based on mathematical technologies and computational equipment.

The theoretical level of studying the reality yields the deepest knowledge and allows us to solve properly the problems of forecasting and decision making. In this case the investigation is based on using complicated theoretical constructions (mathematical models), which may be investigated by using powerful computational means (numerical algorithms and computers in the capacity of the establishment).

In the mathematical modeling the investigation begins with the construction of a mathematical model and the formulation of the related mathematical problem that will be investigated later in detail. Mathematical models are based on the fundamental laws on a concrete applied science, on the accepted theoretical constructions of describing the phenomena and objects under investigation in the given branch of knowledge.

Life support problems are studied in diverse branches of sciences. In this situation it looks impossible to give a classification of mathematical models under use. Furthermore, we do not need such a classification because these issues are properly reflected in the other chapters of this theme.

The universality and inter-disciplinary nature of mathematical modeling as a means of scientific researche is brightly seen in applications of the same mathematical models to different phenomena of living and non-living systems. While discussing the problems of classification of mathematical models of life support systems this enables us to concentrate mainly on the peculiarities of mathematical models exactly as mathematical objects.

We are interested first of all in the mathematical problem that is generated by an applied research effort. Choosing the most specific features of the mathematical problem allows us to pick up adequate mathematical (analytical and numerical) tools for investigation with proper completeness. We add to our text some simple examples from different fields of knowledge. This collection is rather arbitrary, but it can be easily extended.

2. Mathematical Models.

In an applied investigation a mathematical model is constructed for the object (phenomenon, process) under investigation. At the theoretical level of researches the mathematical model reflects the most important features of the object under investigation. In the form of mathematical correlations (equations, inequalities, functionals, etc.) the fundamental laws of the applied field, the connections between the individual components of the investigated object, the conditions (real or forecast) of the object existence, etc; are expressed at first.

Different branches of science are characterized by different levels of theoretical researches and different degrees of mathematization of knowledge. Often, for instance, in the social sciences, we are in need to use the simplest mathematical models whose investigation allows us to make only some conclusions of a qualitative character. In particular, the fundamental laws of some applied fields, as they are, do not possess an exact quantitative character. We speak in this case about qualitative mathematical models.

As a specific example, let us consider the qualitative mathematical models of biological processes. The mathematical model of the simplest two-entity *predator-prey* system is based on the following basic assumptions:

- The populations N and M of prey and predators depend only on time;
- in the absence of interaction the population of a species satisfies the Malthusian law when the rate of change of the population is proportional to its current magnitude;
- the natural mortality rate of the prey population and the natural birth rate of predators are considered as non-essential;
- the growth rate of the population of prey decreases proportionally with the population of predators, i.e., to the value cM, $\mathrm{c} > 0$, and the rate of growth of the predator population increases proportionally with the population of prey, i.e., to the value dN, $\mathrm{d} > 0$.

With these assumptions we arrive at the Lottka-Volterra system of equations

$$\frac{dN}{dt} = (\alpha - \mathrm{cM})\,\mathrm{N}, \qquad (1)$$

$$\frac{\mathrm{dM}}{dt} = (-\beta + dN)\,\mathrm{M}. \qquad (2)$$

Setting the initial values $\mathrm{N}(0),\ \mathrm{M}(0)$ we can find from this system the the population at any time moment $\mathrm{t} > 0$.

Such a mathematical model allows us in many cases to explain the observed phenomena, and it is constructed with such an aim. However, it is difficult to set this model as a foundation for precise quantitative investigations.

The capabilities of mathematical methods can be especially well seen at the investigation of quantitative mathematical models. This situation is usual for the natural sciences (first of all, for physics and mechanics). The fundamental laws have an exact quantitative character. To the mathematical model of an investigated object the demands of a certain accuracy of the description of given experimental data are made. Hence, the mathematical model must describe one or other properties of the investigated object with the prescribed accuracy.

The mathematical model has to reflect the essential characteristics of the investigated object; in the capacity of a model (an ideal, theoretical prototype) it must reveal (by simulation) certain important characteristics of the object as it is. The circumstance reflects the demand of the adequacy of the mathematical model. It means that the model must be close to the investigated object, to show correctly the behavior of the object in accordance with the totality of the chosen properties - it is with this aim that the mathematical model is constructed as it is

We may speak not just about the adequacy of a model but also about the accuracy of the description of the phenomenon or the process. This accuracy must be in the concordance with the data accuracy, by which the mathematical model is calibrated.

At the stage of mathematical modeling in the cycle of the computational experiment, the check of the correctness (verification) on the basis of the given data is performed. The mathematical model is specified during the investigation, and it is possible to say that the order of adequacy of the mathematical model increases.

The adequacy of the mathematical model is one of the basic demands on the mathematical model. It is achieved due to the specification of the model that is usually connected with its complication. More complicated models yield, probably, more exact description, however, they are more difficult for the investigation and therefore we require a mathematical model to be sufficiently simple.

The principle of simplicity in constructing a mathematical model has to satisfy two, generally speaking, contradictory conditions. On the one hand, the mathematical model must be sufficiently complete, i.e., give an adequate description of the investigated object. On the other hand, it should as simple as possibe for the investigation (analytical or numerical).

Improvement of the adequacy of a mathematical model is achieved by hierarchical organization of a class of models. A model from one level to another (better) level in terms of accuracy and detail of description is achieved by specifying the underlying fundamental laws and correlations.

3. Some Classes of Mathematical Models

In practical systems, in which the components are associated with uncertainty or imprecision, the corresponding mathematical model needs to include probabilistic descriptions of scalar or vector valued quantities and the methods of probability and statistics are applied in the study of such models. The notions of mathematical validity and the aspects of dispersion of the random values, distribution functions, stochastic processes etc. are fundamental to the study of such models.

Let us consider an example of a probabilistic mathematical model connected with a random Markov process. We describe the one-dimensional motion of a small rigid particle in a liquid, which undergoes chaotic collisions with the molecules of the liquid (the Brownian motion). Its position at any time moment $t \geq t_0$ is given by the coordinates x.

We assume that the position of the point x at the time t uniquely defines the probability of the particle being at any time $t' > t$ in a certain area, that the events happened during the time interval between t and t' do not influence the position of the point at time t'.(a Markov random process)

The Markov process is completely characterized by the probability density function

$$p\left(t,x,t',x'\right), \quad -\infty < x < \infty, \tag{3}$$

that enables us to calculate the probability of the presence of particle in the neighborhood of the point x' at the time moment t'. The function *p* satisfies the normality condition

$$\int_{-\infty}^{\infty} p\left(t,x,t',x'\right) dx' = 1. \tag{4}$$

It is assumed that during a small time interval Δt the probability that the particle can move through a considerable distance $\Delta x \geq \delta$ is small. This means that for any $\delta > 0$

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{|x'-x| \geq \delta} p\left(t - \Delta t, x, t, x'\right) dx = 0. \tag{5}$$

It is also assumed that for any $\delta > 0$ there existthe following limits that are uniform with respect to x:

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{|x'-x| < \delta} \left(x' - x\right) p\left(t - \Delta t, x, t, x'\right) \mathrm{d}x' = b > 0, \tag{6}$$

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{|x'-x| < \delta} \left(x' - x\right)^2 p\left(t - \Delta t, x, t, x'\right) dx' = 2\mathrm{a} > 0, \tag{7}$$

Where a, b are the main parameters of the process, which have a clear physical interpretation for the considered Brownian motion. The values a and b depend generally speaking, on the point x and on the time moment t; for the simplicity we assume that a and b are constants.

The basic equation for the considered Markov process is the Kolmogorov equation for the probability density

$$\frac{\partial p(t,x,t',x')}{\partial t} = \mathrm{a}\frac{\partial^2 p(t,x,t',x')}{\partial x^2} + b\frac{\partial p(t,x,t',x')}{\partial x}. \tag{8}$$

So, we arrive at the standard linear parabolic equation of the second order, which is the basic one for lots of processes and phenomena. The peculiarity of the probability model is reflected by the fact that this standard partial differential equation is written for the determination of the characteristics of the random process. The investigation of such mathematical models is performed similarly for deterministic models.

While using probability models the situation, when not only the solution possesses a stochastic nature but also the coefficients of the equations and other input data, is typical. In the above case of the parabolic equation the coefficients a and b may by random. Such a nature of equations should be taken into account at the the time of elaboration of numerical algorithms for investigation of applied mathematical models.

It is necessary to specify the models with lumped parameters (point models) and the models with distributed parameters. Point models do not take spatial effects into account; they are usually connected with systems of algebraic equations and with systems of ordinary differential equations.

A realistic model is often connected with the construction of a geometric model, taking into account the dependence of the investigated phenomenon and process behavior on a spatial point. In this case the key point of the mathematical model is that it contains partial differential equations.

Multidimensional mathematical models are difficult to analyze. Analytical methods are utilized only for geometrically simple problems, so, computational facilities are actually the only tool for complex models. The mathematical problems of large dimension are, as a rule, more adequate but they are more difficult for investigation. This is called as the curse of dimensionality.

The stationary and non-stationary mathematical models are distinguished according to the influence of time. In non-stationary (dynamic) models the temporal description of the investigated object is just the goal of analysis. Stationary mathematical models are applied in the case if the investigated object does not change its characteristics in time.

More detailed investigation of non-stationary processes is often based on separating out the quasistationary regimes, by considering the asymptotic (over large intervals of time) behavior.

4. Linear and Nonlinear Models

Realistic mathematical models of real world systems and processes are, as a rule, nonlinear. Linear models are often considered as particular cases and usually they serve as the first approximation to the reality. The non linear mathematical models are essentially more complicated for investigation by both numerical and analytical methods, even more complicated by the latter.

For linear mathematical models the superposition principle holds; it implies that any linear combination of solutions (e.g., their sum) is also a solution of the problem. Using the superposition principle it is not difficult, starting from a solution in particular case, to construct the solution in a more general situation. Some qualitative properties of the general solution may be seen from the properties of the particular one - distinctions between two solutions are only quantitative in character.

For nonlinear systems and processes, whose mathematical models do not satisfy the superposition principle, the knowledge about the behavior of a part of the object does not guarantee knowledge about whole object and its response to a change of conditions may qualitatively depend on the value of this change. The general solution can be found only in seldom cases for the simplest nonlinear mathematical models. Separate particular solutions of nonlinear equations may not reflect properly the behavior of the object in a more general situation.

A practical investigation, as a rule, is connected with the necessity of the consideration of nonlinear mathematical models. Linear models are used for description of non-essential deviations of the values characterizing the object.

Nonlinear mathematical models are often characterized by the fact that small deviations of input data, acting on the investigated object, lead to a qualitative change of the solution. To illustrate such nonlinear effects let us consider the simplest nonlinear model.

We deal with the ordinary differential equation with a quadratic nonlinear term

$$\frac{du}{dt} = au^2 - \mathrm{b}u \qquad (9)$$

With the positive constants a, b and a certain initial condition $u(0) = u_0 > 0$. Such a mathematical model is typical, e.g., in the description of chemical reactions.

The stationary state holds at $u(0) = w$ where $w = \mathrm{b}/\mathrm{a}$. The general solution takes the form.

$$u(t) = u(0)\frac{w\exp(-\mathrm{a}t)}{w - u(0)\left(1 - \exp(-\mathrm{a}t)\right)}. \qquad (10)$$

Depending on the initial condition $u(0)$ we obtain two fundamentally different features of behavior of the solution.

If $u_0 < w$ the solution monotonically decreases to zero as $t \to \infty$. If $u_0 > w$ the

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Biographical Sketches

Alexander A. Samarskii is a professor at the Institute of Mathematical Modelling, Russian Academy of Sciences, Moscow, Russia. He born in 1919 in Donetsk region of Ukraina and graduated from the

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His long-time career as an educator has resulted in the creation of a world-known scientific school in the field of Computational Mathematics and Mathematical Modeling including not only Russian researches, but also colleagues from Germany, Bulgaria, Hungry and some other countries. There are many highly experienced specialists, professors, associate members and members of the RAS among his students. Academician Samarskii has organized and chaired many international conferences on mathematical physics and difference methods, and served as guest lecturer at many other international forums..

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