The Theoretical Aspects of Biosystem Mathematical Modeling

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Abstract

Computational models play an important role in framing our existing knowledge. Such a formal framework is capable of testing scientific hypotheses about biological systems. Increased numbers of annotated models are being developed in order to facilitate communication, search, comparison, retrieval, and validation. A key part of model description relies on consistent representation of information which has been addressed through structured file formats and community guidelines. As we move towards a more comprehensive representation of model-related information, it becomes ever more important to understand how this information is most easily integrated in order to satisfy complex use scenarios. Here, we review key model-related data and emerging methods for facile integration and analysis. More effective approaches for knowledge representation are essential to decrease the time and efforts involved in data integration and create new opportunities for model-based science.

Keywords: mathematical modeling, biosystems, conceptual, analytic, and computational models.

Introduction

The problem of biological analysis and forecast is very difficult not only due to high number of species of organisms, time-and-space heterogeneity of biological parameters but due to many other factors, such as links between the biosystem elements, cannot be neglected. Results obtained in controlled conditions of mesocosms demonstrate important interactions that often do not have sufficient attention (Sullivan, B.K. & V. Banzon, 1990). Complex, multi-component character of the medium and web of links, that stabilize its properties, are very important and must be dealt with. However, study of interactions of many parts is very difficult, even if they are much generalized.

The complexity of natural systems is often cited as one of the main reasons for difficulties in understanding their inter-relationships and to developing ways to manage natural areas. This complexity arises from (1) the great diversity of entities and interrelationships comprised by biological systems, (2) the intricate dynamics, and webs of interactions among these entities, and (3) their distribution patterns in both space and time (Solbrig, 1991). All these indicate that natural systems are not static but rather are constantly evolving and changing, as evidenced by the highly elaborate dynamics of the life cycle of species, and of energy and nutrient flows which are exchanged among and within entities.

Explaining the complexity of natural systems certainly presents biology with one of its greatest challenges in that answers to questions of complexity should provide keys for sustainable conservation and management of biological diversity, control of environmental pollution and pathogens, and providing better food for human populations in both the developed and developing nations. Fundamentally, a better knowledge of biological complexity in space and time is essential to the promotion of sustainable development for future generations.

2. The three major types of biological models

There are three major types of biological models, which are generally applied to different types of problems: (1) conceptual, (2) analytic models and (3) simulation/computational models. Until computers became available, the equations that described the dynamics of systems had to be solved analytically, severely limiting the level of complexity (as well as the resolution) of the systems that could be studied and the complexity of the dynamics that could be examined for any particular system. Table 1 shows the limits of analytical methods in solving various classes of mathematical problems in general.

Table 1: The limits of analytical methods in solving mathematical problems (after von Bertalanffy, 1968)

	Linear			Nonlinear		
Equation	One Equation	Several Equations	Many Equations	One Equation	Several Equations	Many Equations
Algebraic	Trivial	Easy	Difficult	Very difficult	Very difficult	Impossible
Ordinary differential	Easy	Difficult	Essentially impossible	Very difficult	Impossible	Impossible
Partial differential	Difficult	Essentially impossible	Impossible	Impossible	Impossible	Impossible

The solid line divides the range of problems that are solvable with analytical methods from those that are difficult or impossible using analytical methods and require numerical methods and computers to solve (table 1). Systems problems are typically nonlinear and fall in the range that requires numerical methods. It should be noted that whereas some special problems that fall in the areas labeled impossible in the table are actually possible to solve using analytical methods (frequently requiring special tricks), in general, one cannot depend on a solution being available. Computers have guaranteed that a solution can be found in all the cases listed in the table.

Although almost any subdivision of the universe can be thought of as a system, modelers of systems usually look for boundaries that minimize the interaction between the system under study and the rest of the universe in order to make their job easier. The interactions between ecological and economic systems are many and strong. Therefore, splitting the world into separate economic and ecological systems is a poor choice of boundary. Classical (or reductionist) scientific disciplines tend to dissect their subject into smaller and smaller isolated parts in an effort to reduce the problem to its essential elements. To allow the dissection of system components, it must be assumed that interactions and feedbacks between system elements are negligible or that the links are essentially linear so they can be added up to give the behavior of the whole (von Bertalanffy, 1968). Complex systems violate the assumptions of reductionist techniques and there-fore are not well understood using the perspective of classical science. In contrast, systems analysis is the scientific method applied across many disciplines, scales, resolutions, and system types in an integrative manner.

In economics, for example, a typical distinction is made between partial equilibrium analysis and general equilibrium analysis (Costanza, 1993). In partial equilibrium analysis, a subsystem (a single market) is studied with the underlying assumption that there are no important feedback loops from other markets. In general, equilibrium analysis, on the other hand, the totalities of markets are studied to bring out the general interdependence in the economy. The large-scale, whole-economy, general equilibrium effects are usually quite different from the sum of the constituent small-scale partial equilibrium effects (Clark, 2010). Add to this observation the further complication that in reality, equilibrium is never achieved and one can begin to see the limitations of classical, reductionist science in understanding complex systems.

Economic and biological analysis needs to shift away from implicit assumptions that eliminate links within and between economic and natural systems because, due to the strength of the real-world interactions between these components, failing to link them can cause severe misperceptions and indeed policy failures (Costanza, 1987). Because reductionist thinking fails in the quest to understand complex systems, new concepts, and methods must be devised**.** Achieving a comprehensive under-standing that is useful for modeling and prediction of linked biological economic systems requires the synthesis and integration of several different conceptual frames. Conceptual models are often flow charts that demonstrate the relation between different organisms in community and their environment, including the transfer of energy and nutrients.

Conceptual models are representative a model that is represented by conceptual representations of the relationships between different organisms in a community and their environment Analytic models are often more complex mathematically, and work best when dealing with relatively simple (often linear) systems, specifically those that can be accurately described by a set of mathematical equations whose behavior is well known. Simulation models on the other hand, use numerical techniques to solve problems for which analytic solutions are impractical or impossible. Simulation models tend to be more widely used, and are generally considered more biologically realistic, while analytic models are valued for their mathematical elegance and explanatory power. Simulation model utilizes mathematical algorithms to predict complex responses in biosystems dynamics (Jorgensen 1996, Grant 2008, Hall 1990).

3. Situation in the Sphere of Computational Resources

According Annals of Biomedical Engineering (1999) until computers became available, the equations that described the dynamics of systems had to be solved analytically, severely limiting the level of complexity (as well as the resolution) of the systems that could be studied and the complexity of the dynamics that could be examined for any particular system. Table 1 shows the limits of analytical methods in solving various classes of mathematical problems in general. A computational model is a mathematical model in computational science that requires extensive computational resources to study the behavior of a complex system by computer simulation (Olayiwola, 2016). The system under study is often a complex nonlinear system for which simple, intuitive analytical solutions are not readily available. Rather than deriving a mathematical analytical solution to the problem, experimentation with the model is done by adjusting the parameters of the system in the computer, and studying the differences in the outcome of the experiments. Operation theories of the model can be derived/deduced from these computational experiments.

Examples of common computational models are weather forecasting models, earth simulator models, flight simulator models, molecular protein folding models, and neural network models Because of the complexity of biosystems (in terms of numbers of species/biological interactions), biosystem models typically simplify the systems they are studying to a limited number of pragmatic components. These may be particular species of interest, or may be broad functional types such as autotrophs, heterotrophs or saprotrophs. In biogeochemistry, biosystem models usually connect with representations of non-living «resources» such as nutrients, which are consumed by (and may be depleted by) living components of the model.

4. The process of simplification in biosystems.

This simplification is driven by a number of factors:

Ignorance: while understood in broad outline, the details of a particular food web may not be known; this applies both to identifying relevant species, and to the functional responses linking them (which are often extremely difficult to quantify).

Computation: practical constraints on simulating large numbers of biological elements; this is particularly true when biosystem models are embedded within other models (such as physical models of terrain or ocean bodies, or idealised models such as cellular automata or coupled map lattices)

Understanding: depending upon the nature of the study, complexity can confound the analysis of a biosystem model; the more interacting components a model has, the less straightforward it is to extract and separate causes and consequences; this is compounded when uncertainty about components obscures the accuracy of a simulation. The process of simplification described above typically reduces a biosystem to a small number of state variables. Depending upon the system under study, these may represent biological components in terms of numbers of discrete individuals or quantify the component more continuously as a measure of the total biomass of all organisms of that type, often using a common model currency (e.g. mass of carbon per unit area/volume).

The components are then linked together by mathematical functions that describe the nature of the relationships between them. For instance, in models which include predator-prey relationships, the two components are usually linked by some function that relates total prey captured to the populations of both predators and prey. Deriving these relationships is often extremely difficult given habitat heterogeneity, the details of component behavioral ecology (including issues such as perception, foraging behaviour), and the difficulties involved in unobtrusively studying these relationships under field conditions. Typically relationships are derived statistically or heuristically.

For example, some standard functional forms describing these relationships are linear, quadratic, hyperbolic or sigmoid functions. The latter two are known in biology as type II and type III responses, named by C. S. Holling in early, groundbreaking work on predation in mammals (Holling, 1959). Both describe relationships in which a linkage between components saturates at some maximum rate (e.g. above a certain concentration of prey organisms, predators cannot catch any more per unit time). Some biological interactions are derived explicitly from the biochemical processes that underlie them; for instance, nutrient processing by an organism may saturate because of either a limited number of binding sites on the organism's exterior surface or the rate of diffusion of nutrient across the boundary layer surrounding the organism (see also Michaelis-Menten kinetics).

After establishing the components to be modelled and the relationships between them, another important factor in biosystem model structure is the representation of space used. Historically, models have often ignored the confounding issue of space, utilising zero-dimensional approaches, such as ordinary differential equations. With increases in computational power, models which incorporate space are increasingly used (e.g. partial differential equations, cellular automata). This inclusion of space permits dynamics not present in non-spatial frameworks and illuminates processes that lead to pattern formation in biological systems.

5. *Conclusion*

Twentieth century biology has to a great extent been based on the application of informational concepts to biological phenomena: genetic information, translation, translation, proofreading, editing, neuronal code, positional information-examples in molecular biology, neurobiology, and developmental biology abound. We conclude that computational analysis is a useful, tool for comparative investigations of biosystems, for analyzing trends, development of methods of ecological forecasting and interdisciplinary cooperation. A comprehensive understanding of linked systems requires the synthesis and integration of several different conceptual frames.

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