

# MATHEMATICAL MODELS IN ECOLOGY. THE ROLE OF CRITICAL REGIMES.

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## Introduction.

Ecology is one of the most complicated biological disciplines. Ecosystems are among the most complicated systems for investigation that science has to deal with. Just posing the question about the study of ecosystems became possible only in the XX century, which in itself is already quite an indicator of the magnitude of the field.

Every ecosystem consists of both biotic and abiotic elements. That's why the study of ecosystems is impossible without explicit contribution of geologists and geographers (for description and study of geological, hydro-geographical characteristics as well as of landscape and climate involved). Methods from chemistry and physics are also absolutely crucial (although unfortunately often insufficient) for the study of the abiotic part of the system. The core component of the system - the living creatures, plants and microorganisms - are the focus of study of the entire complex of biological sciences.

When studying ecosystems, one also needs to be familiar with socio-economical sciences, since the main purpose of ecology is to use biospheres for the needs of people. Perhaps, one should add - for humanity, which rises above the purely selfish "exploitation" of the resources, assuming also the role of the *keeper* of the biosphere. The interactions between the biosphere and the quickly developing technology are also quite complicated, since technology makes great use of the resources that are for now still available in ecosystems. On the other hand, the idea of resource conservation and preservation is already starting to take greater stand than before.

Mathematical sciences need to find their place in this important problem. For example, one can identify statistical methods for the qualitative estimations of ecosystem structure, or take the systems approach for description and classification of numerous intra- and interconnections of ecosystems, or focus on the more traditional aspects of the study of system change both in evolutionary and successive (generational) senses.

Even this brief overview of possible mathematical approaches to the problem indicates the vastness of the problem. Is modern science that consists of so many disjoint areas even ready to tackle it? Perhaps, the most sensible approach would be to try and identify the most acutely relevant sub-problems.

## Peculiarities of biological systems.

Proper identification of the main directions for investigation and modeling requires in-depth understanding of the specifics of biological systems. Very generally, one can point at four major characteristics of all living things: 1) the complexity of the inner structure of

each individual, 2) large number of factors that characterize the individual's environment, 3) existence in an open system, both in terms of energy, structure and information, and 4) considerable non-linearity - an enormous range of external characteristics that preserve viability of the system. Let's make a few comments about each of these characteristics.

**Complexity of inner structure.** This section could also be called "Respect towards a biological object". Any more or less complete description of even the simplest biological object requires the entire body of knowledge that was accumulated by the "pre-biological" sciences. Let's clarify this thought through a simple example. In popular literature wheels are often used as a way to stroke the humanity's ego with a claim that "biology did not come up with a wheel". But if we were to understand the concept of a "wheel" as the process of replacement of sliding friction by rolling friction, then any walking, jumping and running animals realize this principle in a much more flexible and elegant manner than does such a clunky object as a wheel. And if one were to pose an even deeper question, about the cyclical process of energy transformation, then biology "came up" with the absolutely magnificent principle of a "chemical wheel" - transformation of chemical energy into mechanical energy on all the levels of muscular contraction. From a purely mathematical point of view, system complexity implies that the description of its state requires a large number of numbers. On the language of mathematics this can be formulated as "*a phase space of a biological system is multidimensional*".

**Many factors to characterize an individual's environment.** Complexity of biological objects is not limited to their "insides". They function in a complex environment that is often prone to change. Moreover, it might not be unreasonable to assume that the very complexity of their structure is "compensatory" in nature. They are so complex precisely to be able to respond to the changes in the environment in such a way as to maximally preserve their "inner structure". Genetic material is of course guarded especially carefully. One can even say that the current complexity of a biological object is a storage of "experiences of interactions with environment" of the object's "mom", "grand-ma" and "great great great great grand-ma".

*A mathematical consequence:* a mathematical model of a biological system must contain a lot of parameters (both continuous and discrete) that define the environment, in which the biological system functions.

**System openness.** Biological systems are never "energetically closed" - by now even school kids know that. However, there exist some much more delicate aspects of this property. For example, for most highly developed plants the leaf is the primary organ for photosynthesis. But in certain climates the trees shed their leaves for the duration of the winter, making them a part of the environment. The interactions with the environment are even more complex for certain insects, for example, the ones that go through being a caterpillar and then a chrysalis. This property of some living organisms could be referred to as "morphological, or structural transience", or openness. The instances of "informational transience", such as "chemical interactions" among social insects, are also not uncommon.

From this we can make an important (although distressing for a mathematical modeler) conclusion: *one must model both the biological system and its environment.*

**Considerable non-linearity.** The range of possible changes of the conditions that a biological system (for example, the organs of hearing or sight) can sustain is much larger than the range of, for example, amplitudes and frequencies of mechanical devices. In many physical theories linear approximation that describes small perturbations from the state of equilibrium, is quite efficient and accurate. Taking quadratic terms into account usually significantly increases model precision. Higher degree of non-linearity is infrequent in “pre-biological” sciences.

The situation in biology is vastly different. Any degree of non-linearity is never high enough. Non-linearity in biology is *exponential* in nature. One of the most clear examples of this is the “Weber-Fechner law” that establishes logarithmic dependence of reaction on interaction. *The evolutionary meaning of such a strong non-linearity is quite understandable: one needs to be able to hear the rustle of a crawling snake and not lose sight at the flash of lightning.* Biological systems that could not take a hold of the enormous range of vitally important changes in the environment have simply died out, having lost in the struggle for existence. One their graves one could write: “They were much too linear for this world!”. *Similar fate awaits mathematical models that do not take into account this important property of life.*

### **Complex pre-biological systems. Limitations of the computational approach.**

In natural sciences one can find objects for which there exist relatively exact mathematical models. For instance, celestial mechanics predicts movement of the planets with as much precision as can be monitored with modern technology. In this sense one can talk about an exact model of a phenomenon. Another extreme example is quantum mechanics that describes behavior of atoms. In principle, there is no reason to doubt that Schrödinger’s equation captures the behavior of the molecules with high degree of precision. It is true at least for relatively small molecules, such as the benzene ring  $C_6H_6$ .

This is a good example, with which to demonstrate the limitations of our computational powers. Let’s try to (hypothetically) calculate the simplest benzene model - Schrödinger’s equation for 24 electrons. We take only 4 valence electrons per each of six carbon atoms, leaving out the “inner” electrons and disregarding the movement of the nuclei. Even in this simplification we end up with a partial differential equation for  $\psi$ -function that depends on 72 variables (24 x 3).

Now try to apply the difference scheme, taking only about ten points (which is very little, 100 would be better) for each variable. We end up with  $N = 10^{72}$  points in total. To fully understand just how enormous this number is, if the computer is capable of performing  $n = 10^{18}$  operations per second, one would need  $T = 10^{54}$  seconds (compared to the age of the Earth  $T_0 : T \gg T_0 = 5 \times 10^9 = 1.5 \times 10^{17}$  seconds just to make one single calculation step for this model.

### **Exact, approximate and elementary models.**

From a technical point of view, direct computation of the exact model of any phenomenon is practically impossible not only in biology, although here it happens especially frequently. This by no means implies that exact models are useless. But it does make tight interactions with pure and applied mathematics indispensable. A cleverly reduced approximate model can reduce the time that would be necessary for calculations by orders of magnitude. For instance, quantum chemistry is really just an approximation method for solving Schrödinger's equation for molecules. Quantum chemistry allows calculation of important (often energetic) properties for not very complicated but typical molecules and active groups. Even though we cannot find an exact solution of the problem, but knowing the exact Schrödinger's equation makes it possible to theoretically estimate the exactness of the approximate solution.

An exact, albeit very complicated mathematical model, allows to create approximate models that address specific questions. This results in "emancipation" of theory from experiment, although it is of course the experiment that has the last word. But "His Majesty Experiment" would now have the possibility of giving a clear, rather than a blurred answer. For instance, one does not need to verify the validity of quantum mechanics on molecules. Theory is verified on an elementary object (in this case, an atom) using relatively simple and exact experiments.

*Moral for a mathematician: specific and limiting cases in theoretical framework are important not just by themselves but also as a method for experimental verification of a fuller, more exact model.*

### **Is axiomatics possible in biology?**

Until recently the development of mathematics was primarily stimulated by the questions, arising in mechanics, physics and technical sciences. It is in the framework of this rather narrow spectrum of disciplines that the axiomatic ideal of the science has shaped. The core of this ideal is in determination (albeit experimentally) of the major postulates, followed by strictly logical construction of the remaining theory. The appeal here is evident: only a relatively small set of postulates is to undergo thorough specification and scrupulous experimental verification. The consequences of these postulates (models of specific events, as they are often referred to) automatically improve as a result of further specification of the postulates.

This ideal is realized in Hellenic (Euclidian) geometry in its most transparent, classical form. The axiomatic structure of the next major step in the development of the scientific thought, the celestial mechanics, is much more complex, where the role of axioms is played by the equation of movement, based on the law of Newtonian attraction.

Not all the consequences are clearly observable. For instance, the "three-body problem" still has no satisfactory solution, although each particular movement is easily traced by the modern computational methods.

Even more complex is the axiomatics of quantum mechanics, Its main postulate - Schrödinger's equation - is a partial differential equation. It has an exact solution only in the simplest (although very important) special cases. Purely computational approach, as has already been mentioned, is very cost-inefficient and as of now not possible.

All this seems to indicate that the axiomatic ideal is unfortunately characteristic only for “pre-biological” life sciences. However, this uninspiring conclusion probably pertains to biology as a whole. *Undoubtedly, some of its branches (not necessarily the ones close to the current subdivision into sub-disciplines) not only can but also should be constructed according to the axiomatic ideal.* Some ideas in support of this point of view are given below.

### “Hierarchy” and the small parameter.

During the past century there has been created a theory of cell-based structure of animals and plants, which was probably the most difficult and crucial step to “atomicity” in biology, a historical shift in understanding of hierarchy, discreteness and “non-mushiness” of living forms. Population is comprised of organisms. Organisms are comprised of cells. Yes, there is an enormous difference between a population and a single organism, and nevertheless there are also enough fundamental similarities to allow the use of the word “comprise” in both cases. Cells in an organ (or a tissue) of course interact with each other. However, this connection is much weaker than the connections that occur within a cell. Relative weakness of intercellular connections is very efficiently used in experimental work. A researcher chooses external forces (whether mechanical, physical or chemical) to be strong enough to cause the tissue to dissociate into individual cells. It is remarkable that a researcher can do this without compromising structure and function of each individual cell.

The relation of the “dissipating force” (whether it is force or acidity, voltage or heat) to the “destructive force” is the “dimensionless small parameter  $\epsilon$ ”, as we refer to it in mathematics. Such small parameters define qualitatively the measure of individuality of a cell in the tissue. Generalization of this notion of “up and out” to ecosystems and biosphere, as well as the “down and in” to cellular organelles and macromolecules is evident. *One cannot underestimate the value of this beautiful property of living organisms for effective implementation of mathematical methods in biology.*

### Neighboring levels.

Mathematics deals with the same reality as do the rest of life sciences. The difference, however, lies in methods, approach, point of view. Mathematics studies connections, relations, analogies of phenomena rather than their factual implementation and realization in the “real world”. The loss in the field of concreteness is, of course, obvious. However, it is more than compensated (and only these topics are worth the effort) in generality and quantity of applications. For example, an ichthyologist that writes prognoses for the changes in the number of a certain type of fish works on a population level, never “descending” to the molecular level and never “ascending” to the level of the biosphere. This possibility to not take into account neighboring (upper and lower) levels is tightly related to the idea of the small parameter, or rather, of two small parameters. Moreover, these parameters gain a different - kinetic, temporal - interpretation. The environment can be considered to be nearly constant: it changes rather slowly on the scale of space and time that is characteristic for an object in question. This is the kinetic “disguise” of the small parameter, of the measure of individuality. The inner environment of the object can also be considered

constant, or rather depending only on the key variables that describe the object in question. However, the reason for it in this case is in a way opposite. Subunits (for instance, individuals within a population or cells within an individual) move, change, oscillate so quickly that only the average values of these fast variables can be of any importance.

Should one “break into an open door” and “give a mathematical proof” of the possibility of doing an investigation on the scale of just one such level? Of course, one probably wouldn’t need to if it weren’t for two issues. *Firstly, it is impossible to remain within just one level - one needs to know the borders of applicability of this “mono-leveled” system.* For instance, one cannot understand patterns of crucial migratory phenomena just on the population level, without physiological (and even biochemical) analysis of the stress factors. *Mathematics helps to understand the general cause of the “break” of the neighboring level, i.e. the loss of stability of the system in question.* *Secondly, mathematical analogies can sometimes help model the phenomenon in question on a different (sometimes more experimentally-friendly) level.* Even the mention of the “avalanche” nature of certain migratory processes is an indication that one can re-read the problem as a possible physical model - analogy.

### **Critical regimes, and oscillatory regimes in particular.**

Biological phenomena are extremely complex. Even within the framework of one level, even after having “zeroed-out” all the small parameters, after having gotten rid of everything possible and simplified everything that is “simplifiable” one rarely ends up with a manageable model. In such cases the following methodological trick can be of help. One can purposefully take the system outside of the boundaries of stability by changing the parameters of the model or experimental conditions. In such critical situations the number of key variables is usually quite small - often they are just one or two. Of course, under different conditions a different set of variables will play the key role. But if one does succeed in taking the system to the “neutrality level”, then the structure and properties of the system in question become much clearer.

From here, one can purely mathematically find all possible types of kinetics of the system that has ended up in this type of a critical situation. Those are different types of oscillatory regimes, well known from the field of radio mechanics. Relaxation analogues of these regimes (explosion or monomolecular decay) are also possible, as well as the combination of all of the above (such as tissue differentiation during embryogenesis). All of these regimes have of course already been well studied by theoreticians.

It is important, though, that in every system, however complex it may be, the simplest type of stability loss will follow one of the scenarios described above. *Mathematical models or radioactive decay (an extremely important example of a monomolecular reaction) or of a valve oscillator are not just examples but typical “representatives”, canonical forms of the most complex systems.* It is obvious how much our respect for these models increases when we fully understand this idea.

### **Ecological aspects of the method of critical regimes**

Ecological systems are examples of objects, where one should legislatively forbid the application of the methods that were so compassionately described in the previous section. This is in fact one of the most important tasks in the interaction of “Man and the Biosphere” - not to let the ecosystem go to the unstable extreme. That’s why one needs to learn to get the models to this edge, to learn about the boundaries and their whereabouts. It is a well-known fact that a number of ecological systems are now exactly in the critical state (by now it is not important whether it was done through ignorance or on purpose). So, one needs to try to turn “lemon to lemonade”, collect information, conduct objective studies, observe and find feasible ways to try and fix the situation. *So, the method of modeling of the critical regimes is most effective in this type of situations, when modeling becomes crucial.*

System analysis approach, a thorough account of all possible, complicated, aimed at finding ties and connections should be supplemented by qualitative estimates about the weight and importance of these connections. One needs to compare different models that stem from alternative hypotheses about which variables are most crucial, and compare the conclusions, generated by the model, with experimental data.

#### **“The limiting reagent” and regulation.**

With the help of Darwin’s theory of evolution we can now quite clearly visualize the process of the appearance of regulatory mechanisms. The idea of a small parameter, which has independently also arisen in chemistry, where it has been termed “the limiting reagent” of the reaction, helps us to understand the evolutionary formation of at least some regulatory systems. At first this is the most “exposed”, the most “vulnerable” stage of development. Then the system either goes extinct, or “takes charge” over the limiting reagent (such as, for instance, increased amount of carbon dioxide stimulates respiratory center in the brain). In general, “turning lemons to lemonade” is probably one of the most fascinating evolutionary inventions.

If this is the case, then maybe one should let time take its course? Of course, it is a possibility. The question becomes - what is the price that the biosphere, humanity and civilization would have to pay for this self-regulation. *Unfortunately, in ecological systems we do not have the luxury of time on evolutionary scale. We are forced to replace consecutive evolution with parallel analysis.* However, if we want (and we do!) to have *anything* left to regulate, and *anyone at all* to do it, this analysis has to be based on a model.

The ideas presented here hopefully elucidate the role and place of mathematical modeling in ecology.

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