



Molecular recognition of the environment and mechanisms of the origin of species in quantum-like modeling of evolution



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ARTICLE INFO

Article history:

Received 26 December 2016

Received in revised form

15 April 2017

Accepted 26 April 2017

Available online 5 May 2017

Keywords:

Speciation

Molecular recognition

Entanglement

Quantum control

Quantum information

A review of the mechanisms of speciation is performed. The mechanisms of the evolution of species, taking into account the feedback of the state of the environment and mechanisms of the emergence of complexity, are considered. It is shown that these mechanisms, at the molecular level, cannot work steadily in terms of classical mechanics. Quantum mechanisms of changes in the genome, based on the long-range interaction potential between biologically important molecules, are proposed as one of possible explanation. Different variants of interactions of the organism and environment based on molecular recognition and leading to new species origins are considered. Experiments to verify the model are proposed. This bio-physical study is completed by the general operational model of based on quantum information theory. The latter is applied to model of epigenetic evolution. We briefly present the basics of the quantum-like approach to modeling of bio-informational processes. This approach is illustrated by the quantum-like model of epigenetic evolution.

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1. Introduction

Speciation mechanisms are currently the subject of debate. This is because the theory of evolution itself is undergoing changes associated with both different forms of inheritance (Jablonka and Lamb, 2006) and different mechanisms of genome restructuring, studied over the past quarter of a century (Shapiro, 2013).

On the other hand, *the problem of origin of complexity, which is important in relation to living beings, is unsolved*. This problem has many aspects. For example, we can highlight the algorithmic complexity, computational complexity, information complexity and statistical processing of information. Different definitions of the complexity of living systems are considered in (Heylighen, 1999; Dawkins, 1986; Miconi, 2008; Piqueira, 2009; Finlay and Esteban, 2009; Marquet, 2000; Gell-Mann, 1994; Crutchfield, 2003; Salthé, 2008). In particular, two papers (Melkikh, 2014a,d; 2015) emphasized that this problem (associated with the need to enumerate an exponentially large number of genomic variants) should be solved on the basis of precise mathematical formulation.

In regard to the evolution of life, we are always dealing with complex structures. This is one of the most important properties of living systems, without exception. Even some of the simplest single-celled organisms, such as Archaea, or cyanobacteria, have genomes that are approximately equal to the 10^6 pairs of nucleotides. These genes encode complex systems of molecular transport, information reception, energy conversion and many other processes.

Consider a chain of nucleotides of length N . There are 4^N variants of such sequences. How large is this number? For example, for $N = 1000$ we receive $4^{1000} = 10^{602}$. Note here that $N = 1000$ corresponds to only one modern gene. For a genome size of 10^6 – 10^9 the number of variants in any case is exponentially large and cannot be enumerated during the lifetime of the universe. In this sense, the problem of enumeration of genomic variants – the combinatorial problem – is the key to evolution. Without its solution it is impossible to speak about the adequacy of the theory.

A. Melkikh (2014a,d) presented some reasons that such an algorithmic formulation of the problem leads to the following dilemma:

- Evolution is a priori undirected, but then it is impossible to prove a rational mechanism for the selection of variants of an exponentially large number. This applies to all mechanisms, including sexual reproduction, the selection of alleles in a population, and phenotypic plasticity.
- Or, evolution is a priori directed (i.e., it is known a priori that certain blocks encode something good). However, it is then difficult to justify the existence of such mechanisms in the framework of Darwinism. The essence of Darwinism is that a priori evolution will not focus elsewhere, it has no purpose, and species cannot know what they will need in the future. These are the axioms without which Darwinism does not exist.

To solve this problem, a mechanism for partially directed evolution was proposed (Melkikh, 2014a,d; 2015, Melkikh and Khrennikov, 2016). The term “partially” reflects the fact that in any case, uncertainty in some form will be present in the environment, even if evolution was completely directed. This is due to the factors such as the uncertainty of the climate, and different random events such as asteroid strikes. In connection with this, it is possible to introduce a criterion for the partial directivity of evolution, as the ratio of the number of nucleotides in the genome, changed according to a priori information to the number of all nucleotides that changed during the same time. Such a ratio can be determined from special experiments on directed evolution (see

Melkikh and Khrennikov, 2015).

In particular, in the frame of the model of partially directed evolution it is possible to consistently explain many different evolutionary phenomena, such as the finite lifespan of organisms, the existence of the sexes, the genetic diversity of populations, the effect of the Red Queen, and phenotypic plasticity (Melkikh and Khrennikov, 2016). The theory of partially-directed evolution can be considered as a continuation of L. Berg’s ideas about nomenogenesis (Berg, 1969) at the new level. Indeed, Berg’s book (1922 in Russian) was written in an era when the understanding of the genetic basis of evolution was only at the beginning. Ideas on the directivity of evolution are necessary, first, to be formalized (i.e. to build a mathematical model of directed evolution), and, secondly, to be reconciled with modern data of molecular biology. Papers (Melkikh, 2014a; 2015, Melkikh and Khrennikov, 2016) are also devoted to this goal.

Of course, the notion of “directed evolution” has to be formalized and this is a complex problem. For the moment, we use it heuristically and its essence is illustrated by important biological and bio-physical examples. The minimalist interpretation of “directed evolution” has the Lamarckian feature: changes in biological organisms are adapted to environment during organisms’ life-time. (Thus not simply Darwinian mutations combined with post-selection generated by the environment.) This type of so-to-say instantaneously directed evolution is illustrated by the quantum-like model of epigenetic evolution proposed by Asano et al. (2013), see section 6 for the brief presentation of its basics. However, one of the coauthors, see Melkikh (2014a,d), proceeds with a stronger interpretation. In his works it is presumed that biological systems (primary at the genetic level) can select the “optimal evolutionary pathway” and this optimization “drive” plays the active role in their evolution.

Among the major challenges to be answered by the theory of evolution are the following:

- Q1:** How does biological complexity arise?
- Q2:** How do new biological systems arise?
- Q3:** How do new species cross the “ravines” in the fitness landscape?
- Q4:** Why are the molecular-genetic control systems stable?

The article is devoted to the detailed mechanisms of partially directed evolution towards evolutionary innovation and speciation.

2. Biological complexity and evolution

From the mathematical point of view, we can identify algorithmic complexity, computational complexity, information complexity and statistical processing of information. In varying degrees, all these types of complexity may be relevant to the modeling of living systems. However, if the underlying problem is to consider the emergence of complex systems during the process of evolution, it seems that computational complexity is the most relevant. Computational complexity is associated with the characteristics of a mass of problems (as opposed to individual tasks of algorithmic complexity).

There are many classes of computational complexity (complexity of algorithms for computing), the most important of which are P and NP . The first is a polynomial algorithm in which the number of steps depends on a power of the number of elements of the system being analyzed. The class NP includes algorithms in which the number of steps depends exponentially on the number of elements. The question of reduction of NP -problems to P -problems is fundamental and has so far not been solved (see, for example, Aaronson, 2005).

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