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Review Article

Quantum information and the problem of mechanisms of biological evolution

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ABSTRACT

One of the most important conditions for replication in early evolution is the de facto elimination of the conformational degrees of freedom of the replicators, the mechanisms of which remain unclear. In addition, realistic evolutionary timescales can be established based only on partially directed evolution, further complicating this issue. A division of the various evolutionary theories into two classes has been proposed based on the presence or absence of a priori information about the evolving system. A priori information plays a key role in solving problems in evolution. Here, a model of partially directed evolution, based on the learning automata theory, which includes a priori information about the fitness space, is proposed. A potential repository of such prior information is the states of biologically important molecules. Thus, the need for extended evolutionary synthesis is discussed. Experiments to test the hypothesis of partially directed evolution are proposed.

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1. Introduction

Despite progress in understanding evolution (including its early stages), a number of fundamental issues remain unresolved. One of the simplest living systems in early evolution is the replicator, a molecule that can reproduce itself. However, the conditions under which this replication is possible remain unknown. Particularly, whether molecules have many conformational degrees of freedom and replication occurs with sufficient accuracy has not been determined. A replicator will typically assume different spatial configurations, most of which will not be able to replicate, which is more important for complex evolving systems, (e.g., protocells).

Even if replication is precise, it is unknown whether the proteins encoded by these replicators accomplish useful work or whether useful proteins evolve from the enumeration of variants. If we start from modern genetic distances between closely related species, these patterns can be observed only for short sequences; however, further complications arise from the question of biological systems on the qualitative change in the mechanism of evolution compared

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with the enumeration of variants. Currently, these mechanisms are considered as modular blocks when existing genetic units are used again for the new encoding species; however, this algorithm implicitly assumes that the genetic system contains a priori information about optimal combinations of nucleotides.

This information should be mathematically included in evolutionary theory via partial-information games. The storage of such large amounts of additional information might be explained using quantum mechanics. In principle, qubits store an exponentially large amount of information, although only for pure quantum states, and the question arises of how to avoid decoherence in this system. The need to consider quantum effects in evolution discussed earlier. In some papers (Ogryzko, 1997; McFadden and Al-Khalili, 1999; Goswami and Todd, 1997), it has been suggested that quantum mechanics plays a fundamental role in the mechanism of adaptive mutations and the models of this process were built. However, the question remains of how fundamental the application of quantum models is for arbitrary processes of evolution.

To answer these questions, this article suggests a model of partially directed evolution based on the quantum processing of biological information.

2. Complexity, early stages of evolution and quantum effects

2.1. Under what conditions do replicators exist?

The conversion of simple molecules into more complex organic molecules could occur abiogenically during early evolution, as observed for organic molecules (polypeptides and polynucleotides) in a circuit under protoatmospheric conditions. One of the most important properties of these molecules, in terms of biogenesis, is replication, with small copying errors that modify the initial components and the subsequent selection of favorable options. Several models describing the evolution of self-replicating molecules, i.e., replicators (Eigen and Schuster, 1979; Koonin and Martin, 2005; Fernando and Rowe, 2007), have been proposed. However the question remains, under what physical conditions can such an evolution occur.

It is obvious that energy is required. Chemical reactions and light are generally considered as sources of free energy.

However, models of replicators do not typically consider how replication will occur with any precision. If the molecules-replicators have a large number of degrees of freedom (mainly conformational), the result of the reaction will depend on the conformations of the molecule (e.g., RNA). For most of these conformations, replication is not possible, and the same principle applies to enzymes (catalysts).

Thus, sequences that generate copies when supplied with a source of free energy are a necessary condition for the evolution of replicators. Therefore, we must consider sufficient conditions.

Melkikh (2013) discussed the issue of complexity with regard to biologically important molecules. If we consider replication as a catalytic chemical reaction, in which the complexity of biomolecules plays a critical role, this process can be divided into two stages: folding the molecules into the native configurations and recognizing the molecules when making copies.

Most biologically important molecules (primarily proteins and RNA) have only a small number (typically one) of configurations in which these entities function. What, for example, will a copy of an RNA molecule look like? Generally speaking, this molecule can fold into a variety of potential spatial configurations. If these configurations are different from the original configuration of the RNA, they are no longer copies; RNA in another configuration represents another material with completely different characteristics.

The problem of protein folding was investigated in more detail. Although many studies have been devoted to this issue (the Levinthal paradox), the complexities of protein folding have not been resolved. In many cases (Berezovsky and Trifonov, 2002; Bai, 2003, 2006; Grosberg and Khokhlov, 2010), the existence of a "good" (i.e., not too rugged) energy landscape is simply postulated (i.e., is not derived from the first principles). However, is this a landscape always exists?

If such a (funnel-like) landscape exists, the Levinthal paradox can be avoided; however, Melkikh (2013) proposed objections to the existence of this landscape. The most important objection is that whatever the folding of the molecule (protein, RNA), energetically equivalent states with equivalent probabilities will be observed. The presence of at least one such fork reduces the probability of obtaining the "right" configuration by half. In addition, Melkikh (2013) showed that in the case of a large molecule of length $N \gg 1$, the number of possible ways of folding due to forks is exponentially large:

$$P(N) = \left(\frac{1}{2}\right)^{N/2}.$$

If the number of such variants is comparable to the total number of molecules, the replicator will not reproduce. Even for a replicator with five domains, the efficiency of proper replication is exponentially small.

Note that the protein, of course, can fold correctly even after a "fork" (that is, after the folding went the wrong way), but such a process is unlikely. Indeed, if the molecule in this step has an incorrect configuration, the probability of the next step returning to a correct configuration (i.e., correct an error) is significantly smaller than moving to the other wrong configuration because there are many incorrect configurations but only one correct configuration. Because this formula is an estimate of the order of magnitude, these processes in such a case can be ignored.

Thus, the problem of folding replicating molecules is that the longer the molecule, the lower the replication efficiency. In other words, the correct folding of a sufficiently long molecule requires an exponentially large amount of time. This problem does not exist for a simple substance without any spatial configuration. Such autocatalytic reactions are well known.

A second important aspect of replication considers the accuracy of the copy.

A large number of reactions between two interacting molecules are possible. Many chemical reactions (including those associated with the transfer of information) involve a "key and lock" (or "hand-glove", see for example (Savir and Tlusty, 2007)) mechanism, under which the shape of one molecule must precisely correspond to the form of another to permit enzymatic reactions. If there is no match, then with overwhelming probability, the reaction does not occur. Thus, how does each "key" find its "lock"? Melkikh and Sutormina (2013) and Melkikh (2013) considered this issue. This problem can be considered as a type of Levinthal's paradox. In fact, if a reaction occurs between two molecules, each of which has a large number of possible degrees of freedom, then during the interaction, a molecular complex is formed that has many more degrees of freedom than the reacting molecules. For the "correct" version of the reaction (matching key and lock) to take place, this complex must somehow move from some initial configuration (keeping in mind that there can be many such configurations at the initial meeting of the molecules) to a well-defined target configuration. Such a transition is fundamentally no different from protein folding, i.e., two reactive proteins can be regarded as a single protein composed of two parts. As shown above, the folding of such proteins requires exponentially long times.