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Non-Darwinists Scenarios of Evolution of Complicated Systems and Natural Neural Networks Based on Partly Dissociated Macromolecules

I. Suleimenov and S. Panchenko

Almaty University of Power Engineering and Telecommunications,
Almaty, Kazakhstan

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Abstract: Additional evidences of existence of the neural network mechanism of evolution of complicated systems that is different from the evolution scenarios based on the Darwinian point of view are given. According to this mechanism, a complicated system can be considered as analog of the neural network. At the first stage, there is evolution of this neural network, which does not change features of the constituent elements. At the second stage, a transformed neural network converts into some filter selecting elements, which features are the most compliant with a new state of the system. It is shown that any partially dissociating macromolecules represent analog of the neural network due to their own physical and chemical properties. It gives possibility to state a hypothesis that evolution preceding a biological one was really in compliance with the neural network mechanism.

Key words: Evolution · Neural networks · Polyelectrolytes · Complicated systems

INTRODUCTION

At present, there are active researches directed for understanding of the mechanism of evolution, which was preceding a biological one [1-4]. However, almost all modern concepts of evolution are based on the point of view coming from the Darwinian theory. This theory, in turn, is based on consideration of spontaneous mutations (fluctuations) supposing that new features provide an element of the system with additional competitive advantages. Generally speaking, modern concepts, in particular [1-4], assume that changing of the constituent elements is primary in respect to changing of the whole system.

However, trying to use analogs of the Darwinian theory (concepts assuming that change of features of the constituent elements is primary in the course of evolution of the complicated system) to determine mechanisms of evolution preceding a biological one, there are some significant hardships. One of such problems is closely connected with a problem of «generation» hereditable information [5, 6].

In terms of physical chemistry of polymers, a problem of generation of information can be formulated as follows. There is a system based on the macromolecules; so, a question is: what conditions are necessary for *spontaneous* creation of a mechanism of self-reproduction of structures able to perform operations close to the logical ones and able to the further evolution.

Answer to this question is interesting not only in the academic field. Effective tools of modern nanotechnology include processes of self-organization enabling to produce nanoscale elements with the help of macroscopic impact [7-9]. There is no need to prove that realization of macromolecule systems able to the controlled evolution will allow significantly extend opportunities of creation of a nanostructure by means of macroscopic impacts.

A new scenario of evolution of the complicated systems based on the non-Darwinian approach was suggested in [10].

The concept [10] can be formulated as follows.

It is well known [11, 12] that such properties of the neural network as ability to recognize some images, store information and so on depend not only on the features of the certain elements but on the structure of connections

Corresponding Author: I. Suleimenov, Almaty University of Power Engineering and Telecommunications, Almaty, Kazakhstan.

and weight coefficients describing impact of neurons (or their analogs) on each other. Therefore, there are some reasons for evolution of neural networks able to be realized *without changing of properties of the constituent elements* because such evolution is only connected with reconstruction of the system of inter-element connections. One can find the corresponding examples in the field of social and economic sciences [10]. In particular, a social system in a whole can be considered as a neural network analog establishing compliance between individuals and formal neurons. In this case, quick evolution of the modern society can be interpreted through the global reconstruction of the system of interpersonal communications caused, particularly, by development of the telecommunication industry. There are also known mathematical models of evolution of the neural networks of the considered or similar type [13-15].

At the next stage of the evolution scenario [10], a transformed neural network is converted into the filter selecting elements with properties compliant with the modified state of the system. Advantages of this concept [10] include an opportunity of interpretation of "jumps" in the evolutionary development. The first stage of evolution of the system is latent and can be quite slow, while speed of the second is significantly higher (here one can see the "directed" selection of elements with the certain features).

The most important difference of the concept [10] from the known earlier, in particular [1-4], is that evolution of the system in a whole is primary (but not evolution of its constituent elements). It enables us to consider evolution as a response to changing external conditions and speak about possible creation of the systems with controlled evolution, which way is determined by the macroscopic impacts.

Scenario [10] is applicable for the complicated system of any nature providing that a certain system can be considered as analog of the neural network (this system can be compliant with a complementary neural network). Therefore, a problem of opportunity of implementation of the non-Darwinist scenarios [10] to description of pre-biological evolution is reduced to the problem of the neural network properties of macromolecules.

It is shown that there is a wide range of macromolecules representing direct analogues of the Hopfield neuroprocessor due to their own properties in this article.

Weak Polyelectrolytes as Analog of the Hopfield's Neural Network: From the physical and chemical point of view, informational biological macromolecules (for example, DNA) represent polyelectrolytes, i.e. substances with partially dissociating functional groups. Dissociation reaction causes appearance of the electrostatic charge of the relevant group of the macromolecular chain due to separation of the low-molecular ion.

There were some efforts to use this feature for interpretation of behavior of polyelectrolytes from the informational point of view (there is an analogy when a logical unit is associated with a charged functional group and logical zero corresponds to electrically neutral one). However, such efforts could not provide significant results, in particular, because a charge of the macromolecular chain is «floating», i.e. it can be transferred from one functional group to another beyond any control. Energy of such transition is comparable with the energy of temperature fluctuations and it does not allowing consideration a certain functional group as a direct analog of the digital memory cell.

One cannot consider a linear chain of the polyelectrolyte as some sequence of memory units because of thermodynamic reasons. Quite different situation appears at consideration of the neural networks. It is known that «errors» connected with uncontrolled changing of state of a certain neuron do not have critical impact on the network as whole [11, 12]; it is generally accepted that neural networks are tolerant to the errors. Information is stored in the neural network as whole and it is often compared with a hologram which separate part can restore the same image that a hologram as whole.

Therefore, answer to the question if a fluctuating system, i.e. polyelectrolyte chain, can have some memory, is reduced to the question whether it is possible to consider such object as analog of the neural network.

Let us show that such analogy is completely competent.

Let us consider a simplified diagram of the linear polyelectrolyte (Figure1). One can see the functional groups able to obtain an electrostatic charge due to dissociation; arrows shown in Fig.1 underline that a charge obtained by a certain functional group impacts on behavior of all the others.

Physical realization of such diagram is, for example, molecule of the polycarbon acid chain, which charge is determined by equilibrium in the following reaction:

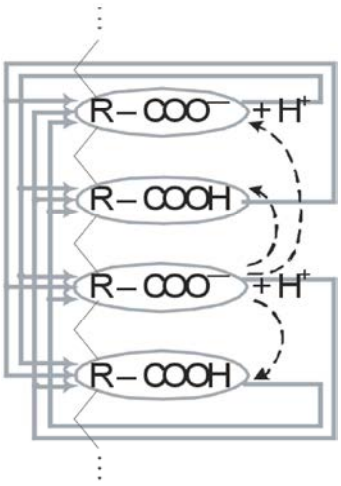

Fig. 1: Simplified diagram of the linear polyelectrolyte behavior

$$R-COOH \Leftrightarrow R-COO^{-}+H^{+} \tag{1}$$

It is of importance that equilibrium constant in the reaction (1) is determined by the electrostatic potential of the point where this group is too. This fact defines a mechanism of impact of the macromolecule state on probability of dissociation of a certain functional group that is highlighted by the arrows in Fig. 1. It is obvious that electrostatic field acting in a certain point depends on state of each functional group and their position in the space.

The fact gives possibility to consider every partially dissociating group as analog of the formal neuron. Indeed, let us suppose that output of this neuron corresponds to a logical one if a relevant functional group obtains electrostatic charge and corresponds to logical zero in the opposite case. Impact of the other groups on probability of dissociation of the separate monomer unit can be interpreted through existence of the feedbacks in the Hopfield neural network shown in Fig.1 at the background, which connect an output of every neuron with inputs of the others.

This analogy can be reasoned considering functional describing energy of the partially dissociating chain in a whole.

At given position of chemical bonds of macromolecules in the space and fixed average degree of ionization of the macromolecule, spatial distribution of charges is described (in the frames of suitable approximation) by the minimum of the next functional:

$$F=\sum_{i,j}\varepsilon_i\varepsilon_j\, w\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right)+\sum_i \varepsilon_i U\left(\mathbf{r}_i\right) \tag{2}$$

where $w\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right)$ - energy of interaction of two charges in the points $\mathbf{r}_i$ and $\mathbf{r}_j$ correspondingly, ε_i - charge number of this functional group, $U(\mathbf{r})$- function describing effect of the cloud of counterions on the charges connected with the macromolecule chain and impact of the external electrostatic fields.

Formula (2) is quite rough because it is assumed that counterions are homogenously distributed in the volumes of the macromolecular coil. However, clarification of the formula (2) does not have impact on the conclusions provided in this work.

Finding a certain position of charges at the macromolecular chain of the considered type, one should take into account that the values of the variables ε_i can be only 1 or 0, i.e. functional (2) is determined on multitude of series of logical variables. Some of them comply with the minimum energy of the considered system.

It is known [12] that finding of the minimum of the functional (2) complies with solution of the problem searching of a sequence of logical variables describing states of outputs of a Hopfield's neural network. Functional (2) can be considered as a formal Hamiltonian for such network and its minimums comply with solution of the following equation:

$$I_i=f\left(\sum_{j\neq i} I_j\, w_{ij}+U_i\right) \tag{3}$$

where w_{ij} - weight coefficients of the neural network, $f(x)$ - function of the neuron activation, U_i - function describing states of the inputs of the neural network. For convenience of the numerical calculation, we can use the following activation function:

$$f\left(x\right)=\begin{cases}+1, & x\geq 0\\ -1, & x<0\end{cases}, \tag{4}$$

and next correspondence:

$$-1 \Leftrightarrow 0$$

at consideration of the logical variables.
Establishing the correspondence:

$$\varepsilon_i=I_i, \quad w_{ij}=w\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right), \tag{5}$$

one can show that solution of the task (5) allows finding the minimums of the functional (2). In other words, energy of interaction between the charges located at the different functional groups can be considered as weight

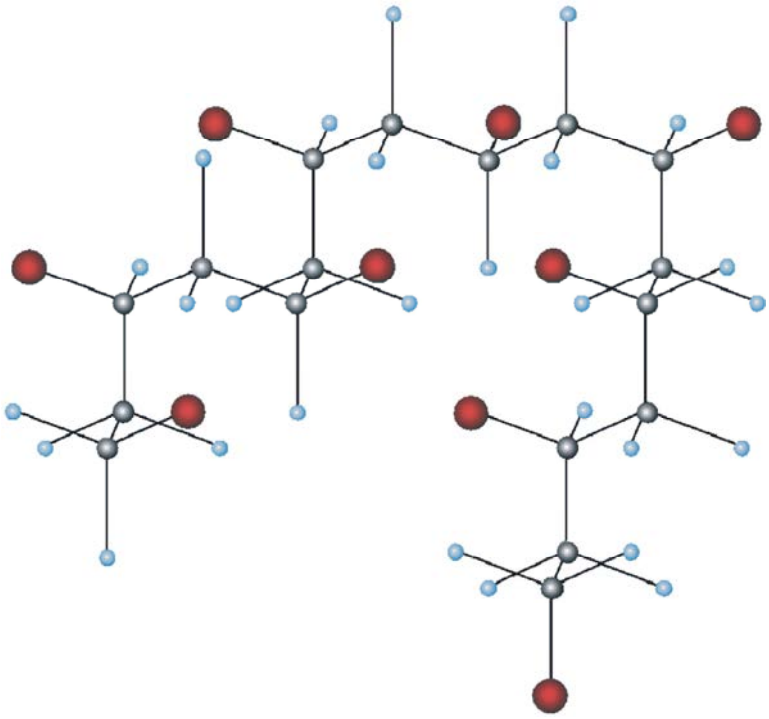

Fig. 2: Example of a special structure modeling polyelectrolyte chain

coefficients of the macromolecular neural network and variations of the chain configuration cause changing of the specified coefficients.

Therefore, analogy between the partially dissociating polyelectrolytes and Hopfield's neuroprocessors is correct.

Results of the Numeric Experiments: Next numeric experiments proving that macromolecules of the considered type demonstrate the main feature of the neural networks – ability to recognize images gives possibility to illustrate constructiveness of this analogy.

Numerically generated special structures complying with the different positions of the macromolecular chain bonds in the space were used; an example of such structure is shown in Fig. 2. An elementary model of the tetrahedral C-C connections was used.

Relating to every produced structure, values of the weight coefficients were calculated (models complying with the Coulomb interaction, interaction with the Debye–Hückel potential and dipole-dipole interaction were used).

Networks with growing number of links complying with the formal neurons of the network (9,10,11…) that corresponds to consideration of the macromolecular chain fragments with growing number of chemical bonds were studied.

All possible combinations of the logical variables were delivered to the inputs of this neural network. It corresponds to the different combinations of the external fields affecting the considered fragment of the macromolecule. Such external fields (relating to the selected segment) take into account the fields generated by charges of the remained fragments of the same macromolecule.

The response of the macromolecular considering as a neural network to all the series of logical variables reflecting condition of its inputs was studied.

An example of the diagram describing the response of such neural network (in respect to the structure presented on Fig. 2) to the different series of the input signals is shown in Fig. 3. Decimal number of the relevant series is shown on the abscissa axis, number of cases when the considered network recognized an image with this decimal number is shown on the other axis.

One can see that there are images recognized more often than the others. Structure of Fig. 2 corresponds to the most frequent recognition of the trivial series consisted of the alternating ones and zeros.

Non-trivial series occur when there are considered structures compliant with «loops» generated by the macromolecule. An example of such frequency diagram of recognizing images and relevant fragment is shown in Fig. 4 and Fig. 5.

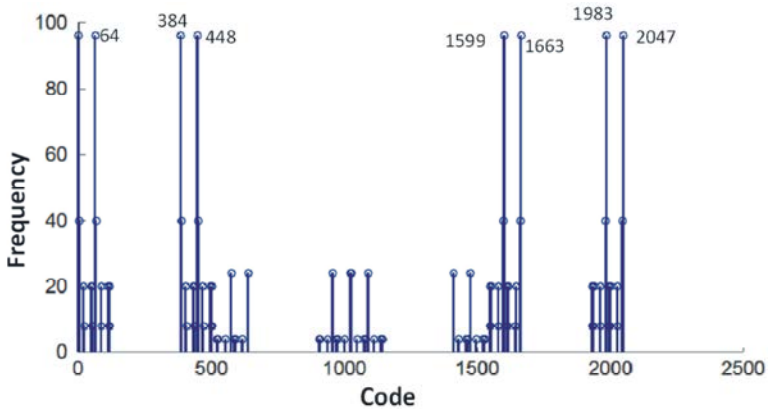

Fig. 3: Diagram of recognizing images by the structure presented in Fig. 2.

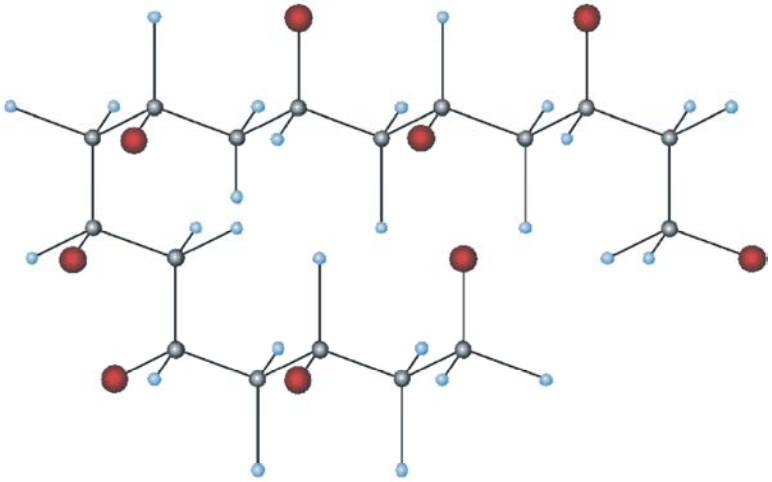

Fig. 4: Special structure compliant with the «loop» configuration

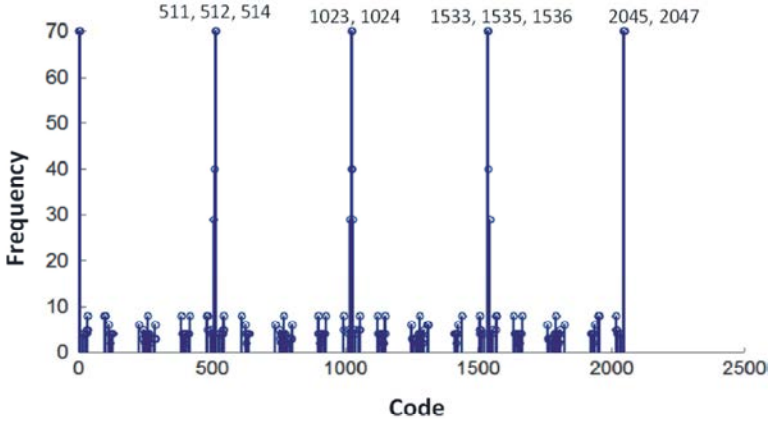

Fig. 5: Diagram of recognition of images by the structure Fig. 4.

The same figure includes decoding of the decimal numbers of series relating to the most expressed peaks.

One can see that there are structures generating quite certain non-trivial code series. These numeric models are simple but they point at the important fact discussed in connection with common ideas on origin of the biologically «valuable» information. (In [5, 6] this problem was interpreted according to the concept of generation of information.)

According to the most general point of view, a problem of generation of the genetic code can be considered as a question on probability of appearance of

structures bearing information in the course of pre-biological evolution. Analogy between the neural networks and partially dissociating macromolecules shows that there are conformations really generating the certain images (code combinations) stored in the «memory» of the relevant macromolecule fragment. Relevant logical series can be interpreted as a prototype of series bearing biological information and we can call them protocodons.

Such images have relative stability. According to the results of the numeric experiments carried out in this work, there are critical sizes of the macromolecular fragment for every potential describing interaction between the charges. Macromolecular neural network with dimensions approximately equal to the critical ones can recognize a certain set of images. Further increase of the network dimensions does not have impact on the series (images) of this set.

One can say that uncontrolled conformation transitions in real time cause creation of the fragments bearing the certain information interpreted as a code combination that this fragment can recognize with the maximal accuracy. This conclusion is important if there are conditions when the relevant information can be fixed, i.e. remembered and reproduced.

Supposedly, such conditions can be realized at creation of the well-studied objects – interpolymer complexes [16-18] and their less stable analogs – hydrophilic associates [19] which existence has been recently proved by the experiments [20].

Complexes and associates stabilized by the hydrogen bonds are the most interesting. It is known that product of the reaction between the macromolecules depends on conformation of each of them. Therefore, according to the general reasons, we can interpret an interpolymer reaction through interaction of the fragments with records of the certain code series. (At least, it relates to reactions between the partially ionized and non-ion polymers studied in [16, 19, 20]). Correspondingly, if an interpolymer reaction is convertible, it is a precondition for the evolution processes with «selection» of the certain code combinations compliant with the most advantageous conditions of a complex appearance.

CONCLUSIONS

Thus, result provided in this work show that 3D structures modeling the partially dissociating macromolecules are really analogs of the neural networks. Taking into account that used simplifications are not significant for description of the electrostatic interaction in the system, one can conclude that real macromolecules are also analogs of the Hopfield's neural networks.

This fact, in turn, means that systems based on the macromolecule able to evolve according to the neural network mechanism. It is admissible to provide a hypothesis that namely this mechanism (or its modification) was the basis of pre-biological evolution.

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