Sequencing for Encoding in Neuroevolutionary Synthesis of Neural Network Models for Medical Diagnosis

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Abstract

Today, artificial neural networks are actively used for various medical tasks. Diagnostics is one of these tasks that can be significantly optimized by using models that will be based on neural networks. Neuroevolution methods are used for synthesis more adaptive models. The work with such methods begins with the initialization of a population contains individuals, each of which is a separate neural network. For further work with them, encoding is used, that is, a certain representation of information about the neural network. The correct encoding method can significantly simplify and speed up further work, which will reduce resource consumption. In this paper, authors propose a new approach to information encoding during neuroevolutionary synthesis, which will expand the practical use of classical methods.

Keywords 1

Medical diagnosis, neuromodels, sequencing, encoding, neuroevolution, ANN, genetic operators

1. Introduction

One of the most relevant areas of medical and biological research is the development and implementation of intelligent systems for the diagnosis and prediction of modern human diseases [1-3]. The basis of this kind of systems are based on various mathematical methods and algorithms. Systems based on the mathematical apparatus of artificial neural networks (ANNs) are particularly effective for solving problems of medical diagnostics and forecasting [2-8]. ANNs are mathematical models, as well as their software or hardware implementations, built on the principle of organization and functioning of biological neural networks [1-7], [9]. Each ANN consists of elements called mathematical neurons [2-5]. A mathematical neuron receives information, assigns weight coefficients to it, performs calculations on it, and passes it on. Connected and interacting mathematical neurons form a neural network that can solve quite complex problems. Models based on ANNs are successfully used for processing large amounts of data, which is typical for complex nonlinear objects [10-13].

Evolutionary methods are often used to synthesize such models [14]. At a high level, the idea is very simple. Instead of relying on a fixed neural network structure, why not let it evolve through evolutionary methods. So, as a rule, when using a neural network, a structure is selected that can work on the basis of empirical data. But it is not known for sure whether this is the best structure that can be used. There's no way to know for sure. Therefore, the idea of gradually synthesizing the best network solves this problem, because the result is the most optimal structure with certain metaparameters (neurons, connections, and weights).

Therefore, the synthesis starts with generating a population of random topologies of ANNs. But an important issue remains the preservation and further development of such ANN. The network

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encoding stage [14] is always one of the research centers of neuroevolution methods. All existing ANN's encoding methods can be divided into direct encoding methods and indirect encoding methods.

Both groups of encoding methods have their advantages and disadvantages [14]. Direct coding should not take into account the close relationship between gene composition and individual performance, but should only prove that its coding design can contribute to effective network evolution. And indirect coding requires developing a set of encoding and decoding rules for transforming gene sequences and individual phenotypes, so there is a need to better understand the genetic and evolutionary mechanisms of biology.

The way genes of individuals are encoded is extremely efficient, and a very short sequence of genes can control complex phenotypes of individuals. Many modern studies of indirect coding are at the research stage, but with the continuous development of research on the mechanisms of biological evolution, research on neuroevolutionary methods based on both directions of coding still has great potential.

Moreover, a number of difficulties with choosing the encoding type are associated with modern ANN topologies. Thus, classical direct coding methods are almost impossible to apply for recurrent ANNs (RNN) [15], where in addition to direct connections between neurons, there are also feedback ones. When encoding deep ANNs (DNN), problems arise in both paradigms, because there is a task to encode not just hidden neurons, but to preserve the structure – distribution by layers.

That is why the task of developing new coding methods that would allow and simplify working with modern ANN's topologies and possibly be less resource-intensive remains urgent.

2. Literature Review

In classical genetics, it is usually distinguish between genotype and phenotype [16-22]. A genotype is a genetic representation of a creature, and a phenotype is an updated physical representation of a creature. Evolutionary algorithms always strongly reflect biology, neuroevolution is no different in this regard.

The coding question comes from the question of how it is wanted to represent the ANN genetically during operation. The way we encode the ANN determines the way the method will handle key evolutionary processes: selection, mutation, and crossover (or recombination) [16], [17]. Any encoding falls into one of two categories, direct or indirect.

Direct encoding operates on chromosomes that represent some linear representation of the ANN, in which all the neurons, weights, and connections of the ANN are explicitly specified. Thus, it is always possible to construct a one-to-one correspondence between the structural elements of the ANN (neurons, connections, weights, etc.), i.e. the phenotype, and the corresponding sections of the chromosome, i.e. the genotype [18].

This method of representing the neural network is the simplest and most intuitive, and also allows to apply the existing genetic search apparatus to the obtained chromosomes (for example, crossing operators and mutations) [19-23]. One of the most obvious disadvantages of this encoding scheme is the swelling of the genotype with an increase in the number of neurons and ANN's connections, and, as a result, low efficiency due to a significant increase in the search space [22].

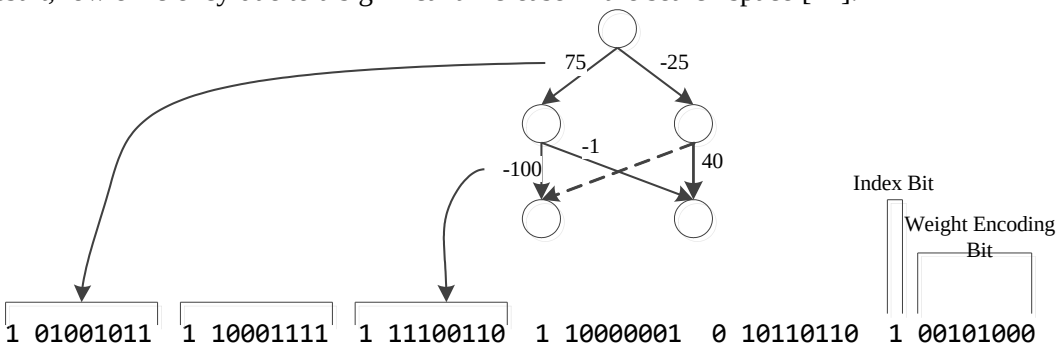

Figure 1: The example of direct encoding the information about ANN

In the example at Fig.1, the Index Bit is used to indicate whether a connection exists or not. Weight Encoding Bits to encode the scale in binary form. A number of researchers have proposed an encoding strategy that encodes weights in real numbers, as well as certain certain mutation operators suitable for encoding [24].

Indirect coding uses a more biological principle: the genotype does not encode the phenotype itself, but the rules of its construction (relatively speaking, a certain program) [16-18]. When decoding a genotype, these rules are applied in a certain sequence (most often, recursively and, most often, the applicability of the rules depends on the current context), as a result of which a neural network is built.

When using indirect coding methods, the genetic representation (and, consequently, the search space for genetic algorithms) is more compact, and the genotype itself allows encoding modular structures, which gives advantages in the adaptability of the results obtained under certain conditions [18], [22-24]. Instead, we get a practical inability to track which changes in the genotype led to the specified changes in the phenotype, as well as many difficulties with the selection of genetic operators, convergence and productivity.

Historically, direct coding has been investigated earlier and more deeply, but a number of disadvantages of this approach are forcing researchers to look more closely at indirect coding methods. However, indirect methods are inherently difficult to analyze [18]. For example, the same mutation of a rule located at the beginning of the program has a huge effect, but applied to the end rules – the effect should not be at all, and as a result: the genetic search has a strong tendency to premature convergence. The selection of crossover operators is also a non-trivial task, since the use of standard binary operators, as a rule, leads to the frequent appearance of non-viable solutions.

There are also a number of other methods of neuroevolution. Let's look at the most popular ones with brief descriptions of each of them [24]:

- Boers and Kuiper approach is using context-sensitive L-systems;
- Dellaert and Beer approach is a similar approach to Cangelosi and Elman, but using random boolean networks;
- Harp, Samad and Guha approach is zone direct encoding of the structure;
- Gruau approach is using a grammar tree to set instructions for cell division (something similar to Cangelossi, Parisi, and Nolfi);
- Vaario approach is cell growth is set by L-systems.

As a result, indirect encoding is usually more compact. On the other hand, setting rules for indirect encoding can lead to a strong bias in the search space, so it is much more difficult to create indirect encoding without significant knowledge of how the encoding will be used.

3. Materials and methods

It is known from the theory of genetics that sequencing of biopolymers (proteins and nucleic acids are DNA and RNA) is the determination of their amino acid or nucleotide sequence [25], [26]. As a result of sequencing, a formal description of the primary structure of a linear macromolecule is obtained in the form of a sequence of monomers in text form. The size of sequenced sections of DNA usually does not exceed 100 pairs of nucleotides (next-generation sequencing) and 1000 pairs of nucleotides during Sanger sequencing. As a result of sequencing overlapping sections of DNA, sequences of sections of genes, whole genes, total mRNA, or complete genomes of organisms are obtained [25], [26].

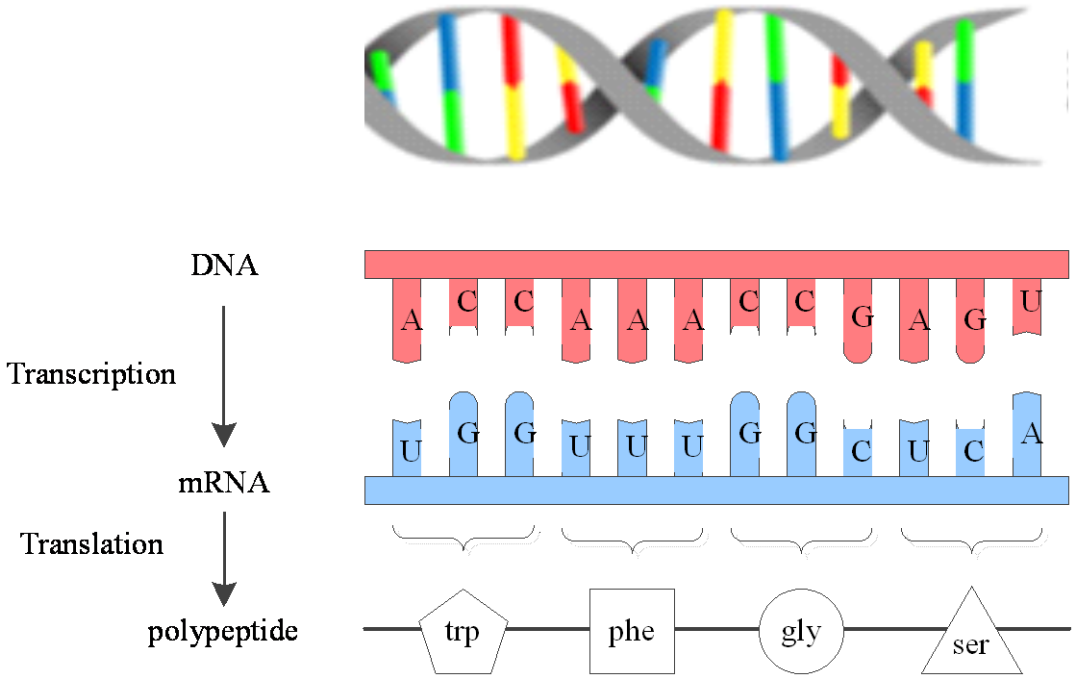

Figure 2: The process of DNA translation

A proposed method of encoding information about the ANN is proposed to be organized based on a similar principle [25-28]. Begin from the coding of connections: in the genotype of an individual, information is provided about the weights of interneuronal connections of the neuromodel, but each gene will contain information about the indices of the initial and final communication neuron, as well as weight of connection. In the case when the method works with RNN, an additional cell is added with the feedback weight, its index is determined by the index of the output neuron.

Some rules for indexing neurons must be introduced [29-33]:

1) since the number of inputs and outputs of the network is a fixed value, the indices of the corresponding neurons are constant and take values in the interval for input neurons $[0; N_i - 1]$, and $[N_i; N_i + N_o - 1]$ for output, where N_i and N_o are the number of inputs and outputs of the network, respectively. Deleting input and output neurons is impossible;

2) new neurons that appear as a result of mutations get the minimum possible index. For example, if an individual represents a network with three inputs and three outputs and does not contain hidden neurons, then the new neuron in this network will be assigned the index "5", the next one – "6", and so on;

3) indices of neurons in a network that is represented by an individual cannot contain missing values, that is, there can be no ANN with neurons that have, for example, indices N_0, N_1, N_2, N_5, N_6. If such a case occurs, for example, after removing a neuron with index 4 from the network, the indices of the neurons that remain are adjusted in this way: $N_5 \to N_4$, $N_6 \to N_5$, while changing the data in the connections related to these neurons.

So it is getting a two-line list, where every four cells (two rows each) form and store information about the neuron. Fig. 3 shows an example.

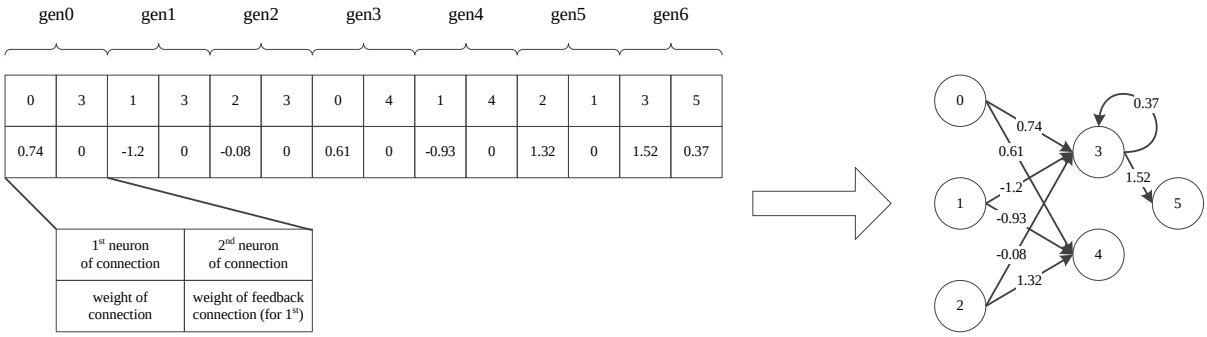

Figure 3: Example of ANN encoding

In addition, it should be noted that the second rule provides a certain ordering of layers: sequencing of orders in lists. In the example on Fig.4 Polymer can be represent as node or component of ANN, but in the case of talking about sequencing it is called polymer.

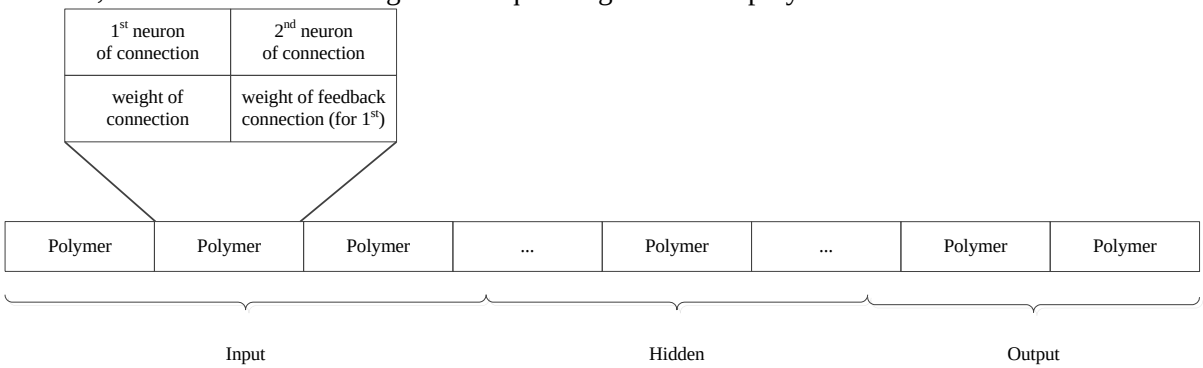

Figure 4: Sequencing of the ANN's layers

4. Experimental research and analysis of results

It should be noted that the most similar method of encoding information in neuroevolution synthesis is the method of Neuroevolution of augmenting topologies (NEAT) [20]. Therefore, in further experimental studies, we will compare the work of the proposed encoding method with NEAT. In addition to modifications with encoding information about an individual, we will use the usual stages of the genetic algorithm for the synthesis of ANN: mutation, rank selection, and dot crossover. The following types of mutation will be used [20-24], [29-33]:

1. adding a hidden neuron;
2. deleting a randomly selected hidden neuron;
3. adding a connection;
4. deleting a randomly selected connection;
5. changing the weight of a randomly selected connection by a random value from the range [-0.5; 0.5].

The choosing the type of mutation based on the values of criteria that characterize the complexity of the problem and the ANN [34-37].

A data set was selected for testing based on the characteristics of patients with pneumonia, which was recently presented by authors M.-A. Kim, J. Seok Park,C. W. Lee, and W.-I. Choi [38]. Total sample size: 77490 values. Table 1 shows the characteristics of the set date.

Table 1

General characteristics of the data set

Total number of values	77490	Number of attributes	54
The type of the data	Numeric (after consideration of)	Number of instances'	1435

For this task, the development of neuromodels will make it much easier to determine the further diagnosis of a person after collecting data on their well-being. Given that pneumonia is one of the most important signs and complications of COVID-19 [39], [40], after additional training on advanced data, this model can be used to diagnose patients or predict the further development of disease dynamics.

Table 2 compares the results of model synthesis using two methods.

Table 2
Test results

Method	Evaluations	Iterations	Population Size
NEAT	14265	97	300
MGA	13949	74	300

The results show that with the same population sizes, the number of iterations and calculations decreased significantly. This may indicate that using the proposed encoding method requires fewer calculations when using genetic operators at the mutation and crossover stage.

In NEAT, connections and weights are encoded directly, and the individual cross is realized by a unique connection mark. The network structure of a population can be effectively developed in an iterative process. Although NEAT is a highly effective neuroevolutionary method, it must encode a large amount of specific information to ensure that information is passed between generations. The encoding method developed in this paper is based on polymer sequencing and uses a more compact encoding and decoding strategy. It can effectively develop the individual structure and weight of a population by simply encoding a small amount of information.

In the proposed method, different people can evolve into different structures, and each structure represents a space of different dimensions. In addition, a simple genetic operator forces the method to try to solve the problem in various ways. The space of modifications (mutations) is very large, and this is beneficial for finding the optimal solution, which further reflects its advantages.

5. Further work

Further involvement and use of probabilistic data structures is quite interesting. Work [41] suggests using a modification of the Scalable Bloom filters. However, this approach does not allow further encoding of feedbacks, and using this approach during mutation with the removal of certain neurons requires the introduction of an additional matrix – a second bloom filter for counting in reverse order. Therefore, the number of calculations increases. Given this, it is more interesting to use the structure: Count-min sketch [42]. CM sketch is a probabilistic data structure that serves as a table of event frequencies in a data stream. It uses hash functions to map events to frequencies, but unlike a hash table, it only uses sublinear space, at the expense of recalculating some events due to collisions.

The use of probabilistic data structures makes it possible to encode information much more compactly. However, when working with such structures, we should not forget about their probabilistic nature. This means that for every hundredth case, a false positive is possible (there is no plural element, but the data structure reports that there is one). When it comes to tasks related to human security, even this percentage of error probability is not acceptable. This is why the use of probabilistic data structures can help encode the ANN more compactly during synthesis, but it is not allowed during use in medical diagnostics.

6. Conclusions

During the work, a new approach to the coding stage in the neuroevolutionary synthesis of ANNs was proposed. The new approach makes it possible to use it without significant modifications in the synthesis of modern ANNs topologies: RNN and DNN. An experimental study confirmed the effectiveness of the method in comparison with its closest competitor, the NEAT method. The best results can be explained by a more compact scheme for encoding information about ANN, which makes it easier to use genetic operators in the future.

During the work, the idea of further development of the proposed approach appeared. However, the proposed technology is based on probabilistic data structures that differ in their probabilistic nature, which is why they cannot be used when working with medical data that require high accuracy.

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