Neural Networks by using Self-Reinforcement Reactions

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Abstract

We consider a chemical reaction network model in which selections of reaction are stochastic and depend on past history. In this chemical reaction network, we found the emergence of Auto-Catalytic Sets (ACS) and complex dynamics in which ACS are repeatedly created and destroyed; we have called this reaction system as the Self-Reinforcement Reactions, SRR. We developed a neural-networks system by using SRR and confirm the neural network of SRR can solve a linear classification problem.

Keywords: Artificial Chemistries, Chemical Reaction Networks, Perceptron, Linear Classification Problem, Self Reinforcement Reaction, Neural Networks

1. Introduction

We consider an abstract model of chemical reactions, a type of "abstract chemistry". The model assumes that substances can interact with each other according to reaction rules which change the amounts of the substance, and that reaction tendencies change depending on the reaction history. Reaction rules are assumed to be of the form $x \rightarrow y$, meaning that the amount of substance x decreases and the amount of substance *b* increases. Reactions occur at rates which depend on the amount of the first substance *x* and the strength of the reaction x → *y*. The strength of each reaction is increased in proportion to how often the reaction has occurred recently.

1.2 An Artificial Chemistry, Abstract Rewriting System On Multisets

We have been proposed an artificial chemistry, based on the Abstract Rewriting System, ARS; the ARS is a theoretical model of computation; we expand ARS on rewriting system on the multiset. A multiset is defined as a simple set and a map, which returns the duplication of element. We denote the duplication (multiplicity) of an element as M (a), for a $\in$ A and in case c /$\in$ A, M (c) = 0; for example M (a) and M (b) of {a, a, b, b} are 2, and M (c) = 0; in the mathematical description, a multiset is described as; < sup, M () >, in which sup is a simple set of elements, in this paper we describe a multiset by denoting the same alphabet in its number of multiplicity such as {a, a, b, b} or a vector w =(M (a1) M (a2) . . . M (an)).

The union of two multisets M1, M2 is the same as the union of simple set and in vector description, the union of multisets is addition of vectors w1 and w2. And inclusion of sets is also the same as the simple set, when M1(a) $\leq$ M2(a) for all a $\in$ A, the multiset M1 is included in M2 and we write M1 $\subseteq$ M2.

A reaction rule is a pair of multiset, we denote A# as a set of all combinations of multisets over A and in the combinations, an empty multiset is included. A reaction rule l $\rightarrow$ r, l, r $\in$ A# is described as a pair of multiset likewise chemical equations or a pair of its vector expression; and in some case, we can describe a reaction rule as a vector r, r = −l + r, it is simple and good for examining the dynamics of an ARMS, but this

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description cannot illustrate when there are the same species of element in the left-hand side and right-hand side such as a, b → a, c; in this case l = (1, 1, 0) and r = (1, 0, 1) and r = −(1, 1, 0) + (1, 0, 1) = (0, −1, 1).

A reaction is described as the rewriting of a multiset, if the left-hand side of a reaction rule is included in a mul- tiset, these elements in the multiset are excluded and the right-hand side of the rule is merged to the multiset; the case when the multiset is a, a, b, b and the reaction rule is a, b → c, d, the left-hand side of the rule is included in the multiset, {a, b} ⊆ {a, a, b, b} so the {a, b} is excluded from the multiset and it is transformed to {a, b} and the left-hand side of the rule {c, d} is merged to the set and we obtain {a, b, c, d} by this reaction.

We have developed a simple computational model, the Abstract Rewriting System, ARMS based on stoichiometric chemistry and reaction rate model. When we consider fundamental mechanism of living systems. ARMS is a hybrid-model and it is a discrete and continuous model, so if the number of elements (molecules) is small, ARMS is discrete model but when the number of element is large it is equal to Differential equation. AC including ARMS, in the most of models, have been described as an algorithm and implemented in digital media and have not been able to communicate with physical environments.

1.3 Self Reinforcement Reaction on ARMS

Specifically, we considered a form of this model which is implemented according to the following procedure. The state of the system is represented by the amounts [x] of the chemical substances, and strengths $w_{y:x}$ of the reaction rules. (For generality, we use "amount" rather than "concentration" or "number of molecules".) Reactions are executed one at a time. The first substance and the reaction rule are each selected stochastically. The probability of selecting substance x is proportional to the relative amount of the substance [x], and the probability of selecting the reaction x → y is proportional to the relative strength $w_{y:x}$ of the reaction. When the reaction x → y occurs, the amount of substance x changes from [x] to [x]-1 and the amount of substance y increases from [y] to [y]+1. The strength of the reaction x→y is $w = (q*R+1)$ where q is the number of times the reaction has occurred in the last M reactions of x and R is the strength of the reinforcement. If reactions have not been selected recently, or there is no reinforcement, then reactions have minimal strength of $w = 1$ (Fig.1).

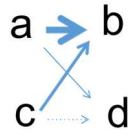

Fig. 1. The schematic example of SRN; in this example, reaction rules are {a → b, a→d, c→b, c→d}; thickness of arrows illustrate speed of reactions (thicker is faster)

The stochastic model we use is based on a well-known model in probabilistic theory, Polya's Urn (Feller 1957) Selecting a node is equivalent to picking up a ball from an urn, where a node name is painted on each ball. In the urn, there are $N-1$ types of balls, excepting itself. Before picking up a ball from the urn, a number R balls is added to the urn for each of the M most recently selected nodes, in addition to one extra ("permanent memory") ball for each node in the network. Initially, the urn will contain just one ball for each node, and the probability of choosing any node will be the same. The model reaction system can be thought of as a network. Each substance corresponds to

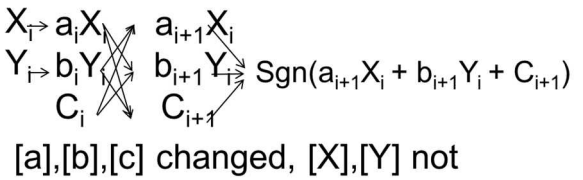

Fig. 2. The schematic example of SRN; in this example, reaction rules are {a → b, a→d, c→b, c→d}; thickness of arrows illustrate speed of reactions (thicker is faster)

a node of the network, and each directed connection between one node to another corresponds to a catalyzed reaction rule. However, since each connection has a

probability which depends on recent activity, it is different from other models such as models based on Random Graph (Erdos and Reny 1960). We can think each node has a "memory storage" where it memorizes the names of the *M* most recent outgoing links and uses this memory to determine the probability for selecting an outgoing link. Another way of description is as follows. There are two types of links. Each node has *(N-1) + M* outgoing links. *(N-1)* permanent links and *M* dynamic links. There is one permanent link to every one of the other *(N-1)* nodes. Other dynamic links which are created and destroyed dynamically. Once a link is activated to a node, then an additional replica link is added, and the oldest dynamic links are destroyed. One of the *(N-1) +M* links is chosen randomly with a bias

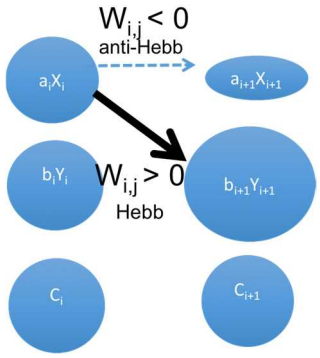

Fig. 3. Schematic image of SRNN; start product is randomly selected in proportion to W^TX, in this example aX is selected and a is decreased by LC and the reaction destination is also randomly selected in proportion to W^TX, in this example by is selected and is increased by LC; and this interaction is memorized.

weight of *R* for dynamic links compared to permanent links (Fig.1).

1.3 Perceptron

A perceptron is an algorithm for learning a binary classifier: a function that maps its input *x* (a real-valued vector) to an output value

$$f(x) = \begin{cases} 1 \; if \; w * x + b > 0 \\ 0 \quad otherwise \end{cases}$$

where *w* is a vector of real-valued weights, $w*x$ is the dot product $\sum_{i=1}^{m} w_i x_i$, where *m* is the number of inputs to the perceptron and *b* is the bias. The bias shifts the decision boundary away from the origin and does not depend on any input value.

2. Neural Networks implemented by ARMS

From Neural Network viewpoints, strength of weight can be regarded as Hebb rule and change of concentrations as anti-Hebb rule; because the concentration of left hand side of the fired rule is decreased and the firing probability of this rule is decreased. We confirmed that Self Reinforcing Neural Network, SRNN (Fig.2 and 3).

2.1. Linear Classification Problem

A linear classifier achieves is making a classification decision based on the value of a linear combination of the characteristics; in this contribution, the classify sample data $X=(x_n, y_n)$, $n=1,2,3,\ldots,N$ by $ax + by + c=0$, the system decide the weight vector $w = (a, b, c)$ and conjectures the sample data is upper or lower than the classification equation. We set an initial weight vector by random value w = (0.1, -0.3, -0.2) and learning coefficient, LC is 0.5.

In the SRNN, reactions exchange value of element in the weight vector by learning coefficient; select an element in w randomly in proportion to $W^T \cdot X$; for example ax is selected, *a is decreased by LC*; in the beginning reaction destination is also randomly selected in proportion to $W^T \cdot X$ and the reaction is memorized as in SR and the selected reaction destination is increased by LC (Fig.3).

3. Result

We compare the ability of system of SRNN with the single layer neural network; in order to characterize difficulty of problems, we change the distance between the center of clusters (x_{center}, y_{center}) from -10 to 10, where the negative distance means that the two clusters are overlapped.

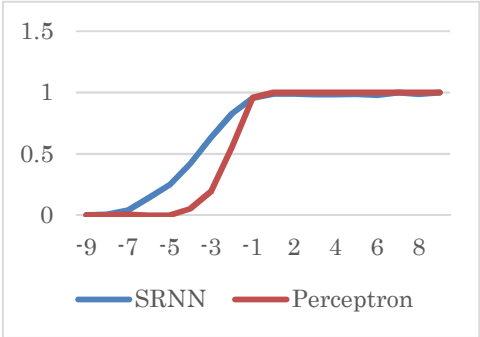

Fig. 4. Compare the SRNN with the single layer Perceptron, the horizontal axis illustrates the distance of the center of clusters, vertical axis illustrates the error rate of clustering.

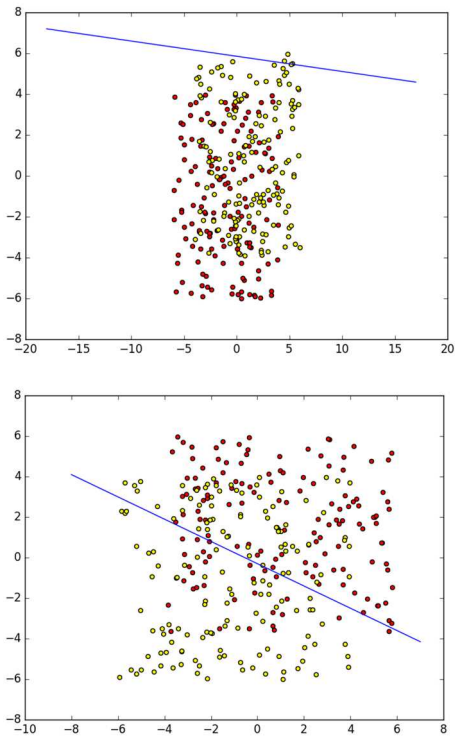

Fig. 4. Fig. 5. The results of sample run of the single layer Perceptron (top) and the SRNN (below) in the same distance of clusters; it shows that SRNN can classify even if the center of clusters are closed.

When the center of clusters are closed, the single layer perceptron cannot classify, while the SRNN can classify the clusters (Fig. 4 and 5).

We compare SRNN with the single layer perceptron by changing the center distance of clusters and examined error rate, where error rate is defined as the ratio of number of correctly classified elements to the total number of data.

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