Biomolecular Computing: Exploring Combining Reservoir Computing with Artificial Chemistry to Improve Classification Problems

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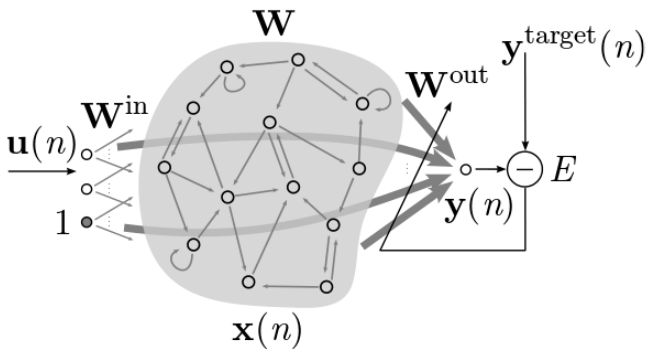
1. Introduction

Artificial chemistry is a rising field of artificial life used to study complex chemistry systems. In this project, reservoir computing and artificial chemistry is explored, and an integration of both is investigated. First, a type of reservoir computing known as echo state network (ESN) was explored with the MATLAB-based ESNToolbox. Next, a type of simple artificial chemistry known as abstract rewriting system on multisets (ARMS) was written in MATLAB based on the paper by Suzuki. The cyclic behavior of variations of the ARMS was recorded, a cycle being defined as when an alphabet repeats itself later on, with the length between the repeats being defined as cycle length. Finally, a combination of reservoir computing and artificial chemistry was implemented by taking the concentrations produced from a perceptron and inputting them to the ARMS system. Various combinations of inputs were put in the perceptron, which was used to recognize AND and NAND functions. The result of project was a preliminary proof-of-concept of using artificial chemistries to improve classification problems in biology, such as better detection of viruses or classifying if heart arrhythmia is present.

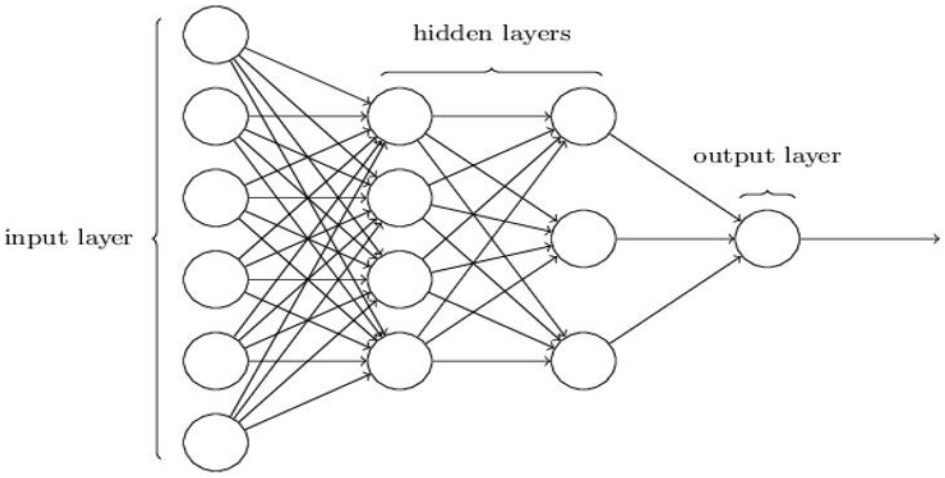
2. Methodology

a. Reservoir Computing

Reservoir Computing is a special type of neural network consisting of input data being fed into a reservoir, in which data randomly interacts with one another. There are two major types of reservoir computing: liquid-state machines and echo state networks. Over the course of this project, echo state networks were explored. The diagram of an echo state network is shown below:



However, for the purpose of this project, a single-layer and multi-layer perceptron was written and adapted to accept molecules as inputs and molecular concentrations as an output. The diagram of a perceptron is show below:



b. Artificial Chemistry

Artificial chemistry is a system that models chemical reactions consisting of molecules interacting with one another according to a set of chemical reaction rules. Instead of physical molecules, however, artificial chemistry uses bits to represent molecular reactions. A specific type of artificial chemistry is the abstract rewriting system on multisets (ARMS), a simple system that rewrites an alphabet based on a set of reaction rules. In this experiment, the following molecules are used:

$$a, b, c, d\ , e, p\ \varphi$$

The following reactions are used, based on the paper by Suzuki:

$$aaa \rightarrow\ \varphi\varphi b$$

$$ba \rightarrow\ \varphi c$$

$$\varphi c \rightarrow\ dd$$

$$de \rightarrow\ \varphi a$$

$$d \rightarrow\ e$$

$$d \rightarrow\ c$$

The following rule orders are used, based on the paper by Suzuki:

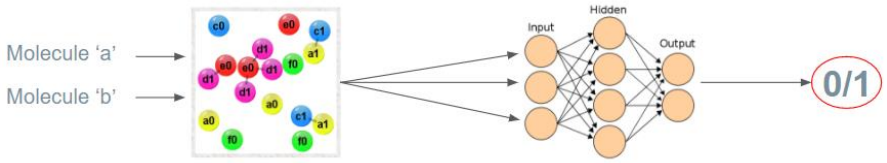
$$r_1 \rightarrow\ r_2 \rightarrow\ r_3 \rightarrow\ r_4 \rightarrow\ r_5 \rightarrow\ r_6$$

$$r_3 \rightarrow r_1 \rightarrow r_2 \rightarrow r_4 \rightarrow r_5 \rightarrow r_6$$

An "input" is determined by replacing a φ with an a, and any reaction according the rule order would occur. These steps occurred for a total of 5050 multiset steps, and the final alphabets were recorded for analysis.

c. Integrating Both

In order to integrate both reservoir computing and artificial chemistry, the following system was used:



The two input molecules 'a' and 'b' are either $a, b, c, d, e, p\ \varphi$, and all 36 combinations were tested. The first part of the system consists of the written ARMS system, and the second part of the system consists of the written perceptron, in this case a single-layer perceptron. Both an AND and NAND functions were tested, with truth tables shown below:

AND Function Truth Table

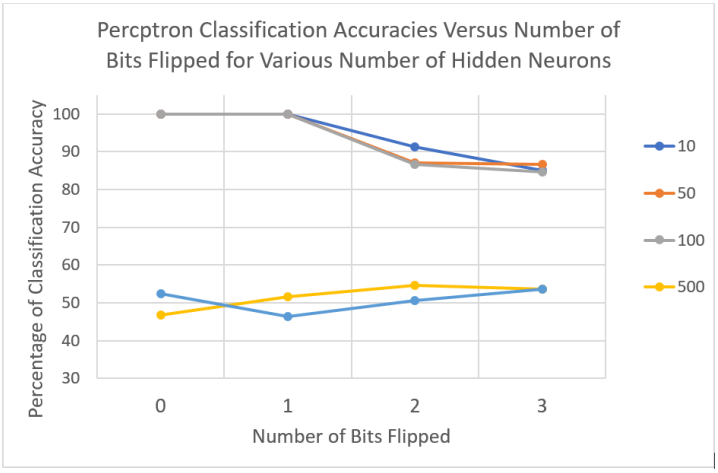
a	*b*	Output
0	0	0
0	1	0
1	1	1
1	0	0

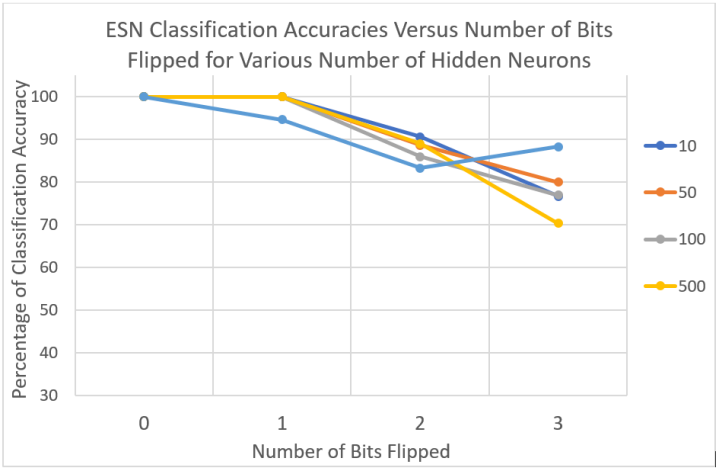
NAND Function Truth Table

a	*b*	Output
0	0	1
0	1	1
1	1	0
1	0	1

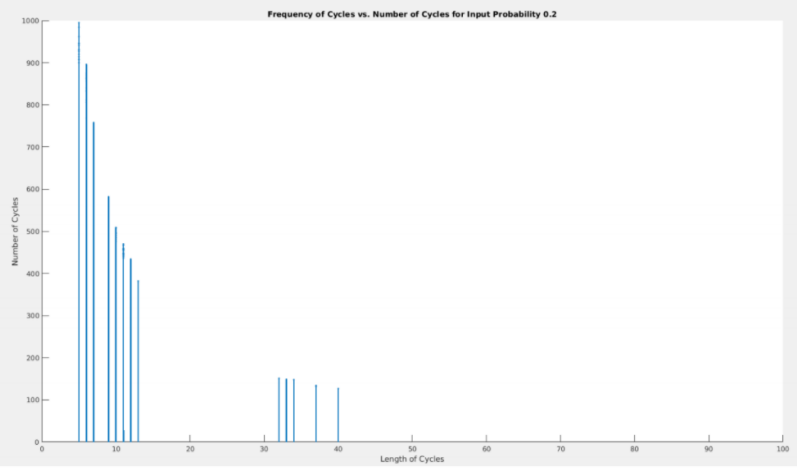
3. Results

1. Reservoir Computing: Classification Accuracies Comparing Perceptron and Echo State Networks

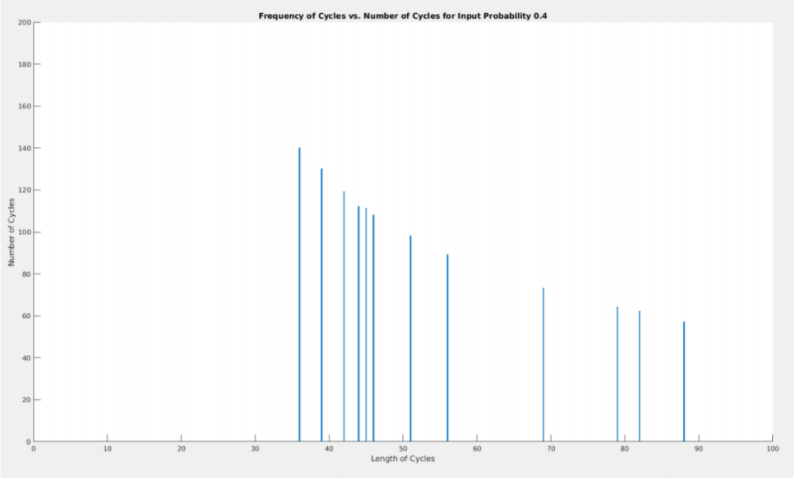




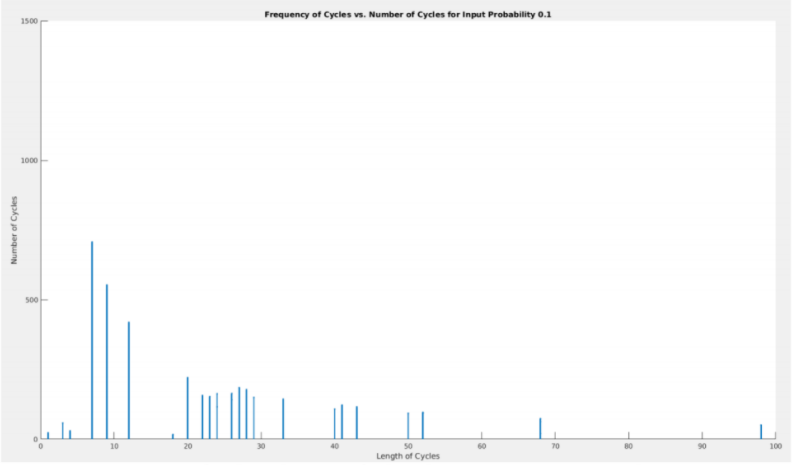
2. Artificial Chemistry: Finding frequency of cycles vs. number of cycles for various input probabilities



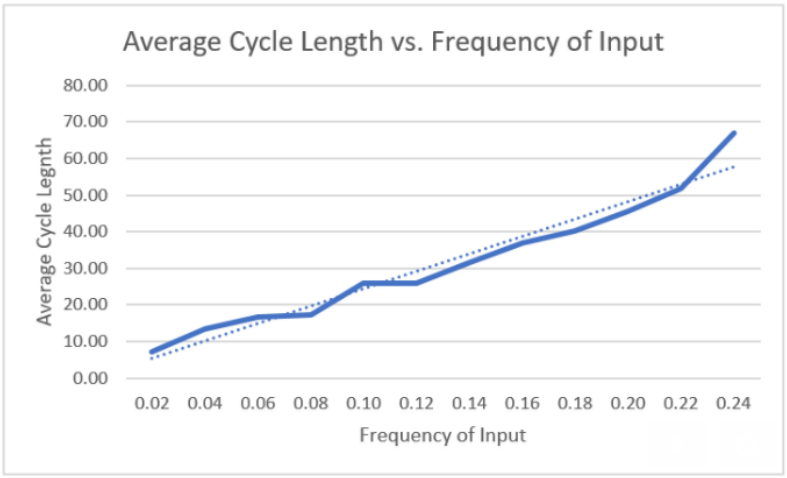
Frequency of Input: 0.2; OR1; Rule order fixed; Percent Terminated: 0%



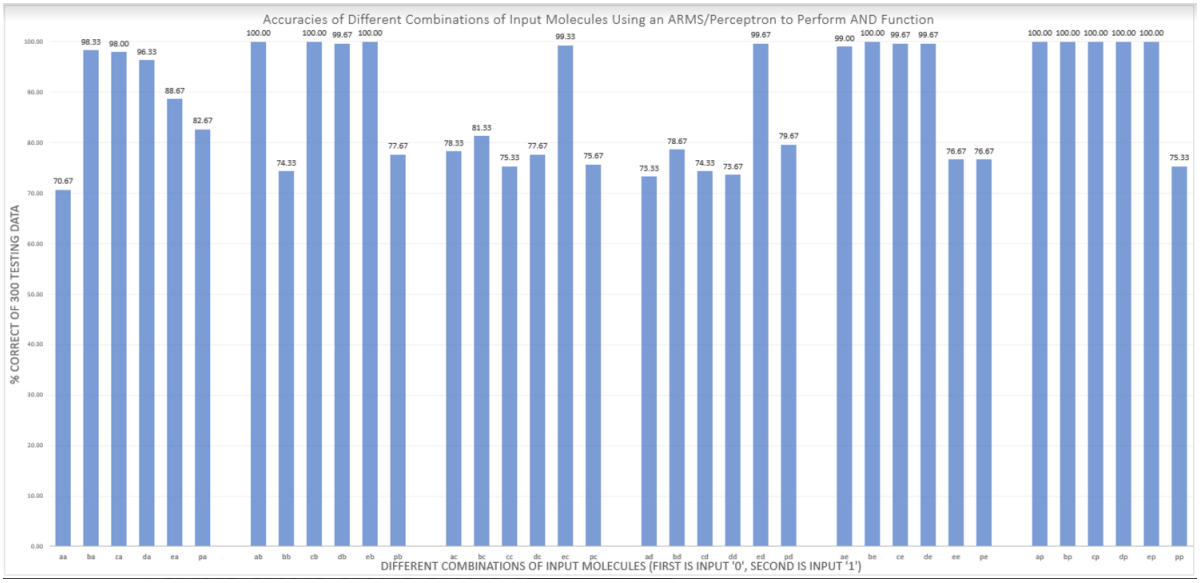
Frequency of Input: 0.4; OR2; Rule order fixed; Percent Terminated: 77%

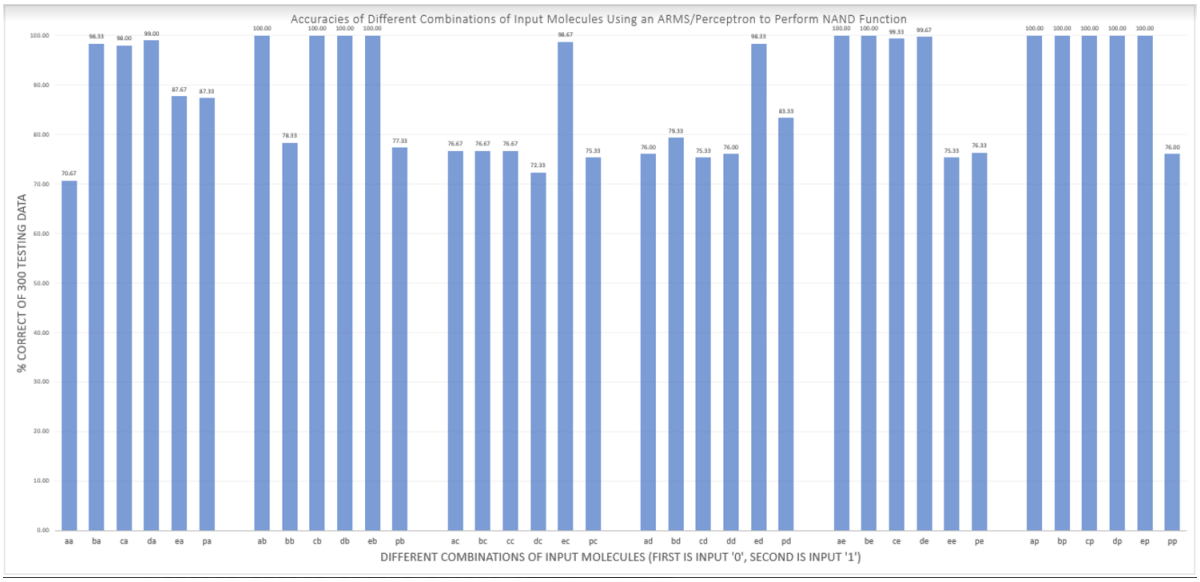


OR2; input: fixed; randomness of rule order: 0.1; Percent Terminated: 53%


Average Cycle Length vs. Frequency of Input
Average Cycle Legnth
80.00
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
0.20
0.22
0.24
Frequency of Input

3. Integrating Reservoir Computing with Artificial Chemistry: Classification accuracies of 36 different combinations of input molecules for AND and NAND functions.





4. Conclusion

In this project, I successfully demonstrated a proof of concept of the potential for reservoir computing to be combined with artificial chemistry to improve complex biological classification problems. Using solely reservoir computing in an X/O image recognition exercise, the system achieved around 100% accuracy with no noise and around 88% accuracy with 3 bits of noise. Analyzing the ARMS system, cyclic behavior within the system is indeed demonstrated, with different cyclic behaviors being exhibited in various frequencies of inputs. On average, increasing the frequency of input would

result in a linear increase of the average length of cycles. Regarding the integration of reservoir computing with artificial chemistry, around 12/36 of the input combinations produced 100% for a system recognizing AND and NAND functions. The range of accuracies span from 70% to 100% accuracy with this implemented system, demonstrating a potential for this combination to be further explored for biological classification problems. This has broader implications in achieving effective medical diagnosis, affordable health care, as well as efficient drug delivery. Future work would include further exploring how to tune both reservoir computing and artificial chemistry systems to see how they would be able to identify pathogens reliably.

5. References

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