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Learning in Bio-molecular Computing Systems

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Emerging Computing Models and Technologies

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Objective

Many potential applications of biochemical computers involve the detection of highly adaptable and dynamic chemical systems, such as emerging pathogens. Current technology is expensive to develop and unique to each application, thus causing limitations in accessibility. In order to make this type of computing a realistic solution to problems in the medical field, a biochemical computer would need to be adaptable to work in a variety of applications.

Background

An artificial chemistry can be used to simulate the behavior of a realistic chemistry. [1] For the purpose of this project a multiset of variables was used to represent concentrations of molecules, as seen in Figure 1. An input variable was added with varying probability, and rules were applied to represent reactions between molecules.

Current State: [A B B D A 0 0 0 0 0]

Input A

Current State: [A B B D A A 0 0 0 0]

Rule: AAA -> 00B

Next State: [B B D 0 0 B 0 0 0 0]

Fig. 1: An example of one term in an ARMS

Simulated Chemistry

An artificial chemistry was used to study concentrations of elements in a multiset when affected by an abstract rewriting system on multisets (ARMS). [2] A multiset of cardinality 10 was applied with varying inputs and a rule set of six rules. Behaviors were studied on 5005 terms of the ARMS, over 100 trials. Figure 2 shows results of varying input probability and rule order.

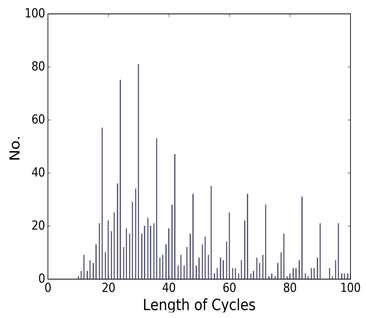


Fig. 2. a

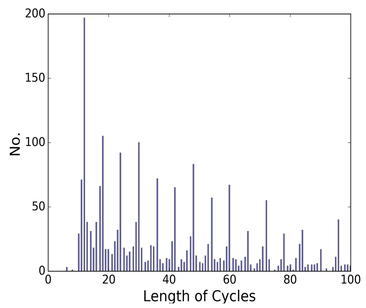


Fig. 2. b

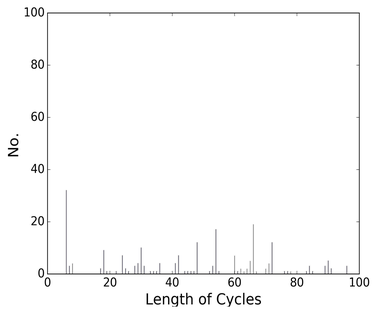


Fig. 2. c

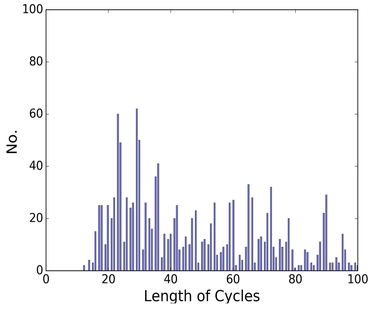


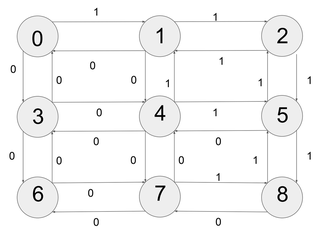
Fig. 2. d

Fig. 2: Frequency of cycle length with input probability of (a) 0.2 (b) 0.4, and (c) 0.8. In (d), input probability is 0.2 and rule order is shifted.

Learning

A reinforcement learning algorithm called Q-learning was applied to a maze-like problem. [3] The Q-learning algorithm uses the Bellman equation to populate a Q matrix. The agent continues training until the matrix converges. [3]

$$Q(s,a) = r + gamma * max(Q(s', a'))$$



Action

State	0	1	2	3	4	5	6	7	8
0	-1	1	-1	0	-1	-1	-1	-1	-1
1	0	-1	1	-1	0	-1	-1	-1	-1
2	-1	1	-1	-1	-1	1	-1	-1	-1
3	0	-1	-1	-1	0	-1	0	-1	-1
4	-1	1	-1	0	-1	1	-1	0	-1
5	-1	-1	1	-1	0	-1	-1	-1	1
6	-1	-1	-1	0	-1	-1	-1	0	-1
7	-1	-1	-1	-1	0	-1	0	-1	1
8	-1	-1	-1	-1	-1	1	-1	0	-1

Fig. 3: State-Action diagram with rewards and corresponding reward matrix.

A grid world was created with “food” at static locations to provide a reward. Figure 4 shows the problem corresponding to the matrix in Fig. 3.

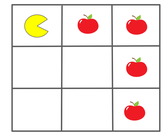


Fig. 4: Grid problem.

Future Work

More results are needed to conclude the effectiveness of the learning algorithm that was used. Once this can be confirmed, an abstract chemistry will be used as the agent to be trained by reinforcement learning. Further development will involve using a realistic chemical system, like DNA, to represent each symbol in the abstract chemistry (Fig 5).

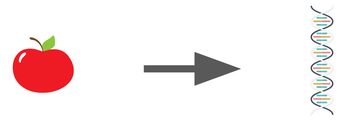
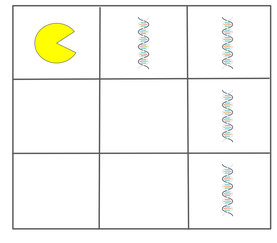


Fig. 5: DNA replaces the food reward. States might be represented by concentrations of certain DNA strands.



Sources

[1] Dittrich, P. et al (2001). Artificial Chemistries - A review. *Artificial Life,* 7: 225-275
[2] Suzuki, Y., & Tanaka, H. (1997). Symbolic chemical system based on abstract rewriting system and its behavior pattern. *Artif Life Robotics,* 1: 211-219
[3] Sutton, Richard S. Barto, Andrew G. (2018). *Reinforcement Learning: An Introduction.* Retrieved from http://incompleteideas.net/book/the-book-2nd.html

Acknowledgments

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