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Learning in Biomolecular Computing Systems

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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.

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.

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]

\[ Q(s,a) = r + \gamma \max(Q(s', a')) \]

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

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

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.

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. 4: Grid problem.

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

Sources

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