In Silco Evolution of Reaction Networks

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Understanding the organization of large biological networks can be made easier if they can be decomposed into smaller functional sub-networks that carry out simpler functions. Construction and analysis of a variety of small functional networks might reveal the design features of reaction networks that are needed to implement a desired function.

To explore the space of simple functional networks, *in silico* evolution (evolutionary algorithms) has been used to construct networks that are capable of realizing small functions. Due to the randomness in evolutionary algorithms, this approach can produce a variety of networks for the same function, allowing one to explore the various strategies that reaction networks can use to realize an objective function. Evolutionary algorithms mimic the basic mechanism of evolution, diversity and selection, thus the networks that they produce may be used to further understand the nature of evolved networks.

Networks have been evolved using various objective functions and using with different reaction kinetics to model the network. Networks capable of calculating roots and polynomial functions have been constructed using mass-action kinetics.

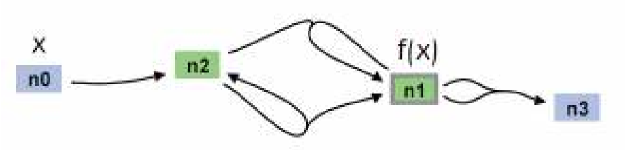

Fig.1: A network where the concentration of n1 is the cube-root of the concentration of n0

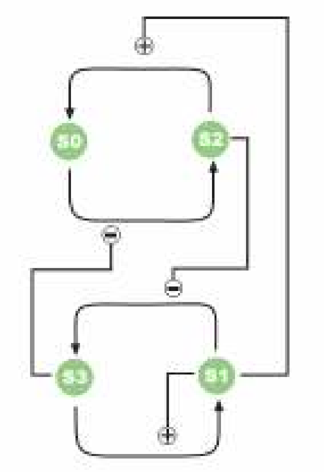

Fig.2: A bi-stable switch that uses Michaelis-Menten kinetics

A series of oscillators, switches, and filters have been constructed using mass-action as well as Michaelis-Menten kinetics and Hill equations (genetic networks).

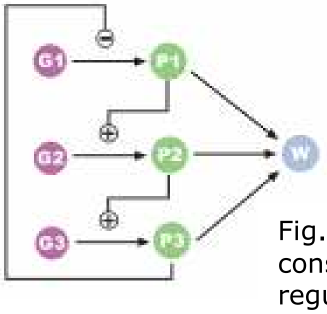

Fig.3: A relaxation oscillator constructed using gene regulation model (Hill kinetics)

Various networks capable of performing chemotaxis have been evolved using different kinetic models, all of which, interestingly, use very similar mechanisms to reach a food source.

Networks with multiple Boolean functions were also evolved to see whether one function would utilize the other or whether they would form a shared modular component.

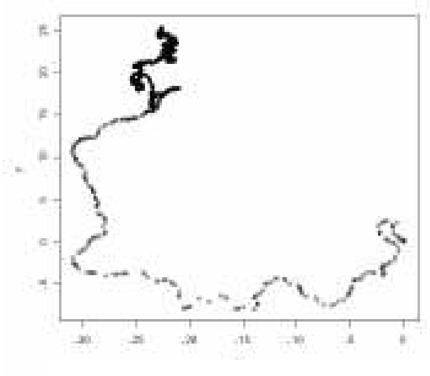

Fig.4: The path taken by a chemotaxis network to reach the target

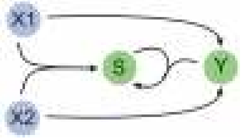

Fig.5: XOR gate

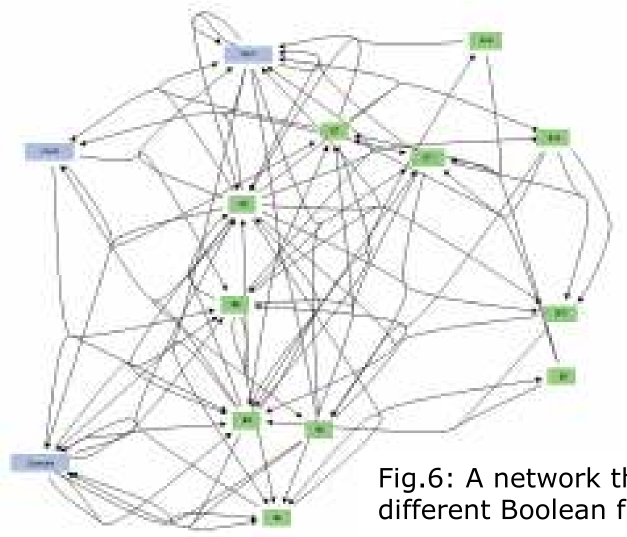

Fig.6: A network that realizes five different Boolean functions.

Classification is a common challenge in artificial intelligence, where a program is trained and then asked to determined what class a given data belongs in. Reaction networks can learn to perform such classification, which required producing a discreet output from continuous inputs.

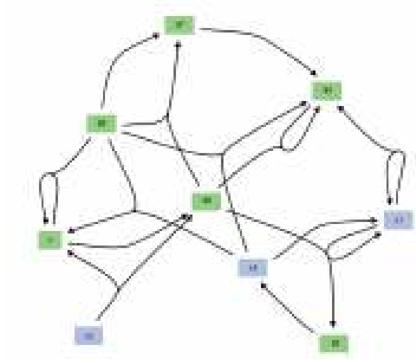

Fig.7: A network that can classify the Iris data (a common dataset used to test classification algorithms).