Complex Dynamics in Random DNA Strand Circuits

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Abstract. DNA strands offer generic combinatorial power to model a wide variety of systems. Yet, due to a high number of required reactions, it is often difficult to predict undesired crosstalk and leakage that makes the design and programming of such circuits challenging. In this work we propose a new approach: we generate random DNA strand networks with influx and efflux using single, full double, and partial double strands, and investigate their complex dynamics. For that purpose we introduce a new measure, the normalized turning point count, which indicates how much the concentration pathways change direction over time. A turning point x of the function $f : \mathbb{R}^n \to \mathbb{R}^n$ is a local minimum or maximum, or more formally

$$\frac{\partial f}{\partial x_i}(x) = 0 \text{ and } \frac{\partial f}{\partial x_i}(x_{-\epsilon}) = -\frac{\partial f}{\partial x_i}(x_{+\epsilon}) \text{ for } i \in \{1, \ldots, n\} \text{ and infinitesimally small } \epsilon.$$

As opposed to related work, we demonstrate how complex dynamics emerge not for a specific instance of reaction networks but rather for a whole range of input parameters such as the number of single strands, ratio of upper to lower strands, and distribution of rate constants, used to generate random DNA strand networks. We show that this behavior is quite sporadic in general, but almost inevitable for specific values of the network generation parameters regardless initial concentration. To search the DNA circuit parameter space we employ standard genetic algorithms, maximizing our turning point measure (TPM).

The TPM of circuits with randomly drawn parameters is on average very low–0.5 turns per species, where each run takes 10^4 time steps (arbitrary time units). During the evolution the TPM fitness teaches the circuit classes to follow different pathways and avoid monotonicity. First, they learn to have a single local minimum or maximum, so they switch direction once on average. After two turns, an evolutionary shift occurs and circuits become complex (periodic or chaotic), and finally their TPM saturates at around 30 turns per run.

We demonstrate that the best class of DNA circuits found by evolution fall into chaotic attractors after a dramatic regime change. This class of DNA circuits is characterized by the specific generation parameter values, which depend on the type of partial double strand ordering. The ordering corresponds to the length of the overlapping subsequences for a given upper or lower strand, so only the strands with longer overlap displace those with shorter overlap from the complex. For a local version only the neighbors of a given single strand are ordered. On the other hand a global version orders the partial double strands from the perspective of the entire system, which prevents cyclic displacement and it is easier to construct. Let (n_L, n_U, k) be a class of DNA strand circuits with n_L lower strands, n_U upper strands, and k partial double strands per each upper strand. The globally ordered type reaches optimal parameters of $(n_L, n_U, k) = (3, 4, 3)$, whereas the locally order type converges to $(n_L, n_U, k) = (3, 3, 2)$. Furthermore, in both cases the circuits require a single full double strand and influx on each species. To prevent an unbound concentration increase we impose an explicit efflux on pure products, such as full double strands.

Future work will focus on using DNA circuits with complex dynamics as a basis for chemical learning and adaptation without explicitly designing the system.