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Discrete Watson–Crick dynamical systems

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ABSTRACT

We generalize previous ideas by Mihalache and Salomaa to define discrete Watson–Crick dynamical systems. We study decision problems for these systems and apply our results to Watson–Crick D0L systems.

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1. Introduction

One of the key ideas of DNA computing is the Watson–Crick complementarity. Mihalache and Salomaa have used this idea to define Watson–Crick D0L systems (see [5]). They start by introducing DNA-like alphabets. Such an alphabet consists of letters $a_1, \ldots, a_n$ and their barred versions $\bar{a}_1, \ldots, \bar{a}_n$. The letters a_i and $\bar{a}_i$ are called complementary. If $\Sigma_n = \{a_1, \ldots, a_n, \bar{a}_1, \ldots, \bar{a}_n\}$ is a DNA-like alphabet, the Watson–Crick morphism $h_W : \Sigma_n^* \to \Sigma_n^*$ replaces each letter by its complementary letter. Now, a Watson–Crick D0L system is a construct $G = (\Sigma_n, g, w, K)$, where Σ_n is a DNA-like alphabet, $g : \Sigma_n^* \to \Sigma_n^*$ is a morphism, $K \subseteq \Sigma_n^*$ is a language and $w \in \Sigma_n^*$ is a word which does not belong to K. The language K is called the trigger of the system. Intuitively, if we apply g to a word u and get a word $g(u)$ which belongs to the trigger language, we replace $g(u)$ by the word $h_W(g(u))$. More formally, the *sequence* $S(G) = (w_i)_{i\geq 0}$ of G is defined by $w_0 = w$ and

$$w_{i+1} = \begin{cases} g(w_i) & \text{if } g(w_i) \notin K \\ h_W(g(w_i)) & \text{if } g(w_i) \in K \end{cases}$$

for $i \geq 0$.

In this paper we will generalize these ideas to define discrete Watson–Crick dynamical systems. A discrete dynamical system in its most general form is a pair (X, f), where X is a set and $f : X \to X$ is a mapping. It is usually assumed that X is a topological space or a measure space and that f is a continuous or measure-preserving mapping.

A discrete Watson–Crick dynamical system is a triple $D = (\Sigma_n, f, K)$, where Σ_n is a DNA-like alphabet, $f : \Sigma_n^* \longrightarrow \Sigma_n^*$ is a mapping and $K \subseteq \Sigma_n^*$ is a language called the trigger of the system. If $x \in \Sigma_n^*$ (and $x \notin K$), the sequence $(x_i)_{i\geq 0}$ of x is defined as above, instead of the morphism g we now iterate the mapping f. The set

$$\mathcal{O}(x) = \{x_i \mid i \geq 0\}$$

is called the orbit of x. The road of x in D is an infinite word indicating the positions in the sequence where the Watson–Crick morphism is applied. The formal definition is given in Section 2.

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In this paper we study decision problems for discrete Watson–Crick dynamical systems. In particular, we study the computability of roads in these systems. We will apply our results to prove new results for Watson–Crick D0L systems. In the general case all problems remain open. In fact, Mihalache and Salomaa have shown that even for Watson–Crick D0L systems with nonregular triggers the simplest nontrivial questions concerning roads are equivalent with the long-standing open problem $\mathbb{Z}_{pos}$ of deciding whether a given $\mathbb{Z}$-rational sequence has only nonnegative terms.

We assume familiarity with notions and results concerning rational series (see [13]). However, we will use rational series mainly in the proofs. Otherwise, the paper is largely self-contained. For further background we refer to [4,7–9].

2. Discrete Watson–Crick dynamical systems

We use standard language-theoretic notation and terminology. In particular, ε is the *empty word* and the *length* of a word w is denoted by $|w|$. If $w \in X^*$ is a word and $Y \subseteq X$, then $|w|_Y$ is the number of occurrences of the letters of Y in w. If u and v are words and $v \neq \varepsilon$, then uv^ω is the infinite word $uvvv\cdots$. An infinite word y is *eventually periodic* if there exist (finite) words u and v such that $y = uv^\omega$.

As usual, $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{Q}$ and $\mathbb{R}$ are the sets of nonnegative integers, all integers, rational numbers and real numbers, respectively. If m and n are positive integers and S is a semiring, then $S^{m\times n}$ is the set of $m \times n$-matrices having entries in S.

Let X be an alphabet. Let the letters of X be $x_1, \ldots, x_d$ in a fixed order. If $g : X^* \to X^*$ is a morphism, then the *matrix* M_g of g is defined by

$$M_g = \begin{pmatrix} |g(x_1)|_{x_1} & |g(x_2)|_{x_1} & \ldots & |g(x_d)|_{x_1} \\ |g(x_1)|_{x_2} & |g(x_2)|_{x_2} & \ldots & |g(x_d)|_{x_2} \\ \vdots & \vdots & & \vdots \\ |g(x_1)|_{x_d} & |g(x_2)|_{x_d} & \ldots & |g(x_d)|_{x_d} \end{pmatrix}.$$

In what follows we will consider *DNA-like alphabets*

$$\Sigma_n = \{a_1, \ldots, a_n, \bar{a}_1, \ldots, \bar{a}_n\}, \quad n \geq 1.$$

The letters a_i and $\bar{a}_i$, $1 \leq i \leq n$, are called *complementary*. The *Watson–Crick morphism* $h_W : \Sigma_n^* \to \Sigma_n^*$ is defined by

$$h_W(a_i) = \bar{a}_i, \quad h_W(\bar{a}_i) = a_i, \quad 1 \leq i \leq n.$$

Hence, the Watson–Crick morphism replaces each letter of Σ_n by its complementary letter. The projections $p : \Sigma_n^* \to \Sigma_n^*$ and $\bar{p} : \Sigma_n^* \to \Sigma_n^*$ are defined by

$$p(x) = \begin{cases} x & \text{if } x \in \{a_1, \ldots, a_n\} \\ \varepsilon & \text{if } x \in \{\bar{a}_1, \ldots, \bar{a}_n\} \end{cases}$$

and

$$\bar{p}(x) = \begin{cases} x & \text{if } x \in \{\bar{a}_1, \ldots, \bar{a}_n\} \\ \varepsilon & \text{if } x \in \{a_1, \ldots, a_n\} \end{cases}$$

If $w \in \Sigma_n^*$, then the *balance* $\mathrm{bal}(w)$ of w is defined by

$$\mathrm{bal}(w) = |p(w)| - |\bar{p}(w)|.$$

In other words, $\mathrm{bal}(w)$ is the difference between the number of nonbarred letters in w and the number of barred letters in w. The languages $PUR \subseteq \Sigma_n^*$ and $PYR \subseteq \Sigma_n^*$ are defined by

$$PUR = \{w \in \Sigma_n^* \mid \mathrm{bal}(w) \geq 0\}$$

and

$$PYR = \{w \in \Sigma_n^* \mid \mathrm{bal}(w) < 0\}.$$

The definition of languages PUR and PYR is from [6].

We now give the central definitions.

Definition 1. A *discrete Watson–Crick dynamical system* is a triple (Σ_n, f, K), where Σ_n is a DNA-like alphabet, $f : \Sigma_n^* \to \Sigma_n^*$ is a mapping and $K \subseteq \Sigma_n^*$ is a language called the *trigger* of the system. A discrete Watson–Crick dynamical system is called *standard* if its trigger is the language PYR.

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