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Ancestors, descendants, and gardens of Eden in reaction systems ☆

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ABSTRACT

This paper analyses several problems related to finding and counting ancestor and descendant states, as well as gardens of Eden (i.e., states without predecessors) in reaction systems. The focus is on the complexity of finding and counting preimages and ancestors that are minimal with respect to cardinality. It turns out that the problems concerning gardens of Eden seem to require the presence of an **NP**-oracle to be solved. All the problems studied are intractable, with a complexity that ranges form $\mathbf{FP}^{\mathbf{NP}[\log n]}$ to **FPSPACE**(poly).

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1. Introduction

Recently many new computational models have been introduced. Most of them are inspired by natural phenomena. This is also the case of Reaction Systems (RS), proposed by Ehrenfeucht and Rozenberg in [4], which are a metaphor for basic chemical reactions. Informally, a reaction system is made of a (finite) set of entities (molecules) and a (finite) set of reactions. Each reaction is a triple of sets: *reactants*, *inhibitors* and *products* (clearly the set of reactants and the one of inhibitors are disjoint). Given a set of reactants T, a reaction (R, I, P) is applied if $R \subseteq T$ and if there are no inhibitors (i.e., $T \cap I$ is empty); the result is the replacement of T by the set of products P. Given a set of reactants T, all enabled reactions are applied in parallel. The final set of products is the union of all single sets of products of each reaction which is enabled in T.

Studying RS is interesting for a number of reasons, not only as a clean computational model allowing precise formal analysis (see [2] for combinatorics issues) but also as a reference with respect to other computing systems. For instance, in [7], the authors showed an embedding of RS into Boolean automata networks (BAN), a well-known model used in a number of application domains. Remark that for BAN the precise complexity of only a bunch of problems about the dynamical behaviour is known. Via the embedding of RS into BAN, all the complexity results about RS are indeed lower bounds for the corresponding ones for BAN.

In this paper, we continue the exploration of the computational complexity of properties of RS started in [7,6]. The focus is on preimages and ancestors of minimal size. In more practical terms, this could be useful when minimising the number of chemical entities necessary to obtain a target compound. Indeed, given a current state T, the minimal preimage (resp.,

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n-th-ancestor) problem or MPP (resp., MAP) consists in finding the minimal set (with respect to cardinality) of reactants which produces T in one step (resp., n steps). Variants of MPP and MAP consider counting the number of preimages (#PP) and of minimal preimages (#MPP); counting the number of ancestors (#AP) and of minimal ancestors (#MAP); or computing the size of a minimal preimage (SMPP) or of a minimal ancestor (SMAP). We also count the number of descendants of a state (#DP). Finally, we investigate problems related to gardens of Eden, namely finding them (GEP) and counting them (#GEP).

More precisely, we prove that (Section 2 recalls the definitions of the complexity classes):

- #PP is #**P**-complete under parsimonious reductions;
- MPP $\in \mathbf{FP}^{\mathbf{NP}}$ and it is $\mathbf{FP}^{\mathbf{NP}}_{\parallel}$-hard under metric reductions;
- #MPP is in $\#\mathbf{P}^{\mathbf{NP}}$ and it is #**P**-hard under parsimonious reductions;
- SMPP is $\mathbf{FP}^{\mathbf{NP}[\log n]}$-complete under metric reductions;
- #AP is **FPSPACE**(poly)-complete under Cook reductions;
- MAP, #MAP, and #DP are complete for **FPSPACE**(poly) under metric reductions;
- SMAP is **FPSPACE**(log)-complete under metric reductions.
- GEP is $\mathbf{FNP}^{\mathbf{NP}}$-complete under metric reductions;
- #GEP is $\#\mathbf{P}^{\mathbf{NP}}$-complete under metric reductions.

These results are important for further understanding the computational capabilities of RS but they also provide clean new items to the (relatively) short list of examples of problems in high functional complexity classes. Remark that the problem of preimage existence has been proved to be in **NP** by Salomaa [12]. However, here the complexity is higher because of the minimality requirement.

The paper is structured as follows: in Section 2 the necessary background notions are recalled; Section 3 is concerned with preimages problems, while Section 4 with ancestors problems. Gardens of Eden are studied in Sections 5. Finally, in Section 6 we draw our conclusions and provide some open questions.

2. Basic notions

This section briefly recalls the basic notions about RS as introduced in [5]. It is important to remark that throughout the whole paper the sets of reactants and inhibitors of a reaction are required to be nonempty, as it is sometimes enforced in the literature. However, the results also hold when empty sets are allowed, unless explicitly specified otherwise.

Definition 1. Consider a finite set S, whose elements are called *entities*. A *reaction* a over S is a triple (R_a, I_a, P_a) of nonempty subsets of S. The set R_a is the set of *reactants*, I_a the set of *inhibitors*, and P_a is the set of *products*. The set of all reactions over S is denoted by $\mathrm{rac}(S)$.

Definition 2. A *Reaction System (RS)* is a pair $\mathcal{A} = (S, A)$ where S is a finite set, called the *background set*, and $A \subseteq \mathrm{rac}(S)$.

Given a *state* $T \subseteq S$, a reaction a is said to be *enabled* in T when $R_a \subseteq T$ and $I_a \cap T = \varnothing$. The *result function* $\mathrm{res}_a : 2^S \to 2^S$ of a, where 2^S denotes the power set of S, is defined as $\mathrm{res}_a(T) = P_a$ if a is enabled in T, and $\mathrm{res}_a(T) = \varnothing$ otherwise. The definition of res_a naturally extends to sets of reactions: given $T \subseteq S$ and $A \subseteq \mathrm{rac}(S)$, define $\mathrm{res}_A(T) = \bigcup_{a \in A} \mathrm{res}_a(T)$. The result function $\mathrm{res}_{\mathcal{A}}$ of a RS $\mathcal{A} = (S, A)$ is res_A, i.e., the result function on the whole set of reactions. In this way, any RS $\mathcal{A} = (S, A)$ induces a discrete dynamical system where the state set is 2^S and the next state function is $\mathrm{res}_{\mathcal{A}}$.

Definition 3. Let $\mathcal{A} = (S, A)$ be a RS. For any $T \subseteq S$, an element $U \subseteq S$ is an *ancestor* of T if $\mathrm{res}^t_{\mathcal{A}}(U) = T$ for some $t \in \mathbb{N}$. In that case T is a *descendant* of U. If $t = 1$, U is called *preimage* of T. An ancestor (resp., preimage) U of T is *minimal* if $|U| \le |V|$ for all ancestors (resp., preimages) V of T, where $|X|$ denotes the cardinality of set X.

A state always admits at least itself as ancestor but might not have a preimage. A state without preimages is called a *garden of Eden*. In dynamical systems admitting only a finite number of states, as RS are, either the next state function is bijective or the system has at least one garden of Eden.

The *orbit* of a given a state T of a RS $\mathcal{A}$ is defined as the sequence of states obtained by iterations of $\mathrm{res}_{\mathcal{A}}$ starting from T, namely the sequence $(T, \mathrm{res}_{\mathcal{A}}(T), \mathrm{res}^2_{\mathcal{A}}(T), \ldots)$. Being finite systems, RS only admit ultimately periodic orbits, i.e., orbits ending up in a cycle.

The complexity of preimage and ancestor problems for RS is conveniently described by complexity classes of function problems. For this reason, the rest of this section recalls the definitions of the relevant ones (for more details, see [10,9]).

Let Σ be an alphabet. We say that a binary relation R over $\Sigma^\star$ is *polynomially-balanced* if there exists a polynomial p such that $R(x, y)$ implies $|y| \le p(|x|)$, where $|x|$ denotes the length of the string x. A "choice function" for R is a function $f : \mathrm{dom}\, R \to \Sigma^\star$ that, for a given x, returns any y such that $R(x, y)$. The class **FP** (resp., $\mathbf{FP}^{\mathbf{NP}}$) consists of all

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